INFORMATION TO USERS

This manuscript has been reproduced from the microfilm master. UMI films the text directly from the original or copy submitted. Thus, some thesis and dissertation copies are in typewriter face, while others may be from any type of computer printer.

The quality of this reproduction is dependent upon the quality of the copy submitted. Broken or indistinct print, colored or poor quality illustrations and photographs, print bleedthrough, substandard margins, and improper alignment can adversely affect reproduction.

In the unlikely event that the author did not send UMI a complete manuscript and there are missing pages, these will be noted. Also, if unauthorized copyright material had to be removed, a note will indicate the deletion.

Oversize materials (e.g., maps, drawings, charts) are reproduced by sectioning the original, beginning at the upper left-hand corner and continuing from left to right in equal sections with small overlaps. Each original is also photographed in one exposure and is included in reduced form at the back of the book.

Photographs included in the original manuscript have been reproduced xerographically in this copy. Higher quality 6" x 9" black and white photographic prints are available for any photographs or illustrations appearing in this copy for an additional charge. Contact UMI directly to order.

UMI
A Bell & Howell Information Company
300 North Zeeb Road, Ann Arbor MI 48106-1346 USA
313/761-4700  800/521-0600
TITAN'S UPPER ATMOSPHERIC STRUCTURE DERIVED FROM
VOYAGER ULTRAVIOLET SPECTROMETER OBSERVATIONS

by

Ronald Joe Vervack, Jr.

A Dissertation Submitted to the Faculty of the
DEPARTMENT OF PLANETARY SCIENCES
In Partial Fulfillment of the Requirements
For the Degree of
DOCTOR OF PHILOSOPHY
In the Graduate College
THE UNIVERSITY OF ARIZONA

1997
As members of the Final Examination Committee, we certify that we have read the dissertation prepared by Ronald Joe Vervack, Jr. entitled Titan's Upper Atmospheric Structure Derived From Voyager Ultraviolet Spectrometer Observations and recommend that it be accepted as fulfilling the dissertation requirement for the Degree of Doctor of Philosophy.

Bill R. Sandel
Date 3 June 97

Donald M. Hunten
Date 3 June 97

William B. Hubbard
Date 6/3/97

Randall M. Richardson
Date 3 June 97

Terry C. Wallace
Date 6/3/97

Final approval and acceptance of this dissertation is contingent upon the candidate's submission of the final copy of the dissertation to the Graduate College.

I hereby certify that I have read this dissertation prepared under my direction and recommend that it be accepted as fulfilling the dissertation requirement.

Bill R. Sandel
Dissertation Director 3 June 97
STATEMENT BY AUTHOR

This dissertation has been submitted in partial fulfillment of requirements for an advanced degree at The University of Arizona and is deposited in the University Library to be made available to borrowers under rules of the library.

Brief quotations from this dissertation are allowable without special permission, provided that accurate acknowledgment of source is made. Requests for permission for extended quotation from or reproduction of this manuscript in whole or in part may be granted by the head of the major department or the Dean of the Graduate College when in his or her judgment the proposed use of the material is in the interests of scholarship. In all other instances, however, permission must be obtained from the author.

SIGNED: Ronald Joe Veveck Jr.
ACKNOWLEDGEMENTS

When I started graduate school, I set a number of goals. Some I’ve achieved and others I haven’t, but I suppose that’s normal. It’s taken longer than I expected, but that’s not unusual either. Anyway, it’s over now, and I look forward to many years of research in space science. I would be remiss, however, if I didn’t thank the people who have brought me to this point in time.

My advisor, Bill Sandel, must be one of the most patient men on the planet. I can’t count the number of times I’ve gone into his office to vent my frustration over one problem or another. Usually, he would quietly listen to my ramblings, waiting to see if I’d solve it myself by thinking “out loud” about it. That was often the case, but if not, he would take the time to make suggestions about how to tackle it. I thank him for his patience and support through the years.

Being “exiled” in LPL-West has had its disadvantages, but the people have not been one of them. I thank Doyle Hall, Roger Yelle, Floyd Herbert, Jay Holberg, and Terry Forrester for invaluable assistance with the Voyager UVS data. Both NASA and Lyle Broadfoot funded this research, so a big thanks to them. I also thank Yiping, Brooke, Tom, and Jim for listening when I needed an ear, Pat and Joe P. for all their help, and everyone else for the good conversations.

My fellow graduate students and I have been through a lot together over the years — classes, exams, basketball, bowling, racquetball, nocturnal events on March 31 — and I’ve enjoyed the ride. I won’t try to name everyone because I’d surely forget someone. They know who they are, and I thank each of them for some great times. I must especially thank the “Thursday night gamers,” who at the expense of their own sanity helped me maintain mine. I’ll miss them the most.

Though they don’t really understand what I do nor why it has taken so long to do it, my family has always encouraged me in this endeavor. Whether the support has been emotional, psychological, or just plain financial, they have been there when I needed them. I especially thank my mother, Donna Agee, and my in-laws, Patricia and Wayne Nipper, for their roles in this drama.

Finally, I must thank my wife, Andrea. More than anyone, she understands what it has taken to get through the last few years. It’s been rough at times, and we’ve had to make sacrifices, but she stuck with me through it all. I hope I can make it up to her in the coming years, and I trust she knows how dearly I love her for believing in me.
DEDICATION

To my grandfather, George D. Carney, Jr.,

who taught me to ask questions and find answers. His love of knowledge was the inspiration for my own. How I wish he had lived to see this day.

To my daughter, Katherine Patricia,

whose precious laugh reminds me that there is more to life than science.
TABLE OF CONTENTS

LIST OF FIGURES .............................................. 9
LIST OF TABLES ................................................... 12
ABSTRACT ............................................................. 13

1 INTRODUCTION ..................................................... 14
  1.1 Pre-Voyager Conceptions of Titan’s Atmosphere .............. 15
  1.2 The Voyager Encounters ....................................... 29
  1.3 Post-Voyager Investigations ................................. 36
  1.4 Recent Work: The Last Ten Years ............................. 40
  1.5 Motivation for the Current Research ......................... 48

2 PROCESSING THE TITAN SOLAR OCCULTATION DATA ............. 50
  2.1 Introduction .................................................. 50
  2.2 The “Raw” Data ................................................. 53
  2.3 Processing the Spectra ......................................... 63
    2.3.1 Linearizing the Spectra .................................. 64
    2.3.2 Descattering the Spectra .................................. 70
  2.4 Generating the Light Curves .................................. 70
    2.4.1 Binning the Reference Spectra ............................ 72
    2.4.2 Ratioing the Spectra ...................................... 73
  2.5 The Geometry of the Titan Occultations ...................... 76

3 DEVELOPMENT OF THE RETRIEVAL METHOD ....................... 85
  3.1 The Basic Theory of Absorptive Occultations ................. 85
  3.2 The Reality of Absorptive Occultations ....................... 89
  3.3 The Reality of Voyager UVS Occultations .................... 91
  3.4 Previous Methods of Voyager UVS Occultation Analyses ....... 96
  3.5 A New Method for UVS Occultation Analysis ................ 101
    3.5.1 Setting up the Atmosphere ............................... 105
    3.5.2 Source Spectrum and Cross Section Wavelength Grids .... 106
    3.5.3 Attenuating the Fluxes ................................... 109
    3.5.4 Modeling the Ratio Spectrum ............................. 116
    3.5.5 Further Considerations of the Finite Sun ............... 120
    3.5.6 Iterating to the Optimal Densities ..................... 121
    3.5.7 Putting It All Together ................................... 128
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5.8</td>
<td>Retrieving the Atmospheric Temperature</td>
<td>130</td>
</tr>
<tr>
<td>3.6</td>
<td>Testing the Method</td>
<td>133</td>
</tr>
<tr>
<td>4</td>
<td>TITAN’S UPPER ATMOSPHERIC STRUCTURE</td>
<td>138</td>
</tr>
<tr>
<td>4.1</td>
<td>Retrieving Titan’s Atmosphere: The Specifics</td>
<td>138</td>
</tr>
<tr>
<td>4.2</td>
<td>The Retrieved Atmosphere</td>
<td>147</td>
</tr>
<tr>
<td>4.2.1</td>
<td>N$_2$ Profiles</td>
<td>148</td>
</tr>
<tr>
<td>4.2.2</td>
<td>CH$_4$ Profiles</td>
<td>152</td>
</tr>
<tr>
<td>4.2.3</td>
<td>C$_2$H$_2$ Profiles</td>
<td>155</td>
</tr>
<tr>
<td>4.2.4</td>
<td>C$_2$H$_6$ Profiles</td>
<td>158</td>
</tr>
<tr>
<td>4.2.5</td>
<td>C$_3$H$_6$ Profiles</td>
<td>160</td>
</tr>
<tr>
<td>4.2.6</td>
<td>C$_4$H$_2$ Profiles</td>
<td>162</td>
</tr>
<tr>
<td>4.2.7</td>
<td>C$_2$N$_2$ Profiles</td>
<td>164</td>
</tr>
<tr>
<td>4.2.8</td>
<td>HCN Profiles</td>
<td>166</td>
</tr>
<tr>
<td>4.2.9</td>
<td>HC$_3$N Profiles</td>
<td>169</td>
</tr>
<tr>
<td>4.2.10</td>
<td>The Thermospheric Temperature</td>
<td>171</td>
</tr>
<tr>
<td>4.3</td>
<td>Comparisons of Data and Model Spectra</td>
<td>174</td>
</tr>
<tr>
<td>4.3.1</td>
<td>Data and Retrieved Atmosphere Model Spectra</td>
<td>175</td>
</tr>
<tr>
<td>4.3.2</td>
<td>Data and Photochemical Model Spectra</td>
<td>186</td>
</tr>
<tr>
<td>4.4</td>
<td>Some Remarks on the Retrievals and Comparisons</td>
<td>196</td>
</tr>
<tr>
<td>5</td>
<td>CONCLUSIONS AND FUTURE WORK</td>
<td>199</td>
</tr>
<tr>
<td>5.1</td>
<td>Summary of Conclusions</td>
<td>199</td>
</tr>
<tr>
<td>5.2</td>
<td>Future Work</td>
<td>204</td>
</tr>
<tr>
<td>A</td>
<td>APPENDIX A THE VOYAGER UVS</td>
<td>206</td>
</tr>
<tr>
<td>A.1</td>
<td>Optical Configuration</td>
<td>206</td>
</tr>
<tr>
<td>A.2</td>
<td>Detector Assembly</td>
<td>210</td>
</tr>
<tr>
<td>B</td>
<td>APPENDIX B THE DETECTOR ASSEMBLY MODEL</td>
<td>214</td>
</tr>
<tr>
<td>B.1</td>
<td>Model Overview</td>
<td>214</td>
</tr>
<tr>
<td>B.2</td>
<td>Detector Thresholds</td>
<td>216</td>
</tr>
<tr>
<td>B.3</td>
<td>Scan Rates</td>
<td>218</td>
</tr>
<tr>
<td>B.4</td>
<td>Charge Spreading Parameterization</td>
<td>222</td>
</tr>
<tr>
<td>B.4.1</td>
<td>Model Descriptions</td>
<td>223</td>
</tr>
<tr>
<td>B.4.2</td>
<td>Parameter Searches</td>
<td>236</td>
</tr>
<tr>
<td>B.5</td>
<td>Detector Gains</td>
<td>238</td>
</tr>
<tr>
<td>B.5.1</td>
<td>HVL 3 Gains</td>
<td>240</td>
</tr>
<tr>
<td>B.5.2</td>
<td>HVL 2 Gains</td>
<td>246</td>
</tr>
<tr>
<td>B.6</td>
<td>Current Limiting</td>
<td>247</td>
</tr>
<tr>
<td>B.7</td>
<td>Even Channel Correction Factor</td>
<td>251</td>
</tr>
</tbody>
</table>
**TABLE OF CONTENTS — Continued**

APPENDIX C PROCESSING VOYAGER UVS SPECTRA  ........................................................................ 256
  C.1 Stellar or Extended Source Spectra ................................................................. 256
  C.2 Solar Spectra ................................................................................................. 258
    C.2.1 Linearization .......................................................................................... 258
    C.2.2 Descattering .......................................................................................... 263

APPENDIX D PHOTOABSORPTION CROSS SECTIONS .......................................................... 267
  D.1 Molecular Nitrogen (N₂) ............................................................................... 268
  D.2 Atomic Nitrogen (N) ..................................................................................... 271
  D.3 Methane (CH₄) ............................................................................................ 272
  D.4 Acetylene (C₂H₂) ......................................................................................... 274
  D.5 Ethylene (C₂H₄) ......................................................................................... 275
  D.6 Ethane (C₂H₆) ............................................................................................ 277
  D.7 Molecular Hydrogen (H₂) ............................................................................ 279
  D.8 Atomic Hydrogen (H) .................................................................................. 282
  D.9 Diacetylene (C₄H₂) ..................................................................................... 285
  D.10 Cyanogen (C₂N₂) ....................................................................................... 286
  D.11 Dicyanogen (C₄N₂) ................................................................................... 288
  D.12 Hydrogen Cyanide (HCN) ......................................................................... 289
  D.13 Cyanoacetylene (HC₃N) ............................................................................ 291

REFERENCES ............................................................................................................. 292
## LIST OF FIGURES

1.1 Titan atmospheric models from July 1973 workshop ................. 21
1.2 Comparison of the predicted temperature profile of Hunten (1978) and the measured profile of Lindal et al. (1983) ............... 32
1.3 Optical depth profiles of G. R. Smith et al. (1982) ............... 35
1.4 Photochemical model of Yung et al. (1984)/Yung (1987) ........... 39
1.5 Mesospheric temperature profile models .............................. 42
1.6 Photochemical model of Toublanc et al. (1995) ................... 44
1.7 Photochemical model of Lara et al. (1996) .......................... 45

2.1 Illustration of the basic principles of absorptive occultations .... 51
2.2 Trajectory of Voyager 1 during the Titan fly-by .................... 54
2.3 Examples of “raw” spectra ........................................ 55
2.4 “Raw light curves” and corresponding $\Delta W$ values ........... 57
2.5 Examples of processed spectra .................................... 67
2.6 Processed “light curves” .......................................... 68
2.7 Illustration of “light curve” scaling ................................ 69
2.8 Illustration of the saturation correction ........................... 71
2.9 Example of a ratioed spectrum .................................... 73
2.10 Final light curves ................................................... 74
2.11 Geometry for altitude calculations ................................. 77

3.1 Comparison of the photoabsorption cross sections for several species in Titan’s atmosphere ........................................... 92
3.2 Examples of model attenuated Voyager UVS spectra .................. 94
3.3 Illustration of the layer-by-layer nature of the retrieval method ... 104
3.4 Geometry for column density calculations .......................... 111
3.5 Illustration of the source’s image on the detector .................. 117
3.6 Illustration of the division of the sun into multiple segments .... 121
3.7 Illustration of a step in the simplex procedure ........................ 124
3.8 Retrieval of profiles in a “noise-free” test case .................... 134
3.9 Retrieval of profiles in a “noisy” test case ........................ 135

4.1 Comparison of data and fit light curves ............................ 140
4.2 Model solar spectrum used in the retrieval procedure ............ 142
4.3 Retrieved $N_2$ profiles compared to models ........................ 149
4.4 Retrieved $CH_4$ profiles compared to models ........................ 153
4.5 Retrieved $C_2H_2$ profiles compared to models .................... 156
4.6 Retrieved $C_2H_4$ profiles compared to models .................... 159
LIST OF FIGURES — Continued

4.7 Retrieved C$_2$H$_6$ profiles compared to models ...................... 161
4.8 Retrieved C$_3$H$_2$ profiles compared to models ...................... 163
4.9 Retrieved C$_2$N$_2$ profiles compared to models ...................... 165
4.10 Retrieved HCN profiles compared to models ......................... 167
4.11 Retrieved HCN profiles compared to observations ................. 168
4.12 Retrieved HC$_3$N profiles compared to models ...................... 170
4.13 Model N$_2$ profiles for various temperatures ...................... 173
4.14 Comparison of data and model spectra: retrieved atmosphere .... 176
4.15 Comparison of data and model spectra: retrieved atmosphere (con­tinued) .............................................................. 177
4.16 Comparison of data and model spectra: Y84/87 ...................... 187
4.17 Comparison of data and model spectra: Y84/87 (continued) .... 188
4.18 Comparison of data and model spectra: T95 ......................... 189
4.19 Comparison of data and model spectra: T95 (continued) ......... 190
4.20 Comparison of data and model spectra: L96 ....................... 191
4.21 Comparison of data and model spectra: L96 (continued) ......... 192

5.1 Light curves illustrating the cut-off at low altitudes .............. 203

A.1 Schematic representation of the Voyager UVS .......................... 207
A.2 Photograph of the Voyager UVS ........................................ 208
A.3 Voyager 2 occultation port slit function .............................. 209

B.1 Schematic representation of the detector assembly model .................. 215
B.2 First threshold levels for the Voyager 1 UVS ......................... 217
B.3 Example of a spectrum with saturated channels .................... 220
B.4 Geometry of the right circular cone model ............................. 224
B.5 Illustration of the volume calculation procedure for the right circu­lar cone model ...................................................... 225
B.6 Illustration of the fractional volume model ............................. 228
B.7 Illustration of the two-triangle total charge fraction model ........ 230
B.8 Illustration of the one-triangle total charge fraction model ........ 235
B.9 Lab-measured charge spreading and best-fit model .................. 237
B.10 Dependence of the pulse height-to-count mode ratios on gain and photoevent rate .............................................. 240
B.11 Comparison of the Voyager 1 Beta Centauri pulse height-to-count mode ratio spectrum and the corresponding best-fit model .... 242
B.12 Best-fit detector gains for Voyager 1 .................................. 244
B.13 Best-fit current limiting function for Voyager 1 ...................... 249
B.14 Comparison of the HVL 2 and HVL 3 sunsals processed with the best-fit current limiting function ................................. 250
B.15 Even channel correction factor grid for Voyager 1 .................. 253
B.16 Illustration of the effectiveness of the even channel correction factor grid ...................................................... 254
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>C.1</td>
<td>Example of an analytical linearization curve</td>
<td>259</td>
</tr>
<tr>
<td>C.2</td>
<td>Illustration of the iterative linearization scheme</td>
<td>262</td>
</tr>
<tr>
<td>D.1</td>
<td>N\textsubscript{2} photoabsorption cross sections</td>
<td>270</td>
</tr>
<tr>
<td>D.2</td>
<td>N photoabsorption cross sections</td>
<td>271</td>
</tr>
<tr>
<td>D.3</td>
<td>CH\textsubscript{4} photoabsorption cross sections</td>
<td>273</td>
</tr>
<tr>
<td>D.4</td>
<td>C\textsubscript{2}H\textsubscript{2} photoabsorption cross sections</td>
<td>276</td>
</tr>
<tr>
<td>D.5</td>
<td>C\textsubscript{2}H\textsubscript{4} photoabsorption cross sections</td>
<td>278</td>
</tr>
<tr>
<td>D.6</td>
<td>C\textsubscript{2}H\textsubscript{6} photoabsorption cross sections</td>
<td>280</td>
</tr>
<tr>
<td>D.7</td>
<td>H\textsubscript{2} photoabsorption cross sections</td>
<td>283</td>
</tr>
<tr>
<td>D.8</td>
<td>H photoabsorption cross sections</td>
<td>284</td>
</tr>
<tr>
<td>D.9</td>
<td>C\textsubscript{4}H\textsubscript{2} photoabsorption cross sections</td>
<td>285</td>
</tr>
<tr>
<td>D.10</td>
<td>C\textsubscript{2}N\textsubscript{2} photoabsorption cross sections</td>
<td>287</td>
</tr>
<tr>
<td>D.11</td>
<td>C\textsubscript{4}N\textsubscript{2} photoabsorption cross sections</td>
<td>288</td>
</tr>
<tr>
<td>D.12</td>
<td>HCN photoabsorption cross sections</td>
<td>290</td>
</tr>
<tr>
<td>D.13</td>
<td>HC\textsubscript{3}N photoabsorption cross sections</td>
<td>291</td>
</tr>
</tbody>
</table>
LIST OF TABLES

B.1 Comparison of In-Flight and Lab-Measured Scan Rates ........ 221

D.1 N₂ Cross Section Data ........................................... 270
D.2 CH₄ Cross Section Data ........................................... 273
D.3 C₂H₂ Cross Section Data ....................................... 276
D.4 C₂H₄ Cross Section Data ...................................... 278
D.5 C₂H₆ Cross Section Data ...................................... 280
D.6 H₂ Cross Section Data ........................................ 283
D.7 H Cross Section Data ........................................... 284
D.8 C₂N₂ Cross Section Data ..................................... 287
D.9 HCN Cross Section Data ....................................... 290
ABSTRACT

The Voyager 1 Ultraviolet Spectrometer (UVS) observations are the only direct measurements we have of Titan's upper atmosphere. Previous analysis of the two UVS solar occultations yielded densities for N₂, CH₄, and C₂H₂, as well as the thermospheric temperature. These results serve as the upper atmospheric boundary conditions in models of Titan's atmosphere; however, there are discrepancies between the observations and models, and the previous analysis itself is known to be internally inconsistent.

We have undertaken a reanalysis of the UVS solar occultations to resolve these differences and to extract the maximum amount of information from the data. In so doing, we have developed a detailed model of the UVS detector and a new analysis method tailored to retrieving multiple species from an occultation of a finite-sized source such as the sun.

Our analysis has yielded density profiles for nine species in Titan's upper atmosphere and a new measurement of the thermospheric temperature. We find higher N₂ densities and lower CH₄ and C₂H₂ densities than those previously determined. We also find a thermospheric temperature of 150–155 K instead of 176–196 K as in the early analysis. Densities for C₂H₄, C₂H₆, C₄H₂, C₂N₂, HCN, and HC₃N are retrieved for the first time.

Titan's atmosphere is one of the most interesting in the solar system. The composition and high degree of photochemical activity elicit comparisons to the early terrestrial atmosphere and considerations about the origins of life. Our results provide improved and expanded constraints for the atmospheric models and should provide scientists with a better view of Titan's upper atmosphere, which is important in planning for the upcoming Cassini mission.
CHAPTER 1

INTRODUCTION

We cannot fully understand the current state of knowledge regarding a topic of scientific interest unless we have an adequate grasp of what has been done in the past. However, we cannot spend all of our time understanding the past or no progress would ever be made. As such, we present here a brief summary of the work that has been done on Titan's atmosphere since its discovery over fifty years ago and use this history as a starting point for the current work.

Before we begin, we should note that the brightness temperature measurements used by many researchers to make inferences about Titan's atmosphere and surface are dependent on the radius of Titan, which was somewhat uncertain at the time. An early estimate of the radius was 2405 km (Harris, 1961). This value was subsequently revised to 2425 km by Dollfus (1970). Morrison et al. (1972), however, pointed out evidence that even this radius was too small and revised the Dollfus value to 2550 km. This evidence was later reconsidered and a value of 2500 km was adopted (Hunten, 1974a; Morrison and Cruikshank, 1974). Shortly thereafter, Elliot et al. (1975) determined a radius of 2916 km using a lunar occultation of Titan by Saturn; however, this value relied on an estimate of the limb darkening of the atmosphere. Believing this estimate to pertain to some level in the atmosphere, many authors adopted a value of 2700 km as the radius of the "true" surface (cf. Caldwell, 1978).

The uncertainty in the radius, while affecting the absolute values of the brightness temperatures, did not affect the relative structure of Titan's infrared spectrum because all the brightness temperatures could be normalized to a given
radius. Rather than do this here, we will simply quote the brightness temperatures as determined by the observers and include the radius value they used in parentheses after the quoted temperature value.

1.1 Pre-Voyager Conceptions of Titan's Atmosphere

The story of Titan's atmosphere began during World War II with the startling discovery by Kuiper (1944) of methane (CH$_4$) absorption bands in the spectrum of Titan. Although this represented the first concrete evidence for an atmosphere on Titan, Kuiper points out the following statement by Jeans (1925): "An atmosphere has been observed on Titan." Because he could find no reference to such an observation in the literature, Kuiper refers to this statement as having "doubtful status;" however, a visual observation of limb darkening was reported by Comas Solá (1908) and it may be this report upon which Jeans based his statement. [Note of interest: In the same paragraph, Jeans also remarks on the "suspected atmospheres on two of Jupiter's satellites," something known for Io for over thirty years (Binder and Cruikshank, 1964) and which recent observations have proved true for Ganymede and Europa as well (Hall et al., 1995; Hall et al., 1996).]

A few years later, Kuiper followed up on his discovery with a laboratory comparison, in which he concluded that a pure-CH$_4$ atmosphere on Titan must contain 200 meter-amagats (m-A) of CH$_4$ (Kuiper, 1952). Despite this remarkable observation, very little was done regarding Titan's atmosphere for nearly twenty years. A notable exception is the observation of Low (1965), who noted that Titan has an anomalously high temperature in the infrared (IR) if it radiates as a black body. His observation seems to have been overlooked, however, and Low later refers to the flurry of infrared observations in the early seventies as the "rediscovery" of Titan's anomalous IR spectrum (Low and Rieke, 1974).

In the early seventies, the study of Titan's atmosphere emerged from its dormant state, triggered primarily by three separate discoveries. First, Trafton
(1972b) reported the detection of weak absorption features in Titan's spectrum at the wavelengths of the 3-0 S(1) and 3-0 S(0) quadrupole lines of hydrogen (H₂). From this he estimated a column abundance of 5 km-A of H₂. Second, Allen and Murdock (1971) and Morrison et al. (1972) measured the thermal IR spectrum of Titan and found it to be anomalous. Allen and Murdock noted that the brightness temperature of Titan at 12.4 μm was 125 ± 3 K (2405 km) and not 116 K as expected for a black body at Titan's distance from the sun. Morrison et al. measured a brightness temperature of 93 ± 1 K (2550 km) at 20 μm, which in combination with the 12.4-μm measurement of Allen and Murdock showed that Titan's thermal IR spectrum is distinctly different from a black body. Both Allen and Murdock and Morrison et al. suggested that a greenhouse effect might be at work on Titan. Finally, McCord et al. (1971), who cited similar work by Harris (1961), showed that the albedo of Titan dropped dramatically from visible to ultraviolet wavelengths.

After these three discoveries, interest in Titan soared to new heights. Trafton (1972a) demonstrated that the methane bands in Titan's spectrum are saturated and noted that either Kuiper's estimate of 200 m-A would have to be revised to 1.6 km-A if CH₄ is the dominant gas or another gas, possibly H₂, is the bulk constituent. Both Veverka (1973) and Zellner (1973) concluded on polarimetric evidence that the drop in albedo in going to the ultraviolet must be caused by an opaque cloud layer with a constituent that absorbs strongly in the ultraviolet. Hunten (1972), in a short but remarkably insightful paper, remarked that retention of the amount of H₂ required by Trafton (1972b) is difficult to conceive unless a heavier gas is present to stabilize it against blow-off. Although CH₄ was known to be present, Hunten used the results of Lewis (1971) to propose that photolysis of ammonia (NH₃) would result in the accumulation of nitrogen (N₂), which could be the bulk constituent of the atmosphere.

Based upon the presence of H₂, Sagan (1973) and Pollack (1973) proposed greenhouse models for Titan. In Sagan's model, the opacity to drive the greenhouse was provided by pressure-induced transitions of hydrogen. This model had a surface
pressure roughly equal to Earth’s, a surface temperature as high as 200 K, and a somewhat staggering H₂ abundance of 100 km-A. Pollack’s model used pressure-induced transitions of hydrogen and methane to drive the greenhouse. While his surface pressure and temperature were similar to Sagan’s, his abundances of H₂ and CH₄ were comparable to the values measured by Trafton (1972a). Both authors pointed out that methane condensation clouds should form and that these could be responsible for the low ultraviolet albedo. Additionally, both authors stated N₂ could not be ruled out as a major constituent but considered it unlikely for that to be the case. A third greenhouse model using neon and/or argon was proposed by Cess and Owen (1973), and they also considered a N₂-dominated atmosphere to be unlikely.

The large amount of H₂ measured by Trafton (1972b), and the even larger amount necessary in the model of Sagan (1973), raised questions about the ability of Titan to retain such amounts of H₂. This concern was addressed in detail by Hunten (1973), who showed that the escape of H₂ is inevitable but can be limited if a heavier gas is present. As in his earlier paper (Hunten, 1972), Hunten advocated an atmosphere in which N₂ was the major constituent but conceded that CH₄ could also provide the necessary stabilization. In response to this, Lewis and Prinn (1973) confirmed on chemical grounds that a CH₄-rich atmosphere was possible and should be considered as a viable alternative to a N₂-rich atmosphere. An interesting consequence of the inevitable escape of H₂ was noted by McDonough and Brice (1973a, 1973b), who showed that the hydrogen should be captured in Saturn’s gravitational field and form a torus following the orbit of Titan.

While models of Titan’s atmosphere were debated, other topics were addressed as well. Khare and Sagan (1973) had produced a dark, reddish-brown substance in the laboratory through the irradiation of gases abundant in the outer solar system. They noted that this substance had properties very similar to those required of the particles composing the suspected clouds on Titan. Leovy and Pollack (1973) investigated the dynamics of Titan’s atmosphere. They found the
temperature variations of the atmosphere to be too small to permit the storage of volatiles in polar caps and concluded that the present methane abundance was probably a balance between outgassing and photodissociation.

The interesting nature of the thermal IR spectrum was further investigated by Joyce et al. (1973) and Gillett et al. (1973). Joyce et al. used measurements at 4.9 $\mu$m, a supposedly absorption-free “window”, to constrain the surface temperature. They concluded that the surface temperature must be less than 190 K (2550 km) if they were seeing the actual surface. If, however, the 5-$\mu$m window was “closed” by absorption in the cloud layer, no constraint could be placed on the surface temperature. Gillett et al. made measurements in the 8-13 $\mu$m range and for the first time saw detailed structure in the spectrum. This structure led them to two conclusions: 1) at least one spectroscopically active component other than CH$_4$ and H$_2$ must be present and 2) the high brightness temperature at 8.0 $\mu$m indicates the presence of a temperature inversion. The other component was suspected to be ethane (C$_2$H$_6$), a suspicion supported by the photochemical model of Strobel (1974), which predicted large column abundances of C$_2$H$_6$. Measurements in the infrared by Trafton (1974) supported the idea of other spectroscopically active species although he was unable to specify what they might be.

With these new observations in hand, Danielson et al. (1973) proposed a non-greenhouse model of Titan’s atmosphere in which a layer of “dust” causes a temperature inversion in the atmosphere. In the model, the dust particles absorb blue and ultraviolet solar radiation, thereby explaining the drop in the ultraviolet albedo. The absorbed radiation is then reradiated by the dust and by molecules having long wavelength bands (e.g., CH$_4$, C$_2$H$_6$). The dust particles are assumed to be poor emitters, so the temperature of the dust rises as does the temperature of the surrounding gas molecules through collisions with the dust. Based upon the measurements of Gillett et al. (1973), Danielson et al. modeled the thermal IR spectrum with a surface of temperature 80 K and emissivity $\epsilon = 1$, dust particles having a temperature of 160 K and an emissivity proportional to the inverse wavelength,
and emission lines from CH$_4$ and C$_2$H$_6$. Danielson et al. noted that their model requires less CH$_4$ than the greenhouse models, that it requires no H$_2$ although it could be accommodated, and that the reddish-brown substance of Khare and Sagan (1973) qualitatively has the properties necessary in the dust particles. Their model also predicted a surface pressure of roughly 20 mbar rather than the bar to kbar levels of the greenhouse models.

The Danielson et al. model was qualitatively supported by further observations of Titan's ultraviolet albedo by Barker and Trafton (1973). Barker and Trafton found no trace of any absorption bands in the spectrum and showed that it was similar to that of Saturn's rings. These results implied that Rayleigh scattering and gaseous ultraviolet absorption are subdued in Titan's atmosphere; however, they determined that an absorber with a weak dependence upon wavelength could satisfy the observations if the absorber were inhomogeneously distributed, as it would be in the Danielson et al. model. The observations of Younkin (1974) also supported the thermal inversion model. Younkin compared the methane bands in the spectrum of Titan to those in spectra of Jupiter and Saturn and concluded that differences between the morphology of these bands on Titan and Saturn could be due to the presence of dust in Titan's atmosphere.

Measurements by Briggs (1974), however, did not support the thermal inversion model so strongly. Briggs determined a brightness temperature of 115$\pm$40 K (2500 km) at 8085 MHz (3.7 cm) and estimated the surface temperature to be 135$\pm$45 K. This high surface temperature tended to support the greenhouse models rather than the thermal inversion model, but the accuracy was such that the thermal inversion model was not ruled out.

Because of the rapid increase of both interest in and knowledge of Titan's atmosphere, a workshop was convened at NASA's Ames Research Center in July of 1973. The conclusions of that workshop are presented in Hunten (1974b) and are summarized in Hunten (1974a). Most of these have been referenced above, and two atmospheric models were supported at the outcome: the thermal inversion model
of Danielson et al. (1973) and a modified greenhouse model in which a warm dust layer overlay a cold cloud layer over a warm surface. These models are qualitatively illustrated in Figure 1.1.

An important result of the workshop was that the presence or absence of a greenhouse caused by H$_2$ could be decided by the shape of the IR spectrum near 17 $\mu$m. In view of this, Low and Rieke (1974) made measurements of the thermal IR spectrum from 1.6 to 34 $\mu$m. Their observations did not show the structure that would be expected from a H$_2$-rich atmosphere, and they ruled out any greenhouse models based on H$_2$. Based on estimates of the surface temperature of 80–90 K (2550 km), they also noted that the thermal inversion model could be ruled out if the bolometric albedo exceeded 0.2, proposing instead a weak greenhouse model powered by pressure-induced absorption in CH$_4$. In addition, their measurement at 5 $\mu$m constrained the surface temperature to be less than 165 K if the 5-$\mu$m window is “open” (cf. Joyce et al., 1973), and they found no evidence for a possible ethylene (C$_2$H$_4$) emission at 10.5 $\mu$m.

Continuing his work on Titan’s atmosphere, Trafton (1975a) compared the CH$_4$ bands in Titan’s spectrum to those in Saturn’s and found the Titan bands to be “washed out” relative to Saturn’s. He concluded that a clear, absorbing gas could not entirely explain this band morphology and that particulate scattering must play a role, confirming the similar conclusion by Younkin (1974). In a second paper, Trafton confirmed his earlier conclusion (Trafton, 1972a) that CH$_4$ must have an abundance of 1.6 km-A or higher, found further evidence for a constituent other than CH$_4$ and H$_2$ in unidentified absorptions between 1.05 and 1.06 $\mu$m, and confirmed that the absorption feature at the wavelength of the 3-0 S(1) line of H$_2$ was real although the one at the 3-0 S(0) line was not definitively established (Trafton, 1975b).

Other observers pursued the investigation of Titan’s IR spectrum as well. Consistent with the results of Low and Rieke (1974), Knacke et al. (1975), assuming
Figure 1.1: Qualitative illustrations of the two models of Titan's atmosphere resulting from the July 1973 workshop. The top panel illustrates the modified greenhouse model. The solid lines bracket a hypothesized CH$_4$ cloud layer which could form at the tropopause. The dotted line represents the nominal surface level, but the temperature profile is extended beyond this level to illustrate that the surface may be deeper. The lower panel represents the thermal inversion model of Danielson et al. (1973). The solid line represents the actual surface level in this model because the surface temperature is assumed to be measured directly and not hidden by the atmosphere as in the greenhouse model.
that the 5-\mu m window is "open," determined an upper limit to the surface temperature of 160 K (2550 km) and found the structure of the spectrum near 17 \mu m to be inconsistent with large amounts of H_2. They concluded that the H_2-rich greenhouse models were unlikely given these two results. Gillett (1975) made further observations of the 8-13 \mu m range and his spectrum was a good match to the predicted spectrum of the thermal inversion model. In addition, he found evidence for emission from acetylene (C_2H_2), C_2H_4, and monodeuterated methane (CH_3D), and commented that the peak of the CH_3D emission was lower than expected if the CH_4 abundance was as large as most observers were requiring for the IR absorption bands. Based on this, he suggested that the CH_4 abundance might be lower than the accepted values owing to the presence of a large amount of a broadening gas or that the bulk of the atmosphere was not in the temperature inversion region, which would reduce the amount of CH_3D seen in emission.

Using a somewhat experimental technique, Owen and Cess (1975) constructed a band model for CH_4 using the known CH_4 abundance of Jupiter and observations below 6000 \AA, where they believed the continuum could be better defined than in the longer IR wavelength region. They determined a surface pressure for Titan of P_s \geq 1.3 atm (the inequality allowing for a cloud over the surface) and a CH_4 column abundance of 20 m-A. This column abundance gave a CH_4 partial pressure of 0.2 mbar, which indicated that a large amount of another gas must be present. Consistent with the earlier work of Cess and Owen (1973), they suggested that the other gas might be neon, but they also stated that it could be N_2 as proposed by Hunten (1972).

Owen and Cess (1975) remarked that a laboratory study was needed as an absolute calibration for their method before their results could be fully accepted. This was provided soon after by Lutz et al. (1976), who made a number of laboratory measurements of CH_4 absorption below 6000 \AA. Based on these, they determined a CH_4 abundance of 80 m-A, a factor of twenty smaller than that estimated...
by Trafton (1972a). They noted that Trafton's estimate was made assuming a CH$_4$-dominated atmosphere but that their lab measurements contradicted his assumptions about the band formation. Their CH$_4$ abundance yielded a surface pressure $P_s \geq 0.4$ atm, though they note that this might have to be revised to $P_s \geq 1.2$ atm depending on certain assumptions they made. The corresponding CH$_4$ partial pressure was 0.9 mbar, confirming that a large amount of another gas was necessary. As Owen and Cess did, Lutz et al. suggested that this gas could be neon or N$_2$.

The IR spectrum was not the only area in which work on Titan was being done at this time. Golitsyn (1975) and Leovy and Pollack (1975) continued the theoretical studies of the dynamics of Titan's atmosphere. One of the more interesting conclusions was made by Golitsyn, who commented that superrotation might occur in Titan's upper atmosphere in a fashion similar to that of Venus. Caldwell (1975) summarized OAO-2 observations of Titan and reached conclusions similar to those of Barker and Trafton (1973) regarding Titan's ultraviolet albedo.

Because the H$_2$ abundance was of critical importance to the greenhouse models, Münch et al. (1977) made high-resolution measurements at the wavelength of the H$_2$ 3-0 S(1) line. They found no evidence of the H$_2$ absorption and quoted an upper limit on the H$_2$ abundance of 1 km-A, a factor of five lower than that of Trafton (1972b). Although they stated that this abundance could be slightly higher if some of their assumptions were incorrect, they concluded that no abundance consistent with their observations would be large enough to provide the opacity necessary for the H$_2$-greenhouse models.

The smaller H$_2$ abundance determined by Münch et al. effectively closed the door on the H$_2$-dominated greenhouse models, leaving two models in contention. The first was the thermal inversion model of Danielson et al. (1973), which Caldwell (1977) summarized and updated to include the more recent data. The second, summarized by Hunten (1977), was the modified greenhouse model, which incorporated the thermal inversion model by placing it on top of a cloud layer under which the temperature increased down to a surface value of 100 K or greater through a
weak CH$_4$ greenhouse effect. Both models acknowledged the requirement of a warm stratosphere and a thermal inversion, most likely caused by an absorbing dust layer.

Beyond this, however, they differed quite a bit. The thermal inversion model placed the surface around the 15-20 mbar level, had CH$_4$ as the dominant gas with an abundance of 1.6 km-A, and had a surface temperature of 78 K. From the surface, the temperature increased to roughly 160 K in the dust layer, above which the atmosphere was isothermal. Because the thermal inversion made formation of clouds unlikely, the clouds required by Veverka (1973) and Zellner (1973) to explain the ultraviolet albedo and polarization data were replaced by appropriate properties in the dust. The modified greenhouse model, on the other hand, placed the surface near the 1 bar level, had CH$_4$ as a minor species with an abundance of order 100 m-A, had either N$_2$ or Ne as the dominant gas with an abundance of 20-30 km-A (although Hunten argued against Ne because of its rarity elsewhere in the solar system), and had a surface temperature in excess of 100 K. From the surface, the temperature decreased to 75-80 K at a tropopause where clouds were likely to form. Above this tropopause, the structure was similar to the thermal inversion model with the temperature peaking near 160 K in the dust layer. Almost as an aside, Hunten included the possibility of a mesosphere above the warm stratosphere. The temperature in such a mesosphere could decrease to a lower value at a mesopause because of a decrease in the amount of dust at higher altitudes. Hunten somewhat arbitrarily chose 100 K as the mesopause temperature. Above this level, the atmosphere was assumed to be isothermal at the mesopause temperature.

With the dust layer and its corresponding thermal inversion more or less generally accepted, researchers began to investigate the properties of the required dust. Podolak and Danielson (1977) used Mie theory to model the scattering and absorption properties of the dust. They concluded that particles with a maximum radius of 0.1 \(\mu\)m would have the necessary properties. Contradictory to the results of Lutz et al. (1976), Podolak and Danielson also determined a CH$_4$ abundance of 1 km-A. They argued that this discrepancy lay in Lutz et al.'s neglect of the dust in
their analysis and stressed that the dust must be included in any future modeling of the CH$_4$ IR bands. The results of Podolak and Danielson tended to support the thermal inversion model because of the relatively high CH$_4$ abundance they derived.

Support for the modified greenhouse model, however, came from the work of Scattergood and Owen (1977), who irradiated various gas mixtures in the lab and observed the resulting ultraviolet spectra. They found that mixtures of CH$_4$ and H$_2$ alone produced colorless spectra inconsistent with the observed ultraviolet spectrum of Titan. To obtain spectra consistent with the color of Titan, they determined that nitrogen (as either NH$_3$ or N$_2$) or sulfur (as H$_2$S) were necessary. With no indication that sulfur was present in Titan's atmosphere, they favored the presence of nitrogen, which supported the modified greenhouse model.

In early 1978, a workshop was held to discuss the current state of understanding of the Saturn system. Caldwell (1978) provided another summary of the thermal inversion model for Titan's atmosphere, citing the work of Podolak and Giver (1979) and Jaffe et al. (1979) as further evidence for the model. Podolak and Giver investigated the IR spectrum of Titan using inhomogeneous scattering models for Titan's atmosphere and concluded that the CH$_4$ abundance must be at least 2 km-A. It should be noted, however, that Podolak and Giver pointed out that it was not possible to distinguish between the "surface" of the thermal inversion model and the top of a cloud layer below which a greenhouse atmosphere might exist. Jaffe et al. measured a brightness temperature of 87 ± 13 K (2700 km) at 6 cm for Titan, which favored the lower-surface-temperature thermal inversion model.

Hunten (1978) provided another version of the modified greenhouse model in which the surface temperature was now 200 K, the surface pressure was 21 bars, and the mesosphere of his previous summary (Hunten, 1977) was removed. Hunten cited the work of Conklin et al. (1977), who observed a brightness temperature of 178 ± 38 K (2916 km) at 3 mm wavelength, as the motivation for the high surface temperature. The measurement of Conklin et al. was in serious conflict with that of Jaffe et al., which led the latter to conclude that one or more of the measured
brightness temperatures were in error, though they did not comment on which ones. Although his preference was for the higher temperature surface, Hunten stated that his model could equally provide for a surface temperature near 100 K by simply placing the surface at the 2 bar level and leaving the remainder of the atmosphere unchanged.

In support of his model over the thermal inversion model, Hunten pointed out the work of Rages and Pollack (1978) and Fink and Larson (1979). Rages and Pollack investigated the physical properties of Titan's aerosols (dust) and concluded that the particles must have radii between 0.2 and 0.4 μm, contradicting the results of Podolak and Danielson (1977), which had been supportive of the thermal inversion model. Fink and Larson measured the IR spectrum of Titan between 0.8 and 2.5 μm and showed that it was quite different from the laboratory spectrum of pure CH₄, supporting the view that CH₄ is a minor constituent in Titan's atmosphere. Additional support came from the work of Atreya et al. (1978), who proposed a scheme for the evolution of a dense, nitrogen-rich atmosphere on Titan.

In response to both Caldwell and Hunten, Trafton (1978) commented that his previous work could be used to support either model. He also stated that he believed Münch et al. (1977) underestimated the H₂ abundance and that in his opinion the features at the wavelengths of the 3-0 S(1) and 3-0 S(0) lines of hydrogen were real, even if they did not arise from H₂.

While the debate continued on which atmospheric model was correct, other researchers focused on the chemistry of Titan's atmosphere. Strobel (1978) examined the photochemistry of a pure-CH₄ atmosphere and found C₂H₂ and C₂H₆ to be the most abundant products of CH₄ photolysis until high in the atmosphere where C₃H₄ and short-lived radicals became more abundant. Bar-Nun and Podolak (1979) also examined the photochemistry of a pure-CH₄ atmosphere and came to other conclusions, differing primarily in estimating a C₂H₂ abundance that was two orders of magnitude smaller than Strobel's. The photochemical model of Allen et al. (1980) provided a third perspective on this issue, though their main conclusion was
that photochemically-produced polyacetylenes are the most likely precursors of the molecules composing the stratospheric dust. Finally, Chang et al. (1978) examined organic chemistry in a Titan atmosphere containing both CH$_4$ and N$_2$. They concluded that nitrogen was necessary for the reddish color of Titan and that the surface of Titan should be covered with both hydrocarbon and N-organic materials which have condensed and fallen out of the atmosphere.

The aerosols in Titan's atmosphere, as the dust particles were now referred to, continued to receive a great deal of attention as well. Podolak and Bar-Nun (1979) examined the physics of the aerosols and determined an upper limit to the aerosol production rate that was five times smaller than required by the models of Podolak and Giver (1979) and Rages and Pollack (1978). This upper limit was, however, consistent with the results of Podolak and Danielson (1977), but those results had been shown to be inconsistent with the CH$_4$ absorption in the IR (Podolak and Giver, 1979). Podolak and Bar-Nun noted that the presence of roughly five times more gas, possibly N$_2$, than implied by either Podolak and Giver or Rages and Pollack could help bring those models into agreement. This seemed to lower the balance in favor of the modified greenhouse model, but the results of Podolak et al. (1979) maintained the balance. Podolak et al. examined the optical properties of various polymers and found that aerosols composed of polyethylene could provide the reddish color of Titan without any N$_2$. This negated the argument by Scattergood and Owen (1977) and Chang et al. (1978) that N$_2$ was necessary.

To place further constraints on the aerosol particles, Rages and Pollack (1980) examined Titan's solar phase variation as a function of wavelength together with the continuum geometric albedo. They concluded that the radii of the particles must be between 0.2 and 0.35 $\mu$m, consistent with the earlier results of Rages and Pollack (1978). They also estimated the CH$_4$ abundance in Titan's atmosphere to be on the order of 2 km·A, consistent with the thermal inversion model, and stated that their derived aerosol properties were consistent with both the products of irradiation of CH$_4$ and N$_2$ mixtures observed by Scattergood and Owen (1977).
and the polyethylenes observed by Podolak et al. (1979). Work by Podolak and Podolak (1980), however, determined that the particle sizes necessary to explain the spectrum of Titan could not form at pressures less than 2 mbar. Because the thermal inversion model required the layer at pressures less than 0.11 mbar, they argued that the thermal inversion model seemed to be ruled out, leaving the modified greenhouse model as the only contender.

As the pre-Voyager era of Titan’s atmosphere drew to a close, attention was also given to a related though not strictly atmospheric topic. Smyth (1981) developed a new model for the Titan hydrogen torus proposed by McDonough and Brice (1973a, 1973b), which had been tentatively detected by Barker (1977) and Barker et al. (1980) and positively detected by Judge et al. (1980). Considerations of the hydrogen supply rate necessary to maintain the torus imposed constraints, albeit mostly theoretical, on the hydrogen density in Titan’s atmosphere.

With no firmly conclusive evidence for either the thermal inversion or modified greenhouse model, researchers had to wait for the Voyager 1 encounter with Titan in November 1980 to know which model was the correct one. It is interesting, especially in retrospect, to note a comment by Hunten, made at the end of the 1978 workshop, regarding the photochemical modeling of Titan’s atmosphere (Hunten and Morrison, 1978, p. 332):

“My personal predilection would be to try to learn something about the upper atmosphere of Titan also. I think this is one of the important insights that’s come out of this meeting, something that perhaps should have been obvious but didn’t occur to me, that methane is liable to be present at very high altitudes and subject to low energy proton bombardment, along with the nitrogen, if it’s there, and produce a great deal of interesting chemistry right at the top of the atmosphere.”

As we shall see in the next section, this statement was almost prophetic in nature.
1.2 The Voyager Encounters

In late 1980, the Voyager 1 spacecraft flew through the Saturn system and gave us our first detailed look at Titan. Its trajectory carried Voyager 1 past Titan while inbound to Saturn, with the closest approach occurring at 0541 UTC (coordinated universal time) on November 12, 1980, at a distance of roughly 6500 km. Voyager 2 also flew through the Saturn system, but its trajectory had been set with the goal of continuing to Uranus and it came no closer than 665,000 km to Titan. As such, the Voyager 1 fly-by is the source of much of what we know about Titan's atmosphere.

The Voyager spacecraft are equipped with a suite of instruments whose varied capabilities are in line with the reconnaissance nature of their missions. Of these, five are most important in studying Titan's atmosphere: an imaging system (ISS), an infrared spectrometer (IRIS), a photopolarimeter (PPS), an ultraviolet spectrometer (UVS), and a radio science system (RSS). We will briefly cover the major results from these five instruments in this section. The remaining instruments are oriented more toward the study of the local space environment surrounding the planets and satellites rather than the bodies themselves. We will not discuss them here; however, excellent summaries of the results from these instruments may be found in several special journal issues: Science 212 (1981), Science 215 (1982), Nature 292 (1981), J. Geophys. Res. 87 (1982), and J. Geophys. Res. 88 (1983).

The ISS results summarized here are from Smith et al. (1981) and B. A. Smith et al. (1982). The Voyager imaging system is essentially a set of cameras which operate in the visible wavelength range. During the several hours before the closest approach, the ISS covered roughly 90% of the illuminated disk at 3.4-km resolution and roughly 50% at 1.3-km resolution. These images revealed that Titan is surrounded by a global haze layer which completely obscures the surface in the visible. Titan's color is reddish-orange, though it is often referred to as brown. A hemispherical asymmetry was observed, the southern hemisphere being uniformly bright in general while the northern hemisphere is darker and redder and
possesses an even darker polar hood. The source of the asymmetry was qualitatively attributed to a combination of seasonal and solar cycle variations. A quantitative analysis of the hemispherical asymmetry is given by Sromovsky et al. (1981).

Limb observations revealed that the global haze brightness peaks at a radial distance of roughly 2753±22 km at northern mid-latitudes and 2804±22 km at southern mid-latitudes. They also revealed that a secondary, mostly detached haze layer has its peak brightness at a radius of 2884±20 km. Estimates of the aerosol optical depth were made by attributing the lack of small-scale contrast features in the images to aerosol obscuration. The resulting values of τ > 5–10 are consistent with the layer being opaque at visible wavelengths. ISS images were also used to deduce the average aerosol particle radius as between 0.25 and 0.5 μm, although the results are dependent on a number of assumptions.

The Voyager infrared instrument consists of a Michelson interferometer, which covers the range of 180 to 2500 cm⁻¹ with a resolution of 4.3 cm⁻¹, and a single-channel radiometer, which operates at visible and near-infrared wavelengths. This instrument obtained a wealth of information on Titan’s lower atmospheric composition, structure, and dynamics during a period from roughly eight hours before to three hours after closest approach. The following summary is taken from a number of articles: Hanel et al. (1981), Hanel et al. (1982), Maguire et al. (1981), Kunde et al. (1981), Samuelson et al. (1981), Flasar et al. (1981), and Samuelson et al. (1983).

Spectra taken with the IRIS instrument showed a number of emission features superimposed on a background continuum. These features were identified as due to CH₄, C₂H₂, C₂H₄, C₂H₆, C₃H₄, C₃H₈, C₄H₂, C₂N₂, HCN, HC₃N, and CO₂. In addition, H₂ was seen in absorption. The brightness temperature information in these spectra was combined with the radio science data (see below) to infer the temperature structure of the lower atmosphere. Because of the spatial coverage of the IRIS data, it was possible to measure latitudinal variations in both composition and temperature, and the northern high-latitudes were found to be cooler than the
The temperature differences measured by IRIS imply that a meridional gradient in geopotential exists, which must be dynamically balanced. Hanel et al. (1981) proposed that this leads to zonal winds of roughly 100 meters per second, ten times Titan's surface speed. Such superrotation of the atmosphere has been observed on Venus, a planet to which Titan has often been compared, and was predicted by Golitsyn (1975).

Analysis of the Voyager radio science results was presented by Tyler et al. (1981) and Lindal et al. (1983). The radio science experiment consisted of using the spacecraft antenna and the coherent dual-frequency radio system (wavelengths roughly 3.6 and 13 cm) to conduct radio occultations in Titan's atmosphere. Downlink to Earth was established and tracked as the spacecraft passed behind Titan and reemerged on the other side. The measured propagation effects through Titan's atmosphere were analyzed to yield information on the temperature and composition of the lower atmosphere. The experiment also measured the electron content of the upper atmosphere. No evidence for ionization layers was found, with the resolution being $3 \times 10^3$ and $5 \times 10^3$ electrons cm$^{-3}$ at the evening and morning terminators, respectively. Finally, scintillations in the data were observed and were potentially attributed to gravity waves and/or CH$_4$ clouds.

Because the radio occultation experiment only measures the temperature-mass ratio, the RSS data were combined with the IRIS data to yield a consistent view of the lower atmosphere. This combined analysis was consistent with a mass of roughly 28, which implied that N$_2$ was the primary atmospheric constituent. CO also has mass 28, but the UVS (see below) directly observed emissions from N$_2$, confirming that it is the dominant gas. Even if the UVS had not observed N$_2$ directly, the presence of N-bearing molecules and scarcity of O-bearing molecules as inferred from the IRIS spectra would have combined to rule out CO as a dominant species.
Figure 1.2: Comparison of the predicted temperature profile of Hunten (1978) and the actual temperature profile measured by Voyager 1 (Lindal et al., 1983). Hunten's preferred model had the surface at roughly 20 bars with the surface temperature at 200 K, but he commented that the surface could be placed at a higher level and the remaining profile remain valid.

Using a mass of 28 (pure N$_2$), Lindal et al. (1983) inferred the temperature profile of Titan's lower atmosphere shown in Figure 1.2. This profile is for the ingress occultation, and the data are from their Table I. Also shown in this figure is the predicted temperature profile of Hunten (1978). The match between the profiles is remarkable, especially given that the surface temperature and pressure, the existence of a tropopause, and the atmospheric composition were all unknown prior to the Voyager 1 fly-by. In addition to the temperature profile, Lindal et al. determined a surface temperature of 94.0±0.7 K, a surface pressure of 1.496±0.02 bar,
a density of $1.881 \pm 0.002$ g cm$^{-3}$, and a radius of $2575.0 \pm 0.5$ km.

The Voyager photopolarimeter observations of Titan are discussed in detail by Lane et al. (1982) and West et al. (1983). Unfortunately, the Voyager PPS suffered instrumental problems during the Jupiter-Saturn cruise and lost the use of five out of eight filters and four out of eight polarization analyzer positions. Through reprogramming, however, the PPS was still able to make important observations of Titan's whole disk polarization at 2460 Å and 7500 Å, with bandpasses of 300 Å and 250 Å, respectively.

The primary result of the PPS observations is that Titan's atmosphere shows strong positive polarization at all phase angles. The measured phase angles ranged from 2.7° to 154°. The observations are not able to be fit by a single-size distribution if the aerosol particles in Titan's atmosphere are spherical or nearly so, and two alternate models were considered. A vertically inhomogeneous distribution of spherical particles suggested by Tomasko and Smith (1982) to explain Pioneer 11 observations fitted the 2640 Å data reasonably well. With some modifications it somewhat fitted the 7500 Å data. The other alternative was suggested by Smith et al. (1981), who proposed that the aerosol particles are nonspherical. A general theory for nonspherical particles did not exist at the time, so confirmation of this hypothesis was difficult.

The final instrument of interest here is the Voyager ultraviolet spectrometer. Analyses of the UVS observations are discussed by Broadfoot et al. (1981a), Sandel et al. (1982), G. R. Smith et al. (1982), and Strobel and Shemansky (1982). The UVS made several different types of observations at Titan, including disk-averaged spectra of Titan's dayglow, measurements of emission as a function of altitude (limb drifts), observations of the hydrogen torus, and solar occultations by the atmosphere.

The airglow observations provided the best direct evidence that the primary
gas in Titan's atmosphere is N₂. The disk-averaged dayglow spectra showed a number of emissions due to N₂, N, and singly-ionized N (N⁺), as well as the H Lyman α line at 1216 Å. On the night side of Titan, only the H Lyman α line was definitively detected. Most of the nitrogen emissions are caused by electron impact excitation. Modeling of the emissions required that the rate of electron energy deposition is roughly 0.05 ergs cm⁻² s⁻¹. This rate is ten times that from solar EUV absorption and emphasizes that photoelectrons cannot provide the necessary energy directly. Using the limb drift observations, constraints were placed on the altitudes at which this energy deposition occurs. Finally, upper limits were placed on the mixing ratios of Ne, Ar, CO, H₂, and H based on the presence or lack of emissions due to these species.

The solar occultation data also provide direct evidence that N₂ is the dominant gas in Titan's atmosphere, but the similarity of the photoabsorption cross section data for N₂ to those for other gases (e.g., Ar or H₂) makes it less definitive than the airglow data. The occultation data consist of ratios of spectra taken during and before atmospheric attenuation, from which the line-of-sight optical depth can be determined. Figure 1.3 shows the derived optical depths for several channels of the UVS spectrum digitized from Figure 3 of G. R. Smith et al. (1982), who presented a detailed analysis of the solar occultation data. Note, however, that this figure is misleading because a single wavelength is assigned to each curve. Because of spacecraft limit cycle motions, which lead to a shift in the measured wavelength range, and the finite resolution of the UVS instrument, each curve actually pertains to a wavelength range which changes with altitude. As such, this figure is fairly deceiving, and analyses based upon it at face value will yield somewhat erroneous results.

From the optical depth information, G. R. Smith et al. determined an N₂ density of 2.7 ± 0.2 × 10⁸ cm⁻³ at a radial distance of 3840 km, a CH₄ mixing ratio of 8 ± 3% near 3700 km, and a mixing ratio for C₂H₂ which varied from 1–2% above 3400 km to 0.1–0.3% below 3300 km. From the scale height of the N₂ density profile,
Figure 1.3: Optical depth profiles of G. R. Smith et al. (1982). The line-of-sight optical depth was obtained as $\tau = -\ln \left( \frac{f}{f_0} \right)$. As mentioned in the text, this figure is deceiving because a single wavelength does not apply to any given light curve.
they derived temperatures of 176 ± 20 K and 196 ± 20 K at the evening and morning terminators, respectively. Using a simple photochemical model, they estimated the location of the homopause to be at 925 ± 70 km with an eddy diffusion coefficient of $1.8 \times 10^8$ cm$^2$ s$^{-1}$. In addition, they constructed a simple engineering model for N$_2$ in which the atmosphere was isothermal at 186 K above $r = 3840$ km and 165 K (the required average temperature) between 2750 and 3840 km.

Finally, G. R. Smith et al. noted the presence of two absorbing layers. The first one is at high altitudes and is centered near 3350 km. This layer is responsible for the inflection in the optical depth profile for 1540 Å in Figure 1.3 at that distance and coincides with the variation in the C$_2$H$_2$ mixing ratio. The second layer is at lower altitudes and is located near 2960 km. G. R. Smith et al. did not investigate this layer, but Broadfoot et al. (1981a) noted that it was fairly close to the detached haze layer seen in the Titan images of Smith et al. (1981). The presence of these layers, which are unique to the Titan solar occultations and not observed in any other UVS occultation from the giant planets or Triton, is confirmation of Hunten’s prediction that Titan’s upper atmosphere is likely to be host to some very interesting chemistry (see quote at end of Section 1.1).

1.3 Post-Voyager Investigations

The Voyager encounters provided us with a wealth of information on Titan’s atmosphere and answered many of the questions raised during the pre-Voyager era. At the same time, however, the Voyager results prompted a new genre of questions. Whereas before we had asked “What is the atmosphere like?”, we now asked “Why is it like that?” and “What are the implications?” This is not to say that the Voyager data themselves were fully understood. Much was still unknown about the nature of the aerosols and possible clouds, and several authors investigated these topics at the data, model, and laboratory study levels (Rages and Pollack, 1983; Rages et al., 1983; Podolak et al., 1984; Khare et al., 1984; Thompson and
Sagan, 1984; Borucki et al., 1984). For the most part, however, the work from this time period concentrated on explaining the known structure of the atmosphere and investigating the implications of it.

From the perspective of the atmosphere as a whole, two authors provided excellent summaries. Owen (1982) considered the overall composition of the atmosphere and discussed the implications for its origin. Strobel (1982) examined the photochemistry and escape processes of Titan's atmosphere and their role in its evolution. At the same time, new discoveries added to the overall picture as Lutz et al. (1983) identified CO in the near-IR spectrum and inferred a mixing ratio of $6 \times 10^{-5}$. Muhleman et al. (1984) later measured the vertical profile of CO and found it well-mixed throughout the troposphere and stratosphere.

Of relevance to the lower atmosphere is the simple yet elegant radiative equilibrium model of Samuelson (1983). Using this model, he made several general conclusions about the physical nature of the lower atmospheric temperature and opacity structure. Also concerned with the lower atmosphere is the work of Lunine et al. (1983), who proposed a global ocean at Titan's surface with a composition of 70% C$_2$H$_6$, 25% CH$_4$, and 5% N$_2$. Previous analyses (Eshleman et al., 1983; Flasar, 1983) had ruled out a predominantly CH$_4$ ocean, but Lunine et al. demonstrated that a predominantly C$_2$H$_6$ ocean was acceptable. The existence of such an ocean has a tremendous impact on the atmosphere because it is both a source and a sink for many of the major atmospheric gases. [Note: the existence of a global ocean appears to have been ruled out by the radar observations of Muhleman et al. (1990) although smaller oceans or lakes are still possible.]

Titan's upper atmosphere also received attention. Bertaux and Kockarts (1983) used the UVS results as input parameters in an analytical derivation of the H$_2$ distribution in the upper atmosphere. They considered adjustments to the profile caused by a possible return flow of H$_2$ from the torus and found them to be negligible, consistent with the earlier conclusions of Hunten (1977). Friedson and Yung (1984) examined the temperature structure of the upper atmosphere, which
had been considered by G. R. Smith et al. (1982) as approximately isothermal from the stratosphere on up. Although previous authors (cf. Hunten, 1978) had commented that the atmosphere is unlikely to be isothermal in this region, the Friedson and Yung work was the first quantitative attempt to model the mesospheric region. They found that a mesopause should form owing to a balance of solar EUV absorption in the thermosphere and IR cooling, primarily by C$_2$H$_2$, at lower altitudes. They calculated the mesopause temperature as roughly 110 K at 736 km altitude.

By far, however, the most impressive work of the time was the photochemical model of Yung et al. (1984). Using the Voyager UVS and IRIS results and ground-based observations of several species as boundary conditions, they modeled the vertical distribution of the major and minor species known to exist in Titan's atmosphere. Although many of the reaction rates had to be estimated, Yung et al. worked at the fundamental levels of chemical kinetics to yield as physically real an atmosphere as possible, and they thoroughly discussed the implications and limitations of their results. This model was later updated by Yung (1987) to account for new chemical schemes in the formation of nitriles.

Figure 1.4 shows several altitude profiles from the Yung et al. model and its subsequent update by Yung. These profiles are digitized from their figures and, when specified as mixing ratio, converted to number density using their total number density profile (digitized from their Figure 2). The displayed N$_2$ profile is just their total number density profile, which they modeled assuming a purely N$_2$ atmosphere. The remaining profiles are from Yung et al.'s Figures 4a (CH$_4$, C$_2$H$_2$, C$_2$H$_4$, C$_2$H$_6$, H$_2$), 4b (H), and 6a (C$_4$H$_2$) and Yung's Figures 2 (N) and 3 (C$_2$N$_2$, HCN, HC$_3$N).

We should note that Yung calculated two sets of density profiles for the nitriles in the update paper because the uncertainties in the rate coefficients are large. We have displayed the profiles calculated using the slower rate coefficients because these yield larger densities for C$_2$N$_2$ relative to C$_4$N$_2$. The reverse is true for the larger rate coefficients. As we will see in Chapter 4, there is no evidence for
Figure 1.4: Altitude profiles of various atmospheric species for the photochemical model of Yung et al. (1984)/Yung (1987). These profiles were adapted from their figures as described in the text.
C₄N₂ but some for C₂N₂ in the solar occultation data. As such, we have used the model profiles that indicate this relationship. The density profiles of Figure 1.4 are used to model the spectra in Figures 4.16 and 4.17 later on.

Although other work was done on Titan's atmosphere during the years following the Voyager encounters, the above represent the most important ones. A thorough summary of the state of our understanding of Titan's atmosphere at the close of the post-Voyager era may be found in Hunten et al. (1984).

1.4 Recent Work: The Last Ten Years

From 1985 to 1987, research on Titan's atmosphere dropped off from the high-activity levels of the post-Voyager years. Starting in 1987, however, preparation for the Cassini mission sparked a tidal wave of interest in Titan's atmosphere.

The number of papers on Titan's atmosphere in the last ten years is quite large, and even a brief summary of the results is difficult. Because the topic of this dissertation is Titan's upper atmosphere and the majority of the work has been concerned with the lower atmosphere, we will only discuss the papers relevant to the upper atmosphere here. Rather than following a time progression, we will group the papers by topic.

Much work has been done on the mesospheric temperature profile. In constructing their Cassini engineering model of Titan's atmosphere, Lellouch and Hunten (1987) adopted the profile of Friedson and Yung (1984). Later, however, Lellouch et al. (1990) reexamined the mesospheric profile and found a problem with the Friedson and Yung evaluation of the solar heating profile. This problem resulted in an underestimation of the solar heating, which in turn led to a mesopause temperature that is too low. To keep the average temperature in the mesosphere at 165 K as required by G. R. Smith et al. (1982), the stratopause temperature had to be elevated to levels inconsistent with analyses of the Voyager IRIS data (e.g.,
Lellouch et al., 1989). Lellouch et al. (1990) recalculated the mesospheric profile and found the mesopause temperature to be roughly 25 K warmer, which brought the stratopause temperature into line with the observations.

The Lellouch et al. (1990) model profile balanced solar heating against IR cooling as Friedson and Yung (1984) had done. Yelle (1991), however, calculated a different mesosphere profile through a rigorous non-LTE treatment of the atmosphere. In addition, he discovered that HCN cooling is important in the calculations. Yelle's profile has a similar mesopause temperature (≈135 K), but the altitude at which the mesopause occurs is roughly 200 km lower than that of Lellouch et al. (1990). An updated engineering model for Titan's atmosphere by Yelle et al. (1994) uses the Yelle (1991) profile in a slightly modified form. Figure 1.5 summarizes the efforts to model the mesospheric temperature profile.

In 1989, Titan occulted the star 28 Sagittarii. This represented a unique opportunity to investigate Titan's atmosphere from 250 to 450 km, an altitude range not probed by the Voyager instruments. As such, a massive international campaign was mounted to observe this occultation at many sites around the world. Data from fifteen separate stations were analyzed in the herculean effort of Hubbard et al. (1993). They concluded that the Yelle (1991) and Lellouch et al. (1990) model temperature profiles bracketed the range of possible temperatures in the lower mesosphere/upper stratosphere and found no evidence for significant latitudinal or diurnal variations in temperature. They also made several inferences about Titan's stratospheric haze, investigated the zonal wind structure, and found Titan's upper atmosphere to be highly axially but not spherically symmetric.

The composition of the atmosphere has also been investigated in recent years. In a series of papers (Coustenis et al., 1989a; Coustenis et al., 1989b; Coustenis et al., 1991; Coustenis and Bézard, 1995), A. Coustenis and co-workers have reanalyzed the Voyager IRIS data and determined better estimates of the abundances of several species. The vertical distribution of CO was measured by Marten et al. (1988), who found CO depleted in the stratosphere relative to the troposphere. This
Figure 1.5: Comparison of the various model mesospheric temperature profiles. The earlier models of Lellouch and Hunten (1987) and Lellouch et al. (1990) were based on the assumption that hydrocarbons, primarily C$_2$H$_2$, were responsible for the cooling. The later models of Yelle (1991) and Yelle et al. (1994) include the effects of cooling due to HCN as well. The Lellouch and Hunten (1987) profile was based on the work of Friedson and Yung (1984), which had an error in the calculated heating rate, forcing the mesopause to a lower temperature.
result conflicted with the earlier measurements of Muhleman et al. (1984); however, Gurwell and Muhleman (1995) also measured the vertical profile of CO and found it to be well-mixed in the troposphere and stratosphere, consistent with the Muhleman et al. results. Thus, there appears to be a controversy over the CO profile. Tanguy et al. (1990) and Hidayat et al. (1997) both measured the vertical profile of HCN. Their measurements showed moderate agreement below 200 km, but they diverged in the stratosphere. Hidayat et al. (1997) attributed this to improvements in the signal-to-noise ratio, and because the two measurements were made more or less by the same researchers, there is no reason to doubt this.

Motivated by the new information on abundances and advances in our understanding of the pertinent reactions, Toublanc et al. (1995) and Lara et al. (1996) proposed new photochemical models of Titan's atmosphere. These models are displayed in Figures 1.6 and 1.7, respectively. The profiles for the Toublanc et al. model were digitized from their Figures 4a (CH₄, C₂H₂, C₂H₄, C₂H₆, H₂), 4b (C₄H₂), 4c (C₂N₂, HCN, HC₃N), and 5a (H) and converted from mixing ratio to number density using the nominal profile of the Lellouch and Hunten (1987) engineering model on which Toublanc et al. based their model. The profiles taken from their Figure 4a are the ones labeled "catalytic scheme 1 off," arbitrarily chosen as "middle of the road" profiles. The profiles for the Lara et al. model were digitized from their Figures 5a (CH₄, C₂H₄, C₂H₆, H₂), 5b (C₂H₂, C₄H₂, H), 8 (HCN), and 9 (C₂N₂) and converted from mixing ratio to number density using the nominal profile of the Yelle et al. (1994) engineering model on which Lara et al. based their model. The profiles for HCN and C₂N₂ are those labeled "K This Work" in the Lara et al. figures.

Interest in a possible ionosphere of Titan has also increased in recent years, starting with the work of Ip (1990). He used the photochemical model of Yung et al. (1984) as a basis for his chemistry, but he apparently neglected diffusive separation of the species in the upper atmosphere and assumed the mixing ratios all achieved constant values. Because his ionosphere essentially starts at the level where he
Figure 1.6: Altitude profiles of various atmospheric species for the photochemical model of Toublanc et al. (1995). These profiles were adapted from their figures as described in the text.
Figure 1.7: Altitude profiles of various atmospheric species for the photochemical model of Lara et al. (1996). These profiles were adapted from their figures as described in the text.
makes this assumption, his results should be viewed skeptically. His work, however, seems to have sparked interest in the Titanian ionosphere, and several other papers soon followed. Gan et al. (1992) investigated the electron distribution in Titan's atmosphere, and their work was used by Keller et al. (1992) in constructing a new model for the ionosphere. Keller et al. also used the photochemical model of Yung et al. (1984) as basis for the chemistry, but they included both the update by Yung (1987) (also neglected by Ip) and the effects of diffusive separation. Roboz and Nagy (1994) examined the energetics of Titan's ionosphere. Shortly thereafter, a more detailed version of their earlier model was provided by Keller et al. (1994) and Keller and Cravens (1994), who discussed the ramside and wakeside ionosphere, respectively. Somewhat in conjunction with the recent ionospheric work, Lammer and Bauer (1991) and Bauer (1992) investigated nonthermal escape processes in Titan's atmosphere.

Finally, a number of authors have reexamined Titan's airglow and upper atmospheric structure. Hall et al. (1992) reanalyzed the Voyager UVS airglow observations and found that the emissions are distributed on both the day and night side with variable spectral content. They presented evidence for $N_2$ emissions on the night side of Titan, whereas Strobel and Shemansky (1982) had found the $N_2$ emissions confined to the dayside. Strobel et al. (1991) determined that many of the airglow features could be explained by solar and photoelectron excitation only, implying that magnetospheric electrons play a minor role in Titan's UV airglow. However, they also determined that photoelectron excitation could only account for 40% of the observed intensity at 970 Å if the feature is mostly $N_2 c'$-band emission, which implies that magnetospheric electrons play a significant role. In their study of electrons in Titan's ionosphere, Gan et al. (1992) reached similar conclusions about the role of electrons in Titan's UV emissions.

Strobel et al. (1992) revisited the Titan airglow question in greater detail. Because the structure of Titan's upper atmosphere is important in understanding the UV emissions, they also reexamined the solar occultation data of G. R. Smith
et al. (1982) and discovered that the G. R. Smith et al. model thermosphere was not consistent with their observed optical depth profiles (shown in Figure 1.3). As such, Strobel et al. attempted to derive a new model for Titan's thermosphere that is consistent with the G. R. Smith et al. optical depth profiles and merges with the physically-based radiative transfer model for Titan's mesosphere of Yelle (1991). They found it impossible to simultaneously fit all of the optical depth profiles and concluded that the profiles, particularly those dominated by CH₄, are not internally consistent. The best matches they could achieve were for CH₄ tropopause mixing ratios of 0.026–0.05 and exospheric temperatures ranging from 172–175 K. Using these atmospheres, however, they were unable to match either the observed emission intensities or the locations of the emission peaks, primarily because the CH₄ density in the upper atmosphere required by the solar occultation data is too large. This led Strobel et al. to conclude that a serious reanalysis of the solar occultation data was needed. Finally, their analysis reached one other firm conclusion: the magnetospheric power dissipation in Titan's atmosphere is at most 10% of the input solar EUV power. They reached this conclusion on the basis of the shape, rather than the absolute intensity, of the limb profile for the brightest N₂ emissions.

Two final notes on Titan's atmosphere come from the work of Strobel et al. (1993) and Courtin et al. (1995). Strobel et al. investigated the Ar mixing ratio in Titan's atmosphere using the revised UVS spectra of Hall et al. (1992), the limits on the tropospheric mixing ratio of CH₄ from Strobel et al. (1992), and the mean mass constraint of Lellouch et al. (1989). They placed a somewhat conservative upper limit on the Ar mixing ratio of 0.1 because of the problems with the UVS solar occultation analysis of G. R. Smith et al. (1982). Courtin et al. reanalyzed the Voyager IRIS spectra using recent developments in our understanding of collision-induced absorptions involving N₂, CH₄, H₂, and Ar and reached several conclusions. First, they determined the H₂ mole fraction in the lower atmosphere to be 1.0 ± 0.4 \times 10^{-3}. Second, they set an upper limit on the Ar mole fraction of 0.06, the lowest upper limit to date. Third, they concluded that CH₄ supersaturation is likely to occur between 15 and 30 km from which they determined a CH₄ mole fraction
at the cold trap of 0.017–0.045. Fourth, they found the mean molecular mass above the cold trap to be 27.7–28.0. Finally, they reached a few conclusions about the hazes and possible clouds in the lower atmosphere.

1.5 Motivation for the Current Research

As the previous sections have demonstrated, Titan's atmosphere is quite fascinating and has been the subject of numerous scientific investigations. Much has been learned in the years since its discovery, but questions still remain regarding such fundamental properties as composition and temperature as well as the "big picture" topics of origin and evolution.

In the search for answers to these questions, many researchers have revisited the Voyager data. Reanalyses of the IRIS spectra and radio-occultation data have yielded a much better understanding of Titan's lower atmosphere. Photochemical models have utilized these new results on the lower atmospheric composition in conjunction with radiative transfer models of the thermal structure to provide much of the information we have on the extensive middle atmosphere region. At the higher altitudes, detailed reexaminations of the UVS airglow observations have placed certain aspects of the upper atmosphere on firmer ground. At the same time, however, these investigations have revealed inconsistencies in the other UVS observations, the solar occultations, which has prompted a call for a reanalysis of these data.

The importance of the UVS solar occultation data cannot be underestimated. The discrete density and temperature results from the original analysis of G. R. Smith et al. (1982) provide the upper boundary conditions for photochemical and radiative transfer models of Titan's atmosphere, which are in turn the bases for models of ionospheric chemistry, atmospheric escape processes, and UV emissions. While some information can be inferred from the airglow observations, it is usually model-dependent, and the solar occultation data provide the only direct
measurements we have of Titan's upper atmospheric structure and composition. Ground-based observations cannot probe this region of the atmosphere, and the UV emissions are generally too weak to be observed from Earth, even with the Hubble Space Telescope.

Given the wide-ranging applications of the G. R. Smith et al. (1982) results and the conclusion of Strobel et al. (1992) that these results are inconsistent, a detailed reanalysis of the UVS solar occultation data is clearly necessary. Although such an undertaking would be ostensibly to resolve the problems in the original work, analyses of the recent occultations at Neptune and Triton (cf. Yelle et al., 1993; Krasnopolsky et al., 1993) have demonstrated that vertical profiles of density rather than a few values at discrete altitudes can be retrieved from the UVS occultation data. The utility of such profiles would greatly enhance our ability to model the middle and upper regions of Titan's atmosphere, providing more detailed constraints than have been available previously. At the same time, the remarkably successful Galileo prediction paper of Yelle et al. (1996) has shown that reanalysis of UVS occultation data can result in somewhat different conclusions. In light of these more recent results, there is even stronger motivation for a reanalysis of the Titan solar occultations.

As we shall see in the following chapters, this task has not been an easy one. We have had to overcome instrumental and data problems through the development of a detailed detector model and new processing procedures. To handle the retrieval of density profiles for Titan's unique upper atmosphere, we have had to develop a new method which accounts for the finite size of the sun and is robust enough for the simultaneous retrieval of several atmospheric species. At the same time, we have searched the literature for the most up-to-date photoabsorption cross sections so that the retrievals will be as meaningful as possible. Despite these difficulties, our effort has been largely successful and has culminated in a view of Titan's upper atmosphere that is both more detailed and internally consistent than previous work.
CHAPTER 2

PROCESSING THE TITAN SOLAR OCCULTATION DATA

2.1 Introduction

The entire basis of absorptive occultations lies in the simple expression generally known as the Beer-Lambert law:

\[ I(\lambda) = I_o(\lambda) e^{-\tau(\lambda)} \]  \hspace{1cm} (2.1)

In this expression, \( I(\lambda) \) is the intensity of light after attenuation by some amount of absorbing material (in our case, the atmosphere of Titan), \( I_o(\lambda) \) is the unattenuated intensity, and \( \tau(\lambda) \) is the line-of-sight optical depth of the absorbing material. This expression is for monochromatic light, and all three quantities are specified at the wavelength \( \lambda \).

The optical depth \( \tau \) is an important atmospheric parameter. We shall return to this in more detail in Chapter 3. For now, we simply state that knowledge of \( \tau \) theoretically allows one to determine the composition of an atmosphere. Thus, if we measure both the intensity of light as it is attenuated by an atmosphere and the intensity of unattenuated light of the same wavelength, we can construct a ratio of the two that yields the value of \( \tau \) at that wavelength:

\[ \tau(\lambda) = -\ln \left( \frac{I(\lambda)}{I_o(\lambda)} \right) \]  \hspace{1cm} (2.2)

If we make a number of measurements of \( I(\lambda) \) at various points in the
Figure 2.1: Illustration of the basic principles of absorptive occultations. As the line of sight to the source descends through the atmosphere, the light is attenuated. Measurements of the attenuated light may be ratioed to measurements of the unattenuated light to generate a light curve as shown on the right. The goal in an absorptive occultation is to retrieve information about the absorbing species in the atmosphere from the characteristics of the measured light curves.

atmosphere, we can construct a series of ratios known as a "light curve." The basic principles of this are illustrated in Figure 2.1. We usually express a light curve as a function of $r_{\text{ pca}}$, which is the radial distance to the closest point along the line of sight as shown in Figure 2.1. This quantity is often referred to as the "tangent point" or the "impact parameter;" however, we prefer to use the term "point of closest approach" for reasons we outline in Section 2.5. Rephrasing equation 2.1 in terms of $r_{\text{ pca}}$ yields

$$\frac{I(\lambda, r_{\text{ pca}})}{I_0(\lambda, \infty)} = e^{-r(\lambda, r_{\text{ pca}})} ,$$

(2.3)

where the radial distance of $I_0$ is set at $\infty$ merely to emphasize that the measurement occurs well outside of the atmosphere. As illustrated in Figure 2.1, a given light curve will begin at one, where no light is attenuated, and decrease to zero, where attenuation is complete. If the atmosphere is not dense enough, the light curve may be cut off before reaching zero as the line of sight intersects the solid surface.
The measurement of such light curves is usually referred to as an "occultation" because the body with the atmosphere ends up between the source and the instrument making the measurements. This can happen in one of four ways: 1) the source and instrument are fixed but the body moves; 2) the body and instrument are fixed but the source moves; 3) the body and source are fixed but the instrument moves; or 4) all three move in such a way that the body ends up between the source and the instrument. Depending on one's point of view, either the source or the instrument is occulted by the body. For us, an occultation occurs because a spacecraft (Voyager) moves rapidly behind a body (Titan) while an instrument it carries (the Ultraviolet Spectrometer, or UVS) is pointed at a source (the sun). Thus, Titan occults the sun.

In general, one will obtain two occultations because the body cannot remain between the source and instrument indefinitely. As the body moves out from between the two, the line of sight is reestablished and a second series of light curves is obtained, although this second series goes from zero to one as the light becomes less and less attenuated. In the nomenclature of spacecraft occultations, the first occultation is referred to as the "entrance" or "ingress" occultation, and the second is referred to as the "exit" or "egress" occultation.

Although light curves can be measured at a single wavelength, it is better to make the observations at several wavelengths. The primary reason for this is that different atmospheric species have different absorption characteristics at different wavelengths (see Figure 3.1). Thus, measurements at several wavelengths can theoretically allow us to discriminate between various species. We will return to this later (see Chapter 3), but the utility in a measuring a spectrum versus a single wavelength is tremendous.

The Voyager UVS was designed to optimize the information retrieved from ultraviolet absorptive occultations by recording a continuous spectrum over a diagnostic wavelength range at regularly spaced intervals in the atmosphere. On November 12, 1980, the Voyager 1 spacecraft performed a fly-by of Titan, during
which the UVS observed both an ingress and egress occultation of the sun by Titan’s atmosphere. The trajectory of Voyager 1 as it passed behind Titan relative to the sun is shown in Figure 2.2. This figure also shows the location of the solar terminator on Titan and the locations of the ingress and egress occultations. As is always the case with the sun, the occultations took place at the terminator, with the ingress occultation taking place at the evening, or dusk, terminator, and the egress occurring at the morning, or dawn, terminator.

In the next few sections, we will go through the stages of processing which we performed on these occultation data to turn the raw spectra into meaningful light curves. At this point, the reader is advised to read Appendix A, which contains a brief description of the design and operation of the Voyager UVS as well as a few notes on some terminology which will be used throughout this dissertation.

2.2 The “Raw” Data

Any UVS occultation analysis begins with an examination of the “raw” (i.e., unprocessed) spectra returned from the spacecraft. This examination ensures that we understand the state of the data before we begin the processing. Figure 2.3 shows two examples typical of raw UVS spectra, one taken in the HVL 2 gain state and the other in the HVL 3 gain state (see Appendices A and B for more on the gains). There are several features in these spectra that we must keep in mind when processing the data from the raw state through the final step in which we ratio attenuated to unattenuated spectra to obtain our light curves.

The first is the relative scarcity of detector counts in portions of the HVL 2 spectrum. Short of channel 80, this is caused by a combination of the lowered gain in the HVL 2 state with a decrease in the solar intensity at these wavelengths. Longward of channel 80, the detector sensitivity decreases and the recorded signal is subsequently much lower than in the rest of the spectrum.
Figure 2.2: Illustration of the Voyager 1 trajectory during the Titan fly-by. The top view shows the geometry in the plane of the trajectory. The bottom view shows the trajectory as seen from the sun and the ranges over which atmospheric absorption was measured by the UVS. The ingress occultation occurred on the evening (dusk) terminator, and the egress occultation occurred on the morning (dawn) terminator. The geometry of the ingress occultation is more favorable because the spacecraft was closer to Titan during the occultation. The indicated latitudes, longitudes, and ranges refer to the mid-point of the relevant occultation.
Figure 2.3: “Raw” HVL 2 and HVL 3 spectra obtained at the same ΔW value. The lower gains of the HVL 2 state are clearly evident in the reduced level of the HVL 2 spectrum. The bottom panel shows the lowest levels of the HVL 2 spectrum, illustrating the relative paucity of counts in the long wavelength channels. The “comb” structure evident in both spectra is caused by the “even channel problem” (see Section B.7). The HVL 3 spectrum was obtained after the onset of atmospheric absorption, explaining the lowered level relative to the HVL 2 spectrum in channels 1–30. Other channels are also attenuated but this is not as obvious in the “raw” state.
The higher gain of the HVL 3 state eliminates these problems; however, the HVL 3 gain state could not be used throughout the occultation because the brighter portions of the spectrum, especially the H Lyman α line, would have been saturated owing to the high intensity of the solar spectrum. All the HVL 3 spectra from the Titan occultations were obtained during the periods of attenuation so that the incoming solar spectrum would be reduced in intensity. This is the reason for the reduced levels of the short wavelength channels in the HVL 3 spectrum in Figure 2.3. Even so, the H Lyman α line is still saturated and must be treated carefully in the processing that follows.

Another feature of these spectra is something we will refer to as the "even channel problem." The even-numbered anodes of the UVS do not perform correctly when the amount of charge falling on the detector array is large. This problem gets worse as the amount of charge increases, as can be seen in a comparison of the HVL 2 and HVL 3 spectra. The low gain of the HVL 2 state somewhat offsets the high intensity of the solar spectrum, and the problem is less severe. With the higher gain of the HVL 3 state, the problem is quite pronounced.

The spectra of Figure 2.3 were taken from two points in the ingress occultation. To get a different perspective on the occultations, Figure 2.4 shows the recorded signal in three channels of the spectrum as a function of "time" during the ingress and egress occultations. Because these are raw spectra and we have not taken a ratio yet, we refer to these as "light curves" in quotes. Channel 7 is shown because it is illustrative of the shortest wavelength channels in which the absorption is due to the N₂ continuum. To give an example of absorption in the N₂ band region, in which CH₄ also plays a role, we plot channel 35. Finally, we show channel 111 as an example of a long wavelength channel in which the absorption is due to a variety of hydrocarbons and carbon-nitrogen species. These three channels are representative of the signal in other channels and illustrate several more features of UVS data that we must keep in mind when processing the spectra.

The most distinctive feature in Figure 2.4 is the sudden jump in the signal.
Figure 2.4: "Raw light curves" for three representative channels of the UVS spectra are shown in the first three panels. The fourth panel is a plot of the corresponding $\Delta W$ values. The data are plotted versus time, but a number of time gaps have been suppressed in the plots; hence, the x-axis label is "time" in quotes. The large change in signal for the three channels marks the change in gain. The dashed line separates the reference spectra region (to the left) from the attenuation region in the ingress occultation. No line is shown for the egress occultation because all the spectra are considered to be attenuated spectra (see text). The dashed line occurs at a slight discontinuity in the plots, which marks the time at which the picture was taken.
This is caused by a programmed change in the gain of the UVS from the low-gain HVL 2 state to the high-gain HVL 3 state. The reason for this change is that it allows the occultation to proceed to a greater depth in the atmosphere by increasing the recorded signal. This gain change occurred in both the ingress and egress occultations, but it could only occur after the solar spectrum had been somewhat attenuated as noted above. Given that each occultation took between 2–3 minutes, credit must be given to the Voyager sequence planning team for the timing of such a change.

We should note that a time gap occurs at the gain change because several spectra have been eliminated. These spectra were those taken during the gain change, which does not happen instantaneously. Such spectra are hybrids of both HVL 2 and HVL 3 and cannot be processed correctly. Their elimination leaves a gap in the “light curves” at this juncture, but the gap is small enough to be insignificant in the analysis.

A second feature in the raw data of Figure 2.4 is the variation in the level of the recorded signal with time. This is caused by a combination of spacecraft limit cycle motions and the mechanical collimator of the Voyager UVS.

Limit cycle motion is caused by the constant adjustment of the Voyager spacecraft’s attitude (i.e., roll, pitch, and yaw) via the firing of small hydrazine jets located at various points on the spacecraft. These adjustments are necessary to keep the spacecraft fixed in a stable position such that observations can be performed. Unfortunately, although these jets keep the spacecraft in an overall “fixed” attitude, they generate small motions of the spacecraft and, therefore, the instruments mounted upon it. Consequently, although the UVS can be pointed at a source, the limit cycle motion causes the source to move around in the UVS slit. As discussed in Section A.1, this causes the spectrum to shift on the detector. Thus, the wavelength range recorded in any given channel of the UVS is different from spectrum to spectrum. If a line feature in the spectrum of the incoming radiation shifts from one channel to another because of limit cycle motion, the change in the
recorded signal can vary quite dramatically.

Coupled with this shifting spectrum is an attenuation of the intensity of the incoming light owing to the slit function of the UVS (see Section A.1). As the source moves around because of limit cycle motion, it moves toward and away from the center of the slit and the fraction of the incoming radiation that passes through the mechanical collimator of the UVS changes. Thus, not only are features in the spectrum of the incoming radiation moving on the detector, their intensity varies depending on the position of the source in the slit.

Without knowledge of the limit cycle motion of the spacecraft, we would be in trouble. Because of the manner in which the spectrum shifts on the detector, it is critical that we divide a particular attenuated spectrum by an unattenuated spectrum at the same position in the slit when we generate the ratios of the final light curves. Failure to do so will result in spurious features in the light curves as we divide absorption at wavelength X by the unattenuated signal at wavelength Y. Proper ratioing of the spectra relies on using unattenuated reference spectra taken at the same positions in the slit as the attenuated spectra.

The limit cycle motion of the spacecraft is specified as relative changes in the roll, pitch, and yaw angles. We must use relative changes because the spacecraft switched to its own internal gyros during the occultations, effectively negating the ability to pinpoint absolute positions. For our purposes, we convert these angles into a relative change in the position of the UVS slit. This position change is specified by two quantities, $\Delta W$ and $\Delta L$, which refer to the change in position along the width and length directions of the slit, respectively.

Luckily for us, we only need to know the relative position of one spectrum to another. As long as the gyros of the spacecraft are operating, the reference frame of the relative measurements does not change. Thus, a spectrum taken at a particular value of $\Delta W$ and $\Delta L$ is at the same relative position in the slit as another spectrum with the same values of $\Delta W$ and $\Delta L$. We should note that this is not exactly true
because the gyros drift, meaning that the reference frame they established when turned on slowly rotates. However, typical gyro drift magnitudes are too small to affect us over the short durations of the occultations and we neglect them here.

Figure 2.4 also shows the value of \( \Delta W \) corresponding to the raw "light curves." We do not show the value of \( \Delta L \) because it turns out that we do not need it. Ideally, we would want a reference spectrum obtained at the \( \Delta W \) and \( \Delta L \) of each attenuated spectrum. In reality, this is not possible because we have no control over what regions of the slit are covered by the limit cycle motion. Indeed, we can only hope that the reference spectra obtained before and after the occultations cover the same regions of the slit as the attenuated spectra! Through the particular design of the UVS, however, both the shift of the spectrum on the detector and the slit function are tied to the width direction of the slit. Thus, knowledge of \( \Delta W \) is the important quantity. This reduces the number of reference spectra which we need from a large two-dimensional grid to a much smaller one-dimensional array. We still have to rely on luck for the reference spectra to cover the same range of \( \Delta W \) as the attenuated spectra, but our chances of this are much better than if we had to cover the entire \( \Delta W \) and \( \Delta L \) range. We should note that variations in the sensitivity of the detector along the length of the slit have been measured; however, they are small enough that we can neglect them with reasonable confidence.

The \( \Delta W \) values plotted in Figure 2.4 are not the \( \Delta W \) as recorded by the spacecraft. Instead, they are the \( \Delta W \) values after they have been converted to an absolute reference frame with zero located at the slit center. Although we stated above that we could not put the gyro information into an absolute frame, we can use a trick to put the UVS slit position information into an absolute frame.

If the sun ever moves through the center of the slit, the intensity of the recorded signal will peak and then decrease. At the same time, the spectrum will be recorded at the nominal, on-axis location. If we look for a peak in the total intensity summed over all channels of the spectrum and find such a peak, we know that the sun is in the center of the slit. We can check this by confirming that the
H Lyman $\alpha$ line is centered on the proper channels for an on-axis spectrum.

During the reference spectra period before the ingress occultation, such a "peak passage" occurred, allowing us to pinpoint the $\Delta W$ value which corresponds to the slit center. This peak is not actually shown in Figure 2.4 because the data set used to make the plots has been pruned down to include only the unattenuated reference spectra that cover the range of $\Delta W$ corresponding to the attenuated spectra and the attenuated spectra themselves. Several hundred more spectra were recorded during the reference spectra period, but because they were never used, we have eliminated them from the figure. This is the reason the x-axis of the plots is labelled "time" without any tick marks; although they cannot be seen because of limit cycle (and therefore signal) continuity, there are several gaps in time in the plotted curves.

Placing the $\Delta W$ values into such an absolute frame is not necessary for the ingress occultation. We had adequate coverage of the attenuated spectra $\Delta W$ range during the reference spectra period, so we could have used the relative values as they were recorded by the spacecraft without any trouble. The reason for doing this lies in the egress occultation. As with the ingress occultation, there was a period of time during which reference spectra were obtained. In the case of the egress occultation, they came after the attenuated spectra. As hoped, there was adequate coverage of the attenuated spectra $\Delta W$ range during this period. Unfortunately, they were rendered useless by an unusual occurrence. Shortly after the reference spectra period began, the recorded spectra changed dramatically even though the limit cycle motion was steady. After this, the spectrum intensity seemed to vary in a manner uncorrelated with the limit cycle motion. This lasted for the remainder of the reference spectra period.

The best explanation for this is that something caused the spacecraft to move without changing the relative motion information from the gyros. This might occur if something, say a small meteoroid, hits the spacecraft. Such a collision could potentially cause the spacecraft to oscillate a bit, much like a ringing bell. Although
this is purely speculation, such motion uncorrelated with the limit cycle has been observed in other UVS observations (W. T. Forrester, personal communication, 1995). Whatever the cause, the egress reference spectra were unusable.

Without any reference spectra, the egress occultation would have been lost; however, we can use ingress reference spectra if we can match up the limit cycle. Because the scan platform had to be repositioned for the egress occultation, the gyro reference frame was changed and the limit cycle with it. However, we can employ another trick to save the day.

Using one of the few good egress reference spectra, we cross-correlate it with all the ingress reference spectra to determine if we have a match. As chance would have it, we do. This allowed us to establish a link between the two limit cycle reference frames. Further investigation revealed that the entire ΔW range of the egress attenuation region was covered during the ingress reference spectra period. Thus, we were able to use ingress reference spectra to process the egress occultation. Although we could have used the ingress limit cycle frame and not an absolute one, converting both the ingress and egress to a common absolute frame is no more difficult than converting the egress frame to that of the ingress given that we have the "peak passage" discussed above. [Note: When we model spectra as in Chapter 3, we will need to know the spectral shift on the detector (i.e., the absolute position of the sun in the slit), so we would have to do a trick similar to this anyway.]

As a final note on the raw data, we point out the small step in the curves of Figure 2.4 that coincides with the dashed line separating the reference spectra region from the attenuated spectra region. This step is a series of twelve spectra obtained in the GS-3 mode, which has an integration time of 3.84 seconds. Normally, solar occultation spectra are obtained in OC-1 mode, which has an integration time of 0.32 seconds. This is because the longer integration time of the GS-3 mode, while better from a signal-to-noise standpoint, would sample the atmosphere at too large a spacing to be useful and, more problematic, could result in overflow of the
Overflow occurs because the Voyager spacecraft only has a 16-bit processor, limiting the number of detector counts to 65,535. If this number is exceeded, the counter rolls over to zero and continues from there. Taking the H Lyman α line as a typical example, it saturates at roughly 7000 counts (the maximum the UVS can record in a single OC-1 spectrum). If this is multiplied by twelve, which is the ratio of the GS-3 to OC-1 integration times, the H Lyman α line would reach 84,000, but overflow would cause this to be recorded as 18,465. Portions of the spectrum which did not overflow would most likely be at a higher level than the H Lyman α line, making the spectrum somewhat odd in appearance. Although it might be possible to correct for overflow, the situation would be far from ideal.

Given this, one might reasonably ask “Why were any GS-3 spectra obtained?” The answer is that someone wanted to take a picture just prior to the solar occultation, which always occurs during the closest encounter between the spacecraft and the body. The integration mode is tied to the spacecraft and not a particular instrument. The Voyager imaging system requires GS-3 mode to take an image; therefore, the mode had to change to GS-3 for this to occur. Although the mode switched back to OC-1 immediately, the solar spectrum had already begun to be attenuated by Titan’s atmosphere. The twelve GS-3 spectra covered a radial descent of the line of sight of roughly 550 km. If the mode change had occurred even a short time later, the ingress occultation would have been an almost total loss. It is tempting to say that the sequence team did another fine job of timing, but we tend to believe that they just got lucky.

2.3 Processing the Spectra

With the various features of the raw data understood, we next process the spectra from their raw state in detector counts to their final state in descattered photoevents. This is a two-stage process consisting of linearization and descattering. At this
point, the reader is advised to at least peruse Appendices B and C, which contain more detailed descriptions of these processes than will be given here.

2.3.1 Linearizing the Spectra

Linearization is the process of converting detector counts, which are highly nonlinear in the case of solar spectra, into photoevents. This is necessary because it removes many instrumental effects from the spectra. These include charge spreading, current limiting, the even channel problem, gain differences, and saturation effects. In addition, the resulting spectra are completely linear in nature, which is critical if the ratios of the final light curves are to have any physical meaning.

Charge spreading effects are caused by the spreading of the electron cloud as it moves from the microchannel plates to the detector anodes. This effect means that a photon striking the microchannel plates at anode X will be recorded on a number of anodes centered on X. The larger the charge, the greater the spread. We must remove these effects from the spectra because they represent a blending of wavelengths in the recorded spectra.

Current limiting occurs because charge is removed from the microchannel plates faster than it can be replenished when the intensity of the incoming radiation is high. This effectively lowers the gain, which must be taken into account or the inferred photoevent rate will be lower than it actually is.

The even channel problem was noted in the previous section. We must correct the spectra for this feature or the signal on the even channels is useless, effectively reducing our spectral resolution by a factor of two.

Gain differences represent the fact that spectra recorded in the HVL 2 gain state are different from spectra recorded in the HVL 3 gain state, even though the originating source spectrum is the same in each case. This is the most critical of the effects mentioned because the continuity of the final light curves at the gain
change seen in Figure 2.4 depends on how accurately we can correct for the different gains. In addition, because we do not have any HVL 3 reference spectra, we must use HVL 2 spectra as the reference spectra for the HVL 3 spectra. If the gain differences are not handled properly, this could introduce spurious features in the final light curves.

The linearization stage was performed using the procedure outlined in Appendix C, particularly Section C.2.1, in combination with the Monte Carlo model of the UVS detector described in Appendix B. The detector model, which was deemed necessary if a reanalysis of the Titan solar occultations was to be worthwhile, represents a substantial amount of work in this dissertation. The linearization scheme using this model is a significant improvement over previous methods, and it is the first to make use of an empirical correction to the even channel problem. In the past, the problem was treated by simply averaging the adjacent odd channels; however, this method suffered in the presence of spectral lines because lines centered in even channels were truncated.

Because the linearization scheme makes use of a Monte Carlo detector model, processing the same spectrum two different times will yield two slightly different spectra. These differences are representative of the fact that several different incident spectra can result in the same measured spectrum owing to the randomness of the charges associated with individual photons, the effects of the detector thresholds, and the nuances of current limiting and the even channel problem. This works to our advantage, however, because we can run the linearization scheme a number of times and average the results to produce a mean spectrum with associated uncertainties. This is another improvement over previous methods, in which the uncertainties were derived from statistical theory rather than the data themselves. From tests on individual spectra, we determined that twenty iterations of the linearization scheme was sufficient to yield reasonably accurate estimates of the mean spectrum and corresponding uncertainties.
Figure 2.5 shows the two spectra of Figure 2.3 after they have been linearized and corrected for some remaining problems (discussed below). As can be seen, the gain differences and even channel problems have been effectively removed. The spectra, particularly the HVL 3 spectrum, no longer have the "squashed" nature caused by the nonlinearities of the detector. This is best seen in a comparison of the H Lyman $\alpha$ line between the raw and processed spectra.

Figure 2.6 shows the "light curves" of Figure 2.4 after the linearization stage and correction of the remaining problems. The effects of the limit cycle motion and the slit function are still present because they are not removed until we ratio the attenuated and unattenuated spectra. The enormous differences between the HVL 2 and HVL 3 spectra, however, are substantially reduced (though they were not entirely removed during the linearization process and a correction was needed; see below).

Although the linearization scheme represents an improvement in our ability to process Voyager UVS solar spectra, the method is not perfect and a few problems remain. We briefly discuss these here and the corrections we have employed to fix them.

**Problem #1: Remaining HVL 2/HVL 3 Discontinuities**

Despite the advances in the linearization scheme and the detailed nature of the detector model, not all of the HVL 2/HVL 3 gain differences were removed during the linearization procedure. Several explanations for this are possible, but it most likely results from poor statistics in the HVL 2 spectra. The remaining discontinuities are largest in the channels in which the HVL 2 signal is low, particularly the long wavelength channels where we are lucky to have even ten detector counts for a source as bright as the sun.

To remove the remaining discontinuities, we scaled the HVL 3 spectra to a level consistent with the HVL 2 spectra. Although the HVL 2 spectra are most
Figure 2.5: Processed versions of the HVL 2 and HVL 3 spectra shown in Figure 2.3. The attenuated nature of the HVL 3 spectrum is now clearly seen. The corrections discussed in the text have been applied to these spectra.
Figure 2.6: The "light curves" of Figure 2.4 after the linearization step and correction of the problems discussed in the text. The error bars show the 1-σ uncertainties in the data. Only every fifth point is shown for clarity.

likely the source of the problem, many of the attenuated spectra and all of the reference spectra are HVL 2 spectra. Thus, for self-consistency, we chose to scale the HVL 3 spectra.

Figure 2.7 shows an example of a scaled "light curve." We performed the scaling by fitting a line to the HVL 2 "light curves" just prior to the gain change and extending the line across the change. The HVL 3 spectra were then scaled such that the slope of the line was preserved across the gain change. In a few instances, the fit to the HVL 2 data was poor because of high noise levels, and the fit was done visually. The uncertainties of the HVL 3 spectra were adjusted following the methods outlined in Bevington and Robinson (1992) for the propagation of uncertainties.
Problem #2: H Lyman $\alpha$ Saturation

Unfortunately, the linearization scheme is not able to infer the proper intensity in a channel that is saturated in the raw spectrum. This is evident in the truncated nature of the peak of the H Lyman $\alpha$ line, which was thoroughly saturated in the raw HVL 3 spectrum. Because we cannot properly descatter a spectrum unless saturation effects are removed, it was necessary to develop a correction for this.

The H Lyman $\alpha$ line is only saturated over a small region of the "light curves" and only in the peak channels of the line. Thus, we were able to use the wings of the line in each attenuated spectrum to scale the H Lyman $\alpha$ line in the corresponding unattenuated reference spectrum to a level representative of what the H Lyman $\alpha$ line should be in the attenuated spectrum. This scaling was performed.
assuming that CH$_4$ was the dominant absorber, and the scaling factor across the line followed that of the CH$_4$ photoabsorption cross section (see Figure D.3) for these wavelengths. To reduce the noise, the reference spectra used were binned and normalized following the procedure of Section 2.4.

The saturated and corrected “light curves” for the peak H Lyman $\alpha$ channel (i.e., the one most saturated) in the ingress occultation are shown in Figure 2.8. As can be seen, the correction is quite good and matches the unsaturated portions of the “light curves” on either end of the saturated region well.

2.3.2 Descattering the Spectra

Once the raw spectra are converted from detector counts to photoevents through the linearization stage and the remaining problems have been addressed, we are able to descatter the spectra. Scattered light exists in the spectra because of imperfections in the grating (see Section A.1), and it represents light of wavelength X falling on the microchannel plates at the position of wavelength Y and subsequently being recorded in the spectrum as though it were of wavelength Y.

This scattered component of the spectrum must be removed before we ratio the attenuated and unattenuated spectra to produce the final light curves. The reason is that variations in the photoabsorption cross sections of the atmospheric species lead to different amounts of absorption at wavelength X and wavelength Y. The interpretation of absorption at wavelength Y will be incorrect if a scattered component from wavelength X is present. The spectra were descattered through the application of a descattering matrix as described in Section C.2.2.

2.4 Generating the Light Curves

With the spectra fully processed, we are now able to ratio attenuated to unattenuated spectra to generate the final light curves which represent the transmission of
Figure 2.8: Illustration of the correction procedure applied to the saturated "light curves" of the H Lyman α line. The dashed lines bracket the region over which the correction was applied. As can be seen in the bottom panel, the correction works well. All three curves are for channel 73 of the ingress occultation.
the atmosphere as a function of wavelength and altitude. There are two steps in this process: 1) binning the reference spectra and 2) ratioing the spectra.

2.4.1 Binning the Reference Spectra

Ideally, we would like to have a reference spectrum at the exact $\Delta W$ of each of the attenuated spectra. In reality, this doesn't happen, and we are forced to use the closest reference spectrum that we have. In addition, we would like to reduce the "noise" of the reference spectra so that the uncertainties in the final light curves are smaller than they would otherwise be. We solve both of these tasks by binning the reference spectra according to their $\Delta W$ values and then normalizing the binned spectra to have an integration time equivalent to that of a single spectrum.

The limit cycle information obtained from the spacecraft is accurate to four decimal places. Because of this, we bin the reference spectra using a step size of 0.001° and bins centered on integer multiples of this step size. For example, the first bin is centered on a $\Delta W$ value of 0.020° and spans the range 0.0195° to 0.0205°. The second bin begins at 0.0205° and continues to 0.0215°. This pattern continues for 90 bins, with the final bin spanning the range 0.1085° to 0.1095°. For reasons described in Section 2.2, all the reference spectra are taken from the ingress occultation reference spectra region and a single set of binned reference spectra is used for both the ingress and egress occultations.

With the bin ranges calculated, we simply determine into which bin a given reference spectrum belongs and add it to that bin. If a reference spectrum has a $\Delta W$ value falling on the border between two bins, the spectrum is arbitrarily placed into the bin with the smaller $\Delta W$ bin center value. We keep track of the number of spectra going into each bin. Once the reference spectra have all been binned, we normalize the binned spectra by dividing by the number of spectra in each bin.
2.4.2 Ratioing the Spectra

With the reference spectra binned and normalized, we generate the final light curves, where the quotes have been removed because these are now true light curves (i.e., transmission profiles). For each spectrum in both the reference and attenuated spectra regions, we determine which $\Delta W$ bin the spectrum corresponds to and divide it by the proper reference spectrum. As with the binning procedure, any spectrum whose $\Delta W$ value falls on the border between two bins is associated with the smaller $\Delta W$ bin.

Figure 2.9 shows the HVL 3 spectrum from Figure 2.5 after it has been divided by its corresponding binned reference spectrum. The line at a transmission

![Graph showing the HVL 3 spectrum ratioed to its binned reference spectrum. The transmission is plotted against channel number, with a line at transmission of 1 to indicate the unattenuated level.](image)

Figure 2.9: The HVL 3 spectrum of Figures 2.3 and 2.5 after ratioing to its binned reference spectrum. The spectrum clearly illustrates the effects of atmospheric absorption. The line at a transmission of one is shown to represent the unattenuated level.
Figure 2.10: Final light curves and their corresponding 1-σ uncertainties. Only every fifth point has been plotted for clarity. The "dip" artifact described in the text lies between 1100 and 1300 km in the channel 111 light curve for both occultations. Of one is shown to make clear the extent of the atmospheric attenuation in this spectrum. Figure 2.10 shows the final light curves for the three channels that we have been following through the processing steps. The curves are now plotted versus altitude, which pertains to the point of closest approach of the line of sight to the surface of Titan for the given data point. The altitudes were determined through the procedure described in Section 2.5 below. Note that the level of the light curves exceeds one for some data points because these curves represent the ratio of two data spectra. The average level along the light curves is generally equal to or less than one, but any given point may be greater than one because of uncertainties in the measured spectra. The uncertainties for these light curves are also shown, and they have been propagated through the steps of descattering, reference spectra binning, and spectra ratioing using the standard methods for propagation of uncertainties as outlined by Bevington and Robinson (1992).
Problem: The "Dip"

A notable feature in the curve for channel 111 in Figure 2.6 is the "dip" that is centered around the gain change. This "dip" is an artifact of the even channel correction and is caused by poor statistics in the even channel correction factor grid (see Section B.7) at low signal levels.

As noted in Section 2.2, the even channel problem gets worse with increasing signal level. Conversely, at low signal levels, it goes away entirely. The method by which the even channel correction factor grid was determined made it difficult to simulate a realistic spectrum at such low signal levels. Thus, the correction factor is less accurate as the even channel problem goes away.

In addition, the even channel correction method applies a single correction factor to the entire spectrum, but it is possible that local effects are present which are difficult to impossible to model accurately. Local effects are especially likely in the long wavelength channels, where the even channels almost all recorded zero counts in the HVL 2 spectra and were quite small in the HVL 3 spectra as well. The "dip" is only present in the long wavelength channels, lending confidence to this interpretation.

The "dip" begins when attenuation sets in at the shortest wavelengths. It bottoms out when attenuation begins at H Lyman $\alpha$. Because H Lyman $\alpha$ dominates the spectrum, the even channel problem begins to go away as it is attenuated. The "dip" turns up from this point on until it ends when the even channel problem disappears owing to a large enough decrease in the intensity of the incoming radiation. At that point, the even channel correction turns itself off and the light curves represent the true level of the signal again.

There is little we can do about the "dip." Because we fit the final light curves with smooth profiles before we perform the atmospheric inversion (see Section 4.1), we can effectively ignore them by fitting across the "dip" using the good
data on either side. This is not optimal, but it represents the best we can do under the circumstances.

2.5 The Geometry of the Titan Occultations

In order to tie the final light curves we have just determined to the atmosphere of Titan, we need to know the altitude of the point of closest approach between the line of sight and the surface of Titan for each of our spectra. The final light curves in Figure 2.10 already illustrate this relationship.

To calculate the altitudes, we need two vectors: the spacecraft state vector (i.e., the vector between the spacecraft and the center of Titan) and the spacecraft-sun line-of-sight vector. We will refer to the spacecraft state vector as $\vec{S}$ and to the spacecraft-sun line-of-sight vector as $\vec{L}$. These vectors are illustrated in Figure 2.11. To determine these vectors, we use the NAIF (Navigation and Ancillary Information Facility) SPICE (Spacecraft Planet Instrument “C-Matrix” Events) library routines obtained from NASA’s Jet Propulsion Laboratory. For each spectrum, the vectors are determined using the ephemeris time of the observation, which is calculated from the spacecraft event time (SCET) of the spectrum. All times and vectors are referenced to the J2000 inertial reference frame that is used by the SPICE routines. This procedure is relatively straightforward, but we need to digress a moment to understand what the two vectors actually represent.

What we want for $\vec{L}$ is the “true” line-of-sight vector between the spacecraft and the sun. This is the physical direction along which light travels from the sun to the spacecraft. It differs from the “geometrical” position of the sun (i.e., the actual position of the sun relative to the spacecraft at the ephemeris time) by the light-time correction introduced because the sun moves while the light is in transit to the spacecraft. The “true” position is simply the “geometrical” position at the ephemeris time minus the light-travel time. We do not want the “apparent” position of the sun, which would be the vector corrected for the fact that the spacecraft is
Figure 2.11: Illustration of the various vectors involved in the geometry calculations which yield the altitude of the point of closest approach between the line of sight and the surface of Titan.
moving (an aberration effect), because that is only a description of where on the celestial sphere to look for the light. We want the actual vector from the spacecraft to the sun that the light travels along, and this is the “true” position vector.

What we then want for $\vec{S}$ is the vector from the spacecraft position at the ephemeris time to Titan at the ephemeris time minus the light-travel time between the spacecraft and the point along the $\vec{L}$ direction that marks the point of closest approach of the line of sight to the surface of Titan. We are trying to establish the relationship between the line of sight and Titan in these calculations, so we must use the position of Titan when the light is actually passing by it along the “true” $\vec{L}$. This is why we must “back up” Titan from the ephemeris time of a given spectrum.

This is what we want for $\vec{S}$ and $\vec{L}$. The problem is that we have to iterate to get the position of Titan when the light passes by it along $\vec{L}$ because we do not know where along the line of sight the point of closest approach is and therefore do not know the light-travel time to use to “back up” Titan. We can either spend a lot of time iterating to an approximate solution or make a reasonable approximation and go with that, but both of these lead to uncertainties in the relationship between $\vec{S}$ and $\vec{L}$.

An alternative method is that described by Nicholson et al. (1990), who used observations of Saturn’s rings by the radioscience (RSS) and photopolarimeter (PPS) experiments to revise the position of Saturn’s pole and the absolute radius scale for the ring system. Rather than working from the spacecraft point-of-view, we should work with vectors relative to the center of Titan. The line-of-sight vector $\vec{L}$ should be the vector which establishes the “apparent” position of the sun relative to Titan. The “apparent” position is the position of the sun taking into account aberration effects (because Titan is moving) and light-time effects (because the sun is moving). By referencing $\vec{L}$ to the center of Titan and taking the motion of Titan into account, we put $\vec{L}$ into a reference frame that comoves with Titan. Then, by moving $\vec{L}$ out to the spacecraft position, the motion of Titan relative to the line of sight is inherently a part of $\vec{L}$, and we do not have to make any light-travel-time
correction for the distance between the spacecraft and the point of closest approach as we would in the other method. The shift of origin between the center of Titan and the spacecraft shifts \( \vec{L} \) such that the motion of Titan is accounted for. Thus, the vector \( \vec{S} \) that we need is now just the spacecraft position vector relative to Titan at the ephemeris time. This method is more straightforward and more accurate than the one which we previously described because it eliminates the need to perform any iteration or approximations.

Of course, this method has its own drawbacks. There is an implicit assumption that the sun, Titan, and spacecraft are approximately colinear (i.e., the sun-spacecraft-Titan angle is small). This is generally true, but the farther the spacecraft is away from Titan, the more accurate the method is. In the end, however, the uncertainties that arise in this method of determining the vectors are smaller than in the iterative method, making this the preferred one. It is also worth noting that the uncertainties we get from this method are more than likely swamped by uncertainties caused by other effects (e.g., small compared to the projected disk of the sun) or insignificant (i.e., an error of a kilometer or so over a radial distance of thousands of kilometers).

Thus, we obtain the vectors \( \vec{L} \) and \( \vec{S} \) as follows. First, we establish the ephemeris time of the observation by converting the SCET to its corresponding Julian date and using the SPICE routine \texttt{utc2et} to convert the Julian date to ephemeris time. Then, we use the SPICE routine \texttt{spkez} to get the position of Voyager relative to Titan in a Titan-centered reference frame at the ephemeris time. Finally, we use the routine \texttt{spkez} again to get the position of the sun relative to Titan in a Titan-centered reference frame at the given ephemeris time but with the appropriate light-time and aberration effects taken into account.

This procedure yields the vectors \( \vec{L} \) and \( \vec{S} \) that we need to calculate the altitude. We want to calculate other geometry information (e.g., latitude and longitude) as well, so we use the SPICE routines once more to rotate these vectors into a pole/prime meridian reference frame for Titan. This rotation establishes the \( z \)-axis
as the rotation axis and the positive x-axis as marking the point of 0° longitude. In addition, we actually need the line-of-sight vector $\mathbf{\bar{L}}$ in unit vector form in the following calculations, so we divide each element of $\mathbf{\bar{L}}$ by $|\mathbf{\bar{L}}|$ to generate the unit vector $\mathbf{\bar{L}}_u$.

With the vectors $\mathbf{\bar{S}}$ and $\mathbf{\bar{L}}_u$ established, we can now calculate the altitudes connecting our light curves to Titan's atmosphere. The critical parameter to establish in this procedure is the point along the line of sight that is closest to the surface of Titan. Historically, this point has been referred to as the “tangent point” or the “impact parameter.” The latter term is vague and does not impart any physical meaning. “Tangent point,” on the other hand, has a physical basis but is misleading because the line of sight is not always tangent to something.

Altitude, being a plane-parallel concept, is defined along a direction that is perpendicular to the local surface (i.e., along the normal to the surface). The minimum distance between a line of sight and a planetary surface is the distance along a line that is perpendicular to both the line of sight and the surface; in other words, the altitude of the line of sight is the minimum distance between the surface and the line of sight. If the planetary body is a sphere, then the altitude is defined along the radial vector. In this case, “tangent point” is acceptable because the line of sight is tangent to a circle concentric with the center of the body. If, however, the body is an oblate spheroid, the altitude is not along the radial direction except at certain locations (e.g., the axes of the spheroid) and “tangent point” loses its meaning. As such, we prefer the term “point of closest approach” (PCA) to describe the relevant point along the line of sight because it is both meaningful and applicable in all situations.

In the geometry calculations to follow, we assume that the body is an oblate spheroid with an equatorial radius $R_{eq}$, a polar radius $R_p$, and an ellipticity $e$ (also known as the “flattening parameter” or “oblateness”) defined by
The oblate spheroid is spherically symmetric about the rotation axis. Figure 2.11 shows the planet as an extremely oblate spheroid to make this point obvious and also to separate clearly the vectors involved.

The procedure we use to find the PCA is an iterative one. Although we balked at an iterative procedure for finding the vectors \( \vec{L} \) and \( \vec{S} \), we are forced to use one in this situation; however, the associated uncertainty is much smaller. The procedure works by moving around on the surface until a point is found at which the normal to the surface is perpendicular to the line of sight. This criterion is only met at one point on the surface for an outward-directed normal vector. Once that point, which we will refer to as the "surface point," is established, we simply move up the normal vector to the line of sight to establish the PCA.

The first step is to guess a starting point on the body's surface that is close to the final "surface point." For this initial guess, we use the point on the body's surface that lies along the radial direction perpendicular to the line of sight. In the case of a spherical body, this point would be the "surface point" we seek because the normal to the surface is along the radial direction. For an oblate body, this is not the case, but the given point should be a reasonable starting point.

We get the point on the line of sight at which a radial vector from the body's center is perpendicular by finding the dot product of the spacecraft vector \( \vec{S} \) with the line-of-sight unit vector \( \vec{L}_u \). Note that because \( \vec{S} \) is defined as the body-to-spacecraft vector, we must take the negative of each element of \( \vec{S} \) in this dot product. This defines the distance from the spacecraft to the intersection point along the line of sight, which can be multiplied by the components of \( \vec{L}_u \) and added to \( \vec{S} \) to give us the point on the line of sight. This point establishes the vector \( \vec{r}_\perp \), which is shown in the top panel of Figure 2.11 and is mathematically calculated as

\[
e = \frac{R_{eq} - R_p}{R_{eq}}. \tag{2.4}
\]
\[
\vec{r}_\perp = \vec{S} + (-\vec{S} \cdot \vec{L}_u) \vec{L}_u. 
\] (2.5)

Next, we move down \( \vec{r}_\perp \) until we reach the surface to establish our starting point. This point is indicated by the vector \( \vec{r}_{\text{initial}} \). The following equations are used to define \( \vec{r}_{\text{initial}} \):

\[
\theta = \tan^{-1}\left( \frac{(r_{\perp})_z}{\sqrt{(r_{\perp})^2_x + (r_{\perp})^2_y}} \right) \quad \text{(latitude of } \vec{r}_\perp),
\] (2.6)

\[
|r_{\text{initial}}| = \frac{R_{eq}}{\sqrt{\sin^2(90^\circ - \theta) + \frac{\cos^2(90^\circ - \theta)}{(1-e)}}},
\] (2.7)

\[
(r_{\text{initial}})_x = (r_{\perp})_x \left( \frac{|r_{\text{initial}}|}{|r_{\perp}|} \right),
\] (2.8)

\[
(r_{\text{initial}})_y = (r_{\perp})_y \left( \frac{|r_{\text{initial}}|}{|r_{\perp}|} \right),
\] (2.9)

\[
(r_{\text{initial}})_z = z_{\text{sign}}(1-e)\sqrt{R^2_{eq} - (r_{\text{initial}})_x^2 - (r_{\text{initial}})_y^2},
\] (2.10)

\[
z_{\text{sign}} = \begin{cases} 
1 & (r_{\perp})_z \geq 0 \\
-1 & (r_{\perp})_z < 0 
\end{cases}.
\] (2.11)

The \( z_{\text{sign}} \) term is necessary in equation 2.10 because the equation for an oblate spheroid involves the square of the \( z \)-component and, therefore, we cannot infer the sign directly from the equation. However, because \( \vec{r}_\perp \) pertains to the case of a spherical body and any oblate spheroid must necessarily “pull in” from a sphere with the same equatorial radius, the \( z \)-component of the “surface point” vector must be in the same hemisphere as that of \( \vec{r}_\perp \).
With \( r_{\text{initial}} \) established, we begin the iterative procedure of finding the final "surface point." To do this, we use the downhill simplex method of Nelder and Mead (1965) as implemented in the routine \texttt{amoeba} from Press et al. (1992). The vertices of the simplex are \((r_x,r_y)\) pairs. The corresponding \( r_z \) value is obtained from equation 2.10 with the known value of \( z_{\text{sign}} \). The initial simplex vertices are \([(r_{\text{initial}})_x,(r_{\text{initial}})_y]\) and two points randomly perturbed from this point. The quantity to minimize is the distance between the line of sight and the planetary surface (i.e., the altitude, \( z \)), which is calculated for a given surface point \((r_x,r_y,r_z)\) from the following equations:

\[
d_1 = L_z(r_y - S_y) - L_y(r_z - S_z)
\]

\[ d_2 = L_x(r_z - S_z) - L_z(r_x - S_x) \]

\[ d_3 = L_y(r_x - S_x) - L_y(r_y - S_y) \]

\[
z = \sqrt{(d_1)^2 + (d_2)^2 + (d_3)^2} \quad \text{(altitude).} \]

When the value of the altitude \( z \) has been minimized, the resulting \((r_x,r_y,r_z)\) defines the vector \( \vec{r}_{\text{surface}} \) shown in the lower panel of Figure 2.11. From this vector, the following equations are used to establish the remaining quantities that we want:

\[
\vec{p}_{\text{surface}} = \vec{r}_{\text{surface}} - \vec{S}
\]

\[
\vec{r}_{\text{pca}} = \vec{S} + (\vec{p}_{\text{surface}} \cdot \vec{L}_u) \vec{L}_u
\]
\[ \vec{r}_{\text{pca}} = \vec{r}_{\text{pca}} - \vec{S}, \]  
\[ \theta_{\text{pca}} = \tan^{-1} \left( \frac{(r_{\text{pca}})_z}{\sqrt{(r_{\text{pca}})_z^2 + (r_{\text{pca}})_y^2}} \right) \quad \text{(latitude of } \vec{r}_{\text{pca}}), \]  
\[ \beta = \left| \tan^{-1} \left( \frac{(r_{\text{pca}})_y}{(r_{\text{pca}})_x} \right) \right|, \]  
\[ \phi_{\text{pca}} = \begin{cases} 
\beta & (r_{\text{pca}})_z \geq 0, (r_{\text{pca}})_y \geq 0 \\
360^\circ - \beta & (r_{\text{pca}})_z \geq 0, (r_{\text{pca}})_y < 0 \\
180^\circ - \beta & (r_{\text{pca}})_z < 0, (r_{\text{pca}})_y \geq 0 \\
180^\circ + \beta & (r_{\text{pca}})_z < 0, (r_{\text{pca}})_y < 0 
\end{cases} \quad \text{(longitude of } \vec{r}_{\text{pca}}). \]

The above equations were derived for the general case of an oblate spheroid. In the case of a spherical body, the equations work equally well, and the vectors \( \vec{r}_{\perp} \) and \( \vec{r}_{\text{initial}} \) shown in Figure 2.11 are equal to the vectors \( \vec{r}_{\text{pca}} \) and \( \vec{r}_{\text{surface}} \), respectively.

The geometry for the Titan solar occultation was calculated assuming a spherical Titan (i.e., \( e = 0 \)) and an equatorial radius of 2575 km. With the geometry established, the light curves we derived in Section 2.4 are tied to the atmosphere of Titan, and we are ready to begin the retrieval of the atmospheric parameters.
CHAPTER 3

DEVELOPMENT OF THE RETRIEVAL METHOD

3.1 The Basic Theory of Absorptive Occultations

In Chapter 2 we showed how a series of intensity measurements at various points in an atmosphere could be used to construct a light curve, which we then tied to the atmosphere through the use of the Beer-Lambert law:

\[
\frac{I(\lambda, r_{\text{PCA}})}{I_0(\lambda, \infty)} = e^{-\tau(\lambda, r_{\text{PCA}})}.
\]  

(3.1)

Though we did not elaborate, we stated that the line-of-sight optical depth \( \tau \) theoretically allows one to determine the atmospheric composition. The mathematical theory of absorptive occultations describes the relationship between \( \tau \) and the atmospheric composition and how we can extract the composition from the light curve measurements. We give a brief summary of the theory here.

We begin by expressing the line-of-sight optical depth as

\[
\tau(\lambda, r_{\text{PCA}}) = \sum_i \sigma_i(\lambda) N_i(r_{\text{PCA}}),
\]

(3.2)

where \( \sigma_i(\lambda) \) is the total extinction cross section of species \( i \) at wavelength \( \lambda \) and \( N_i(r_{\text{PCA}}) \) is the total column density of species \( i \) along the line of sight with point of closest approach given by \( r_{\text{PCA}} \). Although \( \sigma \) usually represents a photoabsorption cross section, it sometimes represents the sum of photoabsoption and scattering (e.g., Rayleigh scattering) cross sections. The source of the extinction is not critical
to the development of the theory. The total column density $N_i(r_{pca})$ is given by

$$N_i(r_{pca}) = \int_{-\infty}^{\infty} n_i(s) \, ds,$$

(3.3)

where $n_i(s)$ is the atmospheric number density of species $i$ along the line-of-sight direction, specified here by $s$ and having its origin at the point $r_{pca}$. Thus, through equations 3.1, 3.2, and 3.3, we have related the atmospheric number densities to the measured light curve data.

At this point, it is possible to extract the atmospheric number densities by guessing values for the $n_i(s)$, integrating them to yield the column densities $N_i(r_{pca})$, computing light curve values for comparison to the data light curves, and adjusting the $n_i(s)$ values iteratively until convergence is achieved. In general, however, this can be complicated by the number of species involved, the ability to distinguish one absorber ("scatterer") from another, and the shapes of the various number density profiles. As such, the theory has evolved from this point to more specialized cases in which the majority of the complexity is eliminated.

The most common assumption is that of spherical symmetry. This allows us to write the integral of equation 3.3 as

$$N_i(r_{pca}) = 2 \int_{r_{pca}}^{\infty} \frac{n_i(r)}{\sqrt{r^2 - r_{pca}^2}} \, r \, dr,$$

(3.4)

where the number densities $n_i(r)$ now represent vertical profiles as opposed to profiles along the line of sight. Equation 3.4 is in the form of the Abel transform and can be inverted to yield

$$n_i(r) = -\frac{1}{\pi} \int_{r_{pca}}^{\infty} \frac{dN_i(r_{pca})}{dr_{pca}} \frac{dr_{pca}}{\sqrt{r_{pca}^2 - r^2}}.$$

(3.5)

Equation 3.5 allows us to solve directly for the vertical number density profiles $n_i(r)$.
from the column density gradients. This is perhaps a moderate improvement over the situation of equation 3.3, but we still must solve for the number densities in an iterative manner because the measured light curves are a function of the sum of the column densities as expressed in equation 3.2 and the column densities of the individual species are not known a priori.

We are greatly helped in this matter if we have a single absorber or "scatterer" only. In this case, we can use equation 3.1 to rewrite equation 3.2 as

$$N(r_{\text{pca}}) = -\frac{1}{\sigma(\lambda)} \ln \left( \frac{I(\lambda, r_{\text{pca}})}{I_0(\lambda, \infty)} \right), \quad (3.6)$$

which on substitution into equation 3.5 yields

$$n(r) = \frac{1}{\pi \sigma(\lambda)} \int_r^\infty \frac{d}{dr_{\text{pca}}} \left[ \ln \left( \frac{I(\lambda, r_{\text{pca}})}{I_0(\lambda, \infty)} \right) \right] \frac{dr_{\text{pca}}}{\sqrt{r_{\text{pca}}^2 - r^2}}. \quad (3.7)$$

Equation 3.7 allows us to solve directly for the vertical number density profile of a single species using the measured light curve values. The Abel transform is somewhat sensitive to noise (cf. Hays and Roble, 1973); however, this equation can be used successfully in many instances if the wavelength range of the measurements is such that only one species is involved.

A different approach is to start with the integral of equation 3.4 and solve it directly using the so-called "onion-peeling" method. In this case, the atmosphere is broken up into spherical shells and the integral of equation 3.4 is replaced by a sum over the shells from the top of the atmosphere down:

$$N_i(r_j) = 2 \sum_{k=1}^j n_i(r_k) \int_{r_k}^{r_{k-1}} \frac{f_i(r)}{\sqrt{r^2 - r_j^2}} r \, dr, \quad (3.8)$$

where $n_i(r) = n_i(r_k)f_i(r)$. The functions $f_i(r)$ are not normally known, and an approximation is usually made, the most common being the assumption that the
$n_i(r)$ are constant within each shell.

Considering a single species as before, we can rewrite equation 3.8 using equation 3.6 as

$$-\ln \left( \frac{I(\lambda, r_j)}{I_o(\lambda, \infty)} \right) = I_j^* = 2\sigma(\lambda) \sum_{k=1}^{j} n_i(r_k) \int_{r_k}^{r_{j-1}} \frac{f_i(r)}{\sqrt{r^2 - r_j^2}} r \, dr .$$  (3.9)

Equation 3.9 can be written as the matrix equation

$$[I_j^*] = [A_{jk}][n_k] ,$$  (3.10)

where the elements of matrix $[A_{jk}]$ are functions of $\sigma(\lambda)$, $f_i(r)$, and the shell radii. Special attention must be given to the top “shell” because it represents an integral to infinity, and the elements $A_{j1}$ are usually more complicated. This form is convenient because it generally reduces to a triangular matrix that is easily solvable through recursion. In addition, the uncertainties in the number density profiles may be estimated from the uncertainties in the data in a straightforward manner.

The above discussion is only a brief introduction to the theory of absorptive occultations. A complete review of the theory would be quite extensive and is not within the scope of this dissertation. Our goal was to introduce the reader to the basic equations in order to provide a basis for the following sections, in which we discuss the shortcomings of previous methods and the method we have implemented to overcome them. More detailed surveys may be found in Smith and Hunten (1990), Chu (1977), Roble and Hays (1972), and Hays and Roble (1968).
3.2 The Reality of Absorptive Occultations

Theory and reality are often at odds in the physical sciences, and absorptive occultations are no exception. Many of the methods devised to extract atmospheric information from measured light curves are based on assumptions that do not always hold true. The primary assumption is usually that a single absorber ("scatterer") is responsible for the attenuation. Other assumptions include those of spherical symmetry and cross sections that do not vary with temperature and/or pressure.

The assumption of spherical symmetry is generally acceptable in most situations. Even when the planet is highly oblate, axial symmetry is usually a reasonable assumption. Most occultations occur in or near to the equatorial plane of the planet, and the oblateness is of small consequence. Exceptions occur when the line of sight is close to being perpendicular to the equatorial plane or when the line of sight passes through the atmosphere at very high latitudes, both of which can happen with stellar occultations. A notable case of this situation is the occultation of γ Pegasi by Uranus as observed by the Voyager 2 UVS, in which the line of sight passed almost directly over the pole of Uranus because of its large axial tilt relative to the ecliptic. In such extreme cases, the assumption of spherical symmetry may lead to erroneous results.

Photoabsorption cross sections can be highly dependent on temperature and/or pressure, but they are often assumed to be constant in occultation analyses to reduce the mathematical complexity. If the wavelength range of the measurements falls into a region in which the species act as continuum absorbers, then this assumption is usually valid. Continuum absorption is generally insensitive to temperature and pressure differences. On the other hand, if the wavelength range of the measurements falls into a region in which the species act as band absorbers, this assumption is almost assuredly invalid. Band absorption is strongly affected by changes in temperature and/or pressure because of the effect these have on the relative populations of the rotational and vibrational states of the absorbing molecules.
and the width of the spectral lines.

The most important assumption to consider, however, is that of a single absorber. If the species involved are known a priori, then a suitable wavelength range can be chosen for the measurements such that only one species has significant absorption in the range. In this case, the mathematics of the problem are simplified and the basic methods of Section 3.1 apply quite well. If the species involved are not known ahead of time, or if the wavelength range of interest has significant absorption from more than one species, then we must consider several species simultaneously. This can lead to significant complexity in the mathematics of occultation analysis even in ideal situations. If the situation is less than ideal, a physically meaningful retrieval may be difficult to impossible.

One of the factors which defines this "ideal" scenario is the cross section information of the species. If the cross sections are similar, we might not be able to distinguish one species from another. This would yield number density profiles that are averages of the species involved, or the retrieval method may favor one species over another without due cause.

A second consideration is the light curve data. The wavelength resolution of the data must be such that differences in the cross sections of the various species are visible. If the resolution is poor, cross section features that would potentially allow us to separate the contributions from each species could be blended to such an extent that the distinguishing features are wiped out.

Finally, any real instrument will yield spectra with a certain amount of uncertainty. The magnitude of the uncertainties can seriously affect our ability to analyze a multi-species absorption spectrum because features that appear to be real may actually not exist and vice versa. The "classical" methods of occultation analysis are often rigorously based in a mathematics that more or less assume perfect data. The Abel transform, in particular, can be very sensitive to noise. The less "perfect" the data are, the less applicable many of the methods become.
3.3 The Reality of Voyager UVS Occultations

Most of the absorptive occultation work performed to date has been concerned primarily with Earth. As such, occultation analysis methods have been developed with particular concern for Earth's atmosphere. The assumptions of Section 3.2 have been made because they generally hold true for Earth's atmosphere or it has been possible to design the occultation experiments such that they are valid.

For example, O₂ density profiles have been retrieved for Earth (cf. Roble and Hays, 1972) because O₂ absorbs strongly near 1500 Å and dominates the absorption at that wavelength. Because this is a continuum absorption region (the Schumann-Runge continuum), considerations of temperature and pressure are not critical. In addition, because a single absorber is involved, the instrument only needed to make measurements at a single wavelength or with a small bandpass.

This example is representative of an almost ideal scenario for an absorptive occultation. Similar cases exist for other species in Earth's atmosphere, which is why absorptive occultation analysis methods have developed along rather simplified and specific lines. Unfortunately, the Voyager UVS occultations are far from such an ideal situation, and the detailed methods developed for Earth are not generally applicable to the Voyager UVS occultations.

Part of the problem lies in the nature of the atmospheres of the planets (Jupiter, Saturn, Uranus, and Neptune) and satellites (Titan and Triton) at which the UVS obtained occultation data. These atmospheres are dominated by either H₂ or N₂, but all of them possess significant amounts of hydrocarbons and, in the case of Titan, nitriles. These species have very similar photoabsorption cross sections in the wavelength range of the UVS, as can be seen in Figure 3.1.

The problem of similar cross sections is both compounded and helped by the design of the UVS instrument. Because the UVS simultaneously measures a continuous spectrum over a wide range of wavelengths, we have the ability to
Figure 3.1: Comparison of the photoabsorption cross sections for several species in Titan's atmosphere. The sources of the cross section data are outlined in Appendix D. All cross sections shown here correspond to room temperature.
distinguish among the various species. This would not be the case if the UVS were restricted to the wavelength range of 800–1000 Å, in which the cross sections of the pertinent species are generally continuum absorbers. Without large changes in the cross sections, continuum absorption can result in a somewhat featureless spectrum, making it difficult to separate the contributions from various species. Inclusion of wavelengths out to 1700 Å allows the recorded spectrum to contain information on the species in their band absorption regions. This can be seen in Figure 3.2, where several absorption features are prominent in the model spectra. These longer wavelength features are useful in distinguishing among the various species, but, as band absorption features, they also introduce considerations of temperature and pressure dependence into the picture.

Figure 3.2 also shows how the Voyager UVS compounds the problem of similar cross sections. While the absorption features in the cross sections of Figure 3.1 are sharp and well-resolved, the UVS blends the features and smears them somewhat owing to its finite resolution. Each channel of the UVS records a range of wavelengths of width 9.26 Å. Because of spreading effects (scattered light, electron cloud spreading from the microchannel plates, point spread functions), the total range on a given channel can be two to three times this width, representing a substantial overlap of the absorption features.

This is not a problem unique to the Voyager UVS; any instrument with finite resolution will blend the features to some extent. However, given the general similarity of the cross sections of the atmospheric species pertinent to the atmospheres for which the Voyager UVS obtained occultation data, the moderate resolution of the Voyager UVS blends the features more than we might desire. This is not a flaw in the Voyager UVS but simply a matter of circumstance. The Voyager UVS was designed to be able to make a suite of observations without necessarily being optimal for any specific one, and it has performed admirably at the tasks for which it was designed.
Figure 3.2: Examples of model attenuated Voyager UVS spectra. The top spectrum was modeled using a column density of $6 \times 10^{15}$ cm$^{-2}$ of C$_2$H$_2$. The middle spectrum is that for a column density of $6 \times 10^{15}$ cm$^{-2}$ of C$_4$H$_2$. The bottom spectrum is a combined spectrum of CH$_4$, C$_2$H$_2$, and C$_4$H$_2$ with column densities of $2 \times 10^{16}$, $6 \times 10^{15}$, and $6 \times 10^{15}$ cm$^{-2}$, respectively.
A final difference between the Voyager UVS occultations and Earth occultations is the source of the measured intensities. Earth occultations are almost invariably stellar occultations because, as point sources, stars provide the best altitude resolution. More than half of the Voyager UVS occultations, however, are solar occultations for two primary reasons.

First, there are only so many stars that are bright in the wavelength range of the UVS, and they need to be in the proper location relative to the occulting body and Voyager for an occultation to occur. This was not always the case. The sun, on the other hand, is always available.

The second reason is that stellar fluxes suffer from absorption by interstellar hydrogen. With a few exceptions, this effectively wipes out the flux short of the hydrogen continuum edge at 912 Å. Because the Voyager UVS wavelength range extends down to about 500 Å, use of a star renders roughly 35% of the spectrum useless. In addition, the wavelength range from 500–900 Å is diagnostic of several constituents in the atmospheres observed by the Voyager UVS (H₂, N₂, H, N), so use of a star reduces or even eliminates our ability to infer the densities of these species. The sun, however, provides plenty of flux in this wavelength region.

The main problem in using the sun is that it has a finite size and cannot be treated as a point source. The projection of its disk in the atmosphere of the occulting body can be quite large, so the measured intensity can include absorption over a substantial altitude range. In addition, the ultraviolet flux of the sun can be nonuniform over the solar disk such that the incoming intensity at the atmosphere will vary with altitude. These two effects in combination can have a serious impact on the retrieved number density profiles if they are not properly accounted for.

There are other problems in using the sun as the occultation source as well. Solar occultations are restricted to the terminator region of the occulting body. This limits the spatial coverage as well as investigations of the daily variations of the atmosphere. The sun also impacts the instrument design because it is perhaps
too bright a source. Instruments observing the sun usually operate in a highly nonlinear fashion, making the processing of the data critical in the analysis.

In light of the difficulties and restrictions imposed by the sun, it has not been used much in Earth occultation work. As such, analysis methods have not dealt with finite sources in great detail and have focused primarily on the use of a point source. The application of such methods to a solar occultation is not necessarily straightforward and is yet one more reason that the Voyager UVS occultations can be difficult to analyze.

3.4 Previous Methods of Voyager UVS Occultation Analyses

Despite the problems outlined in Section 3.3, many of the Voyager UVS occultations have been analyzed using the methods developed for Earth occultations. This is particularly true when retrieving either H$_2$ or N$_2$ from their continuum absorption in the short wavelength end of the UVS spectrum, where it is possible to assume that the relevant species is the only significant absorber. Under this assumption and using analytical expressions derived for an exponential distribution in a spherically symmetric atmosphere, H$_2$ densities have been retrieved for Jupiter (Atreya et al., 1981; Festou et al., 1981), Saturn (Smith et al., 1983), and Uranus (Herbert et al., 1987), and N$_2$ densities have been obtained for Titan (G. R. Smith et al., 1982) and Triton (Krasnopolsky et al., 1993). After subtraction of the dominant N$_2$ absorption, Krasnopolsky et al. (1993) were also able to obtain a profile for N.

At longer wavelengths, the absorption spectrum becomes more complicated as band absorption from H$_2$ or N$_2$ overlaps with absorption from CH$_4$ and the heavier hydrocarbons. The simple approach used to retrieve the H$_2$ or N$_2$ densities from their continuum absorption does not apply in this situation, and different methods have been used to retrieve these densities. The most common approach has been to assume a distribution for the relevant species and forward model the occultation for comparison against the data. Appropriate changes to the density profiles were
made and the procedure repeated until a satisfactory fit was obtained. This method generally proceeded by “brute force” in that a suite of atmospheres were generated and the best fit found by modeling the occultation data for each atmosphere rather than trying to infer the atmosphere from the data itself. This approach has been used by Festou et al. (1981) at Jupiter (CH₄, C₂H₂, C₂H₆), G. R. Smith et al. (1982) at Titan (CH₄, C₂H₂), Smith et al. (1983) at Saturn (CH₄), Herbert et al. (1987) at Uranus (CH₄, C₂H₂, C₂H₆), and Bishop et al. (1992) at Neptune (CH₄), where the inferred species are indicated in parentheses.

The main problem with this approach is that the included species must be determined ahead of time so that the appropriate density profile can be generated. Inclusion of an additional species meant that the entire process had to be repeated to find the optimal atmosphere. This method is made even more inefficient in that many atmospheres have to be produced to cover all the possible combinations of densities that might yield the observed absorption spectra. Because of this, other methods were developed which attempted to extract the density information from the light curve data in a more direct manner.

One such method was developed by Herbert and Sandel (1991) to retrieve profiles of CH₄ and haze in Triton’s atmosphere. They used a parameterization of the number density profiles in combination with an analytical expression for the spatially-averaged transmission of the projected solar disk to generate a series of linear equations which were then solved using the singular value decomposition (SVD) technique. The advantage of this approach is that the densities were estimated directly from the data so that the optimal profiles were obtained more efficiently. The SVD technique also allowed the uncertainties in the data to be translated to uncertainties in the retrieved profiles in a direct fashion.

The disadvantage of this approach is that the problem has to be phrased mathematically or the SVD technique cannot be used. This involves a number of approximations that may or may not be strictly applicable. For example, the parameterization of the number density profiles uses an exponential function. This
biases the retrieved profiles towards an exponential distribution that might not apply to a photochemically-active species. Another example is that the expression for the spatially-averaged transmission assumes a uniform solar disk, which is almost certainly not the case in the EUV.

A final problem with this method is that only a few discrete altitudes could be directly inferred owing to computational time. This is because the method infers the entire profile (i.e., models the entire occultation) simultaneously. The more points that are specified in the profile parameterization, the longer it takes to perform each retrieval. Computational burden is also a reason for some of the approximations in the equations. The uniform-sun approximation could be replaced with an expression for the variation of the EUV intensity across the solar disk, but the added complexity would increase the computation time significantly.

Despite these problems, the method of Herbert and Sandel represented a substantial evolution in the analysis of absorptive occultations. A slightly modified version of this method was applied by Yelle et al. (1993) to infer profiles for H₂, CH₄, C₂H₂, C₂H₄, and C₂H₆ in Neptune’s atmosphere. However, in an attempt to provide more detailed altitude resolution than allowed by the Herbert and Sandel method, they also developed a different, two-stage method.

In the first stage, Yelle et al. related the transmission through the atmosphere (i.e., the light curve ratio) to the volume extinction coefficient as

\[ T_\lambda(r) = \exp \left( -2 \int_r^\infty \frac{k_\lambda(r')}{\sqrt{(r')^2 - r^2}} r' dr' \right), \quad (3.11) \]

where \( k_\lambda(r) \) is the volume extinction coefficient. They solved for the altitude profile of the volume extinction coefficient in each channel of the UVS spectrum using equation 3.11 and a constrained inversion technique based on the work of Twomey (1977) and Feng (1991).

In the second stage, the inferred profiles of extinction coefficient were related
to the number densities using

\[ k_\lambda(r) = \sum_j \sigma_j(\lambda) n_j(r), \quad (3.12) \]

which was solved using an iterative, least-squares method. However, they also ran into computational burden problems, which they lessened by averaging sets of three adjacent channels in the UVS spectrum. The problem with this is that it combined absorption across a wide range of wavelengths, forcing them to develop a weighted cross section given by

\[ \sigma^j = \frac{\int d\lambda' S_i(\lambda') \sigma_j(\lambda') I_o(\lambda') \exp \left( -\sum_i \sigma_i(\lambda') H_i(r) \right)}{\int d\lambda' S_i(\lambda') I_o(\lambda') \exp \left( -\sum_i \sigma_i(\lambda') H_i(r) \right)}, \quad (3.13) \]

where \( i \) refers to the UVS channel, \( j \) refers to the species, \( S_i(\lambda) \) is the response of channel \( i \) to wavelength \( \lambda \), \( I_o(\lambda) \) is the unattenuated solar flux, and

\[ H_i(r) = 2 \int_r^\infty \frac{n_i(r')}{\sqrt{(r')^2 - r^2}} r' \, dr' \quad (3.14) \]

is the column density along the line of sight. Equations 3.12 and 3.13, therefore, had to be solved together in the iterative procedure.

The Yelle et al. method represents the final development of the UVS occultation analysis methods prior to this work. Despite its mathematical sophistication, it suffers from several drawbacks. First, the two-stage nature of the process is disjoint, and it is unclear how the uncertainties in the first stage carry over into the second stage. Second, the use of a weighted cross section introduces new concerns. Because the solar flux and the response of the instrument are involved in the integrals of equation 3.13, their uncertainties contribute more significantly than in other methods where they tend to divide out. Finally, despite the averaging of channels to reduce the computational burden, they were still restricted in the number of species they could consider for computational reasons.
Although the methods of Voyager UVS occultation analysis have evolved significantly from the simple ones applied to the Jupiter and Saturn occultations to the mathematically sophisticated procedures used for Triton and Neptune, a few drawbacks are common to all of them.

First, no method has accounted for the possibility of temperature and/or pressure dependence of the cross sections in the retrieval procedure. Several authors did take this into account in trying to model the H\textsubscript{2} band absorption region, but they did so using number densities retrieved from the continuum region and were only trying to get a spectral match, not infer density information.

Second, no method has accurately accounted for the blending of wavelengths in UVS spectra. Each channel of the UVS measures a wavelength range. As such, each channel records absorption at a number of wavelengths, and the variation of the cross sections across this range must be considered. Simple weightings have been performed, but these suffer from other problems (see above).

Third, the finite size of the sun has not been treated accurately. All previous analyses have assumed a uniform flux across the solar disk. In addition, the finite size of the sun impacts the recorded spectrum because the sun’s image on the detector can span several channels. This means that the wavelength range of a given channel is even more extensive than the nominal range, further complicating the issue of cross section variations and proper treatment of the absorption.

Finally, issues of computational time have plagued all the methods in one way or another. To deal with this, the methods have tended to include a variety of assumptions (e.g., spherical symmetry, uniform sun). Even so, they have been limited in their ability to handle more than a few species simultaneously, and the assumptions made are usually not ideal.

What we need is a new method. This method should be detailed enough to handle non-spherical geometry, temperature and/or pressure-dependent cross sections, a nonuniform sun, proper treatment of the blending of wavelengths (and
thus absorption features) in the UVS spectrum, and a large number of species
while avoiding the approximations and complex mathematics that have limited
the previous analyses. At the same time, the method should be reasonably fast
and flexible enough to handle a variety of situations (e.g., both stellar and solar
occultations). Fortunately for us, such a method can be developed.

3.5 A New Method for UVS Occultation Analysis

In developing the following method for UVS occultation analysis, we begin with a
very simple question: what happens during an absorptive occultation? In answering
this question, we find that an occultation can be broken down into a series of basic
events. These are:

1. Light from a source arrives at the atmosphere.
2. This light passes through the atmosphere and is attenuated.
3. The attenuated light is received and recorded by the instrument.
4. The spectrum of attenuated light is ratioed to a spectrum of unattenuated
light.
5. We analyze this ratioed spectrum to infer properties of the atmosphere.

The way in which we treat these five events forms the core of any method of occul-
tation analysis that we might develop, and there are basically two ways to approach
the problem: direct and indirect.

The direct way is to focus on event #5. After all, if we have a number of
spectra, we want to know what they tell us. Thus, we develop a method which allows
us to get information directly from the spectra. To do this, we combine the first
four events into a series of connected equations through a number of simplifications
and assumptions. Then, all we have to do is plug the spectra into this mathematical
“black box” we have created and out comes the atmosphere. As we have seen in the previous sections, this can work in some circumstances, but it is somewhat limited in scope and replete with marginally true assumptions.

The indirect way is to focus on events #1–4. In this case, we guess an atmosphere, forward model the spectra, and see how they compare to the data spectra. If the match is good, the atmosphere is good. If not, we adjust the atmosphere and try again. This method has also been used in the past, and its main problem is that it takes a long time to cycle through all the possible atmospheres that might yield good matches to the data spectra. However, unlike the “black box” approach of the direct method, the indirect approach is not constrained by the mathematics. We can break the process down into the basic events above and treat each one separately rather than forcing connections through equations.

In fact, this is exactly the way we should approach an absorptive occultation. If we have an atmosphere and an instrument, and we are able to express the physics of each through an independent set of possibly complex equations, why would we want to complicate the issue by combining them into a single set of relationships if by doing so we are forced to make assumptions to keep the math tractable? Doesn’t it make more sense to keep the two separate, avoid the complicating assumptions, and work with basic concepts for which a physical understanding is possible? Indeed, it does, and this is the approach we take in developing our method. But as we just stated, this approach has the problem of cycling through a large number of model atmospheres to find the optimal one. This problem, however, can be avoided with a simple realization: we do not have to deal with the entire atmosphere simultaneously.

Past methods based on this approach have tried to match the light curves over their entire extent, and this required that the entire atmosphere be specified for the modeling. The truth is, however, that we only have to deal with one spectrum at a time, not the entire series of light curves. By working from the top of the atmosphere down, we can find the atmosphere that best matches the first spectrum,
build on those results to match the second, and so on until we reach the end of the occultation. Thus, instead of iterating an entire atmosphere simultaneously, we are only iterating a small part of it at any given time.

Figure 3.3 shows how this works. We divide the atmosphere into a number of layers, noting that the topmost "layer" is actually unbounded and requires special attention (see Section 3.5.1). We then vary the number densities in this topmost "layer" until the spectrum modeled with the densities is a good match to the first data spectrum. Once a good match has been achieved, we move to the next data spectrum, which corresponds to a line of sight lower in the atmosphere. As the line of sight moves through the atmosphere, it will encounter new layers. When a new layer is reached, the previous layer is frozen and the densities are no longer varied. The reason for this is that the spectra prior to this point contained information on the densities in the previous layer. By iterating the densities in the previous layer until we obtained the best possible match to those spectra, we determined the densities in that layer. In this manner, we work from the top of the atmosphere down, building upon the results as we go.

In concept, this is very similar to the "onion-peeling" method described in Section 3.1. The difference is that the "onion-peeling" method is based on direct mathematical relationships (with the ever-present assumptions and simplifications) and is solved using matrix inversion methods that determine the entire atmosphere at one time. Here, we are simply peeling the layers away one at a time as we work our way down through the atmosphere.

The remainder of this section describes the individual steps we perform to model a ratio spectrum and the means by which we iterate on each data spectrum until we achieve a good match. In each case, we will discuss the general method and the specifics that pertain to the Titan solar occultation analysis. Note that the steps of Sections 3.5.1 and 3.5.2 only have to be performed once at the beginning of the retrieval. The steps of Sections 3.5.3–3.5.6 are performed in each iteration.
Figure 3.3: Illustration of the layer-by-layer nature of the retrieval method. At each point in the occultation, we only retrieve the densities in the lowest layer intersected by the line of sight. As the line of sight descends through the atmosphere, each layer is “frozen” as the line of sight moves to a new lowest layer. The shading indicates the “frozen” layers in this illustration.
3.5.1 Setting up the Atmosphere

As a framework for the retrieval, we begin the process by dividing the atmosphere into a number of layers. Each layer is defined by an altitude, which pertains to the bottom of the layer. Thus, layer 1 extends from \( z_1 \) to \( z_2 \), layer 2 from \( z_2 \) to \( z_3 \), and so on until the top of the atmosphere. The final, topmost "layer" begins at \( z_{\text{num}} \), where \( \text{num} \) is the total number of layers, and is unbounded.

Each layer has several parameters associated with it. These include a temperature, a pressure, and number densities for the various species. All parameters are referenced to the bottom of the layer. In the case of the topmost "layer," this allows us to set up a profile "to infinity" for each species using the standard barometric law including the effects of gravity given by [from Chamberlain (1963)]

\[
n(r) = n(r_{\text{num}}) e^{-[\lambda(r_{\text{num}}) - \lambda(r)]}, \quad (3.15)
\]

in which \( \lambda(r) \) is defined by

\[
\lambda(r) = \frac{G M m}{k T_{\text{num}} r}, \quad (3.16)
\]

where \( G \) is the gravitational constant, \( M \) is the mass of the planet, \( m \) is the mass of the species, \( k \) is the Boltzmann constant, \( T_{\text{num}} \) is the temperature at the base of the topmost "layer," and \( r \) is the radial distance. Note that we assume the various atmospheric species are diffusively separated at the top of the atmosphere. Note also that the top of our defined atmosphere may not be exactly at the critical level for which these equations are defined, but Chamberlain points out that "ballpark" estimates are acceptable. In any event, if we define our atmosphere to high enough altitudes, the resulting attenuation will be minor at best from this unbounded "layer."
3.5.2 Source Spectrum and Cross Section Wavelength Grids

To facilitate the calculations of atmospheric attenuation, we define two wavelength grids, one coarse and one fine. This is necessary because the input source spectrum and the cross section data can be specified at any number of wavelengths and with variable spacings between adjacent data points. While this makes our modeling program flexible to use, it makes the internal calculations a nightmare. Thus, we set up these wavelength grids and put all the input data on a uniform basis.

The coarse wavelength grid spans the entire range of the spectrum which we will model. The grid is a series of bins centered on a given wavelength and having a defined, constant width. In modeling the spectra, each of these bins will be considered as a spectral “line” at the bin-center wavelength with an intensity equal to the bin’s total source intensity. The important consideration in setting up the coarse wavelength grid is that the spacing be smaller than the width of the channels in the data spectra and on the order of the spacing of wavelengths of the input cross sections. The first criterion is necessary so that we have several spectral “lines” per data channel. The second is necessary so that the cross section interpolation does not span too large a wavelength range and, possibly, truncate sharp features in the cross section data. We use a spacing of 0.5 Å in this work, which is on the order of the best cross section resolution and an order of magnitude smaller than the 9.26 Å spacing of the UVS data channels.

The fine wavelength grid is defined within the bins of the coarse wavelength grid. It is used in connection with high-resolution band absorption cross sections, which are generally the result of theoretical modeling. Measured band absorption cross sections are usually at a low enough resolution that they can be interpolated onto the coarse wavelength grid, but modeled band absorption cross sections, as well as a few measurements (e.g., Stark et al., 1992), are often specified with wavelength spacings as small as 1 mÅ, much too small for the coarse grid.

Whereas we specify the parameters of the coarse wavelength grid, the fine
wavelength grid bins are determined by the band absorption cross section data. By default, any high-resolution band absorption cross sections are assumed to be defined on a uniform wavelength grid on input to the modeling program. For each coarse wavelength bin, we determine which species has the highest resolution band absorption cross sections and then center the fine wavelength bins at the wavelengths of these cross sections. By default, the fine wavelength bins then have widths equal to the cross section spacing.

This procedure is repeated for all the coarse wavelength bins, with any potential overlaps at bin boundaries handled appropriately. In this manner, it is possible for the fine wavelength bin widths to vary from one coarse bin to another, and it is possible for many of the coarse wavelength bins to have no fine wavelength bins at all. This design is on purpose because it allows us to perform detailed calculations where they are necessary and avoid them where they are not, saving computational time. Once the wavelength grids have been defined, we set up the input source spectrum and the cross section data on the grids.

The Source Spectrum

The source spectrum for the retrieval is specified through an input file in one of three ways: as a series of continua over wavelength intervals, as a series of lines at specific wavelengths, or as a combination of the two. After it is read in, the source spectrum is assigned to the two defined wavelength grids.

Continua are specified as fluxes over a wavelength range. The proper fraction of flux from each continuum specification is placed into the bins of both the coarse and fine wavelength grids according to the ratio of the wavelength intervals.

Lines are specified as the flux at a given wavelength. In addition, we approximate the lines as a sum of two gaussians, so the half-widths of the gaussians and the separation of the peaks are also specified. We use the sum of two gaussians to allow the lines to have self-absorption in the line center (which occurs for the
H Lyman $\alpha$ line in the solar spectrum, for example). If this is not needed, the peak separation is specified as zero and the sum collapses to a single gaussian. The flux in each line is divided among the coarse and fine wavelength bins by integrating under the gaussians over the wavelength range of each bin.

Note that the flux in each coarse wavelength bin is equal to the sum of the fluxes in any fine wavelength bins contained in that coarse bin. As we will see in Section 3.5.3, we attenuate the flux in either the coarse bin or the fine bins, not both, so we are careful to preserve the total flux at all times.

The Cross Sections

The cross section data are input from files and fall into two categories: “continuum” absorption and high-resolution band absorption. “Continuum” here means anything that isn’t a high-resolution band cross section, so it may refer to continuum absorption, band absorption at low resolution, Rayleigh scattering, or a combination of these. The distinction is along the lines of resolution, not origin. High-resolution band absorption refers to cross sections that are specified on a uniform grid (usually because they are modeled) with spacings on the order of a mÅ.

Once they are read in, the cross sections are specified on one of the defined wavelength grids. The “continuum” cross sections are interpolated onto the coarse grid using linear interpolation. They are not specified on the fine grid because a single cross section (per species) is assigned to each coarse bin and that value is used for any fine wavelength bins within the coarse bin.

The high-resolution band absorption cross sections, conversely, are only specified on the fine wavelength grid. The highest-resolution data correspond to the bin definitions as described above. If high-resolution band absorption data exist for more than one species, the “lower” resolution cross sections are assigned to the fine wavelength bins in a manner consistent with the fine bin definitions. Interpolation is not used because of memory constraints (e.g., high-resolution data spanning the
wavelength range from 700–1100 Å at 1 mA resolution and 10 temperatures require 32MB at single precision).

The cross section data for any given species may be specified at multiple temperatures. In setting up the cross sections on the wavelength grids, each temperature set is treated the same. For example, species A might have a set of cross sections at 200 K and another at 295 K. Both sets will be interpolated onto the coarse wavelength grid (assuming they are “continuum” absorption cross sections). The net result is that we will have, for each wavelength in the grids, a cross section for each temperature input for each of the species.

3.5.3 Attenuating the Fluxes

With the atmosphere, source spectrum, and cross sections set up according to Sections 3.5.1 and 3.5.2, the next step is to reduce the fluxes by the atmospheric attenuation. To do this, we first determine where in the atmosphere the line of sight falls. Next, for each atmospheric layer traversed by the line of sight, we calculate the column density of each species. Then, we cycle through the wavelength grids and add each layer's contribution to the optical depth (basically the product of column density and cross section, but we have to be careful – see below). Finally, we use equation 3.1 with the calculated optical depths and input source spectrum to generate the attenuated fluxes on the coarse wavelength grid.

Where in the Atmosphere is the Line of Sight?

To determine where in the atmosphere the line of sight lies, we compare the altitude of the point of closest approach for the line of sight against the altitudes of the atmospheric layers. The lowest layer in the atmosphere that is pertinent to the attenuation calculations is the one whose altitude, in combination with that of the next higher layer, brackets the altitude of the point of closest approach. All layers
from this lowest layer (referred to as layer \( j_{low} \)) on up must be included in the attenuation calculations. If the point of closest approach is above the altitude of the topmost "layer," the line of sight is completely within the final, unbounded "layer" of the atmosphere and represents a special case.

**Calculating Column Densities**

Once we know the layers of the atmosphere to include, we calculate the column density of each species in each layer. There are two possible cases to consider: the line of sight is completely within the topmost "layer" or the line of sight intersects multiple layers.

If the line of sight lies completely within the topmost "layer," we are forced to make an assumption about the behavior of the number density profiles because we only have information for the base of the "layer." In this case, we assume that the number densities follow the barometric law including gravity, which is given by equations 3.15 and 3.16. Then, the column density of species \( i \) in the topmost "layer" (i.e., layer \( j_{num} \)) is given by

\[
N_{ij_{num}} = n_{ij_{num}} e^{-[\lambda(r_{j_{num}}) - \lambda(r_{pca})]} \sqrt{\frac{2\pi r_{pca}^2}{\lambda(r_{pca})}} \left[ 1 + \left( \frac{9}{8\lambda(r_{pca})} \right) \right],
\]

where \( n_{ij_{num}} \) is the number density of species \( i \) in layer \( j_{num} \) and \( r_{pca} \) is the radius of the point of closest approach of the line of sight. This equation is taken from Chamberlain (1963) and has been multiplied by two to give the total column density.

If the line of sight does not lie completely within the topmost "layer," it must intersect at least two layers. This sets up two different calculations as illustrated in Figure 3.4. The first calculation involves the unbounded, topmost "layer," and the second calculation involves the remaining layers.

To calculate the column density in the topmost "layer," we again assume
Figure 3.4: Geometry for the column density calculations. The column density in the topmost, unbounded "layer" is calculated assuming an exponential fall-off in density and depends on the source zenith angle, \( \chi_p \). The column densities of the remaining layers are calculated assuming spherical symmetry, which leads to straightforward, geometrical relationships for the path lengths in each layer. The \( d_i \)s are the third sides of the triangles formed by the respective \( r_j \) and the sum of the surface radius \( r_s \) and the altitude \( z \) of the point of closest approach of the line of sight (i.e., \( r_{pcs} \)).
that the number density profiles follow the barometric law. However, because the line of sight is interrupted by other atmospheric layers, we cannot use equation 3.17. That equation is defined for a solar zenith angle \( \chi_p \) (see Figure 3.4) of 90°, and we now have a case of \( \chi_p < 90° \). Instead, we turn to the general form for the column density as originally solved (using different notation) by Chapman (1931)

\[
N_p = n_p H \, \text{ch}(x_p, \chi_p),
\]

(3.18)

where \( N_p \) is the column density along the line of sight from point P to the spacecraft, \( n_p \) is the number density at point P, \( H \) is the scale height of the assumed exponential distribution of \( n \), \( x_p \) is the ratio \( \frac{r^2}{H} \), and \( \text{ch}(x_p, \chi_p) \) is the Chapman grazing incidence integral. The Chapman integral is a complex beast, so we use an approximation from Smith and Smith (1972):

\[
\text{ch}(x_p, \chi_p) \approx \begin{cases} 
1.0609693 + 0.55643831y & 0 \leq y \leq 8 \\
1.0619896 + 1.7245809y + y^2 & 8 \leq y \leq 100 \\
0.56498823 & y \geq 100
\end{cases}
\]

(3.19)

where \( y \) is given by

\[
y = | \cos \chi_p | \sqrt{\frac{x_p}{2}}.
\]

(3.20)

We can now calculate the total column density \( N_{ij_{\text{top}}} \) for species \( i \) in the topmost "layer" using equations 3.18 and 3.19 and multiplying the result by two.

The column densities in the remaining layers are calculated in a more straightforward manner, making use of two assumptions. First, we assume spherical geometry, which is a valid approximation for Titan. Second, we assume that the number density of each species is constant within each of these layers. This is reasonably valid as long as the atmospheric layers are thin enough compared to the scale heights of the species involved. Although we have criticized the use of such
assumptions as limiting, we note that the criticism arose from instances in which they were potentially invalid. We also note that because the method we have developed does not incorporate these assumptions into equations for use in an inverse method, they may be changed as the situation demands without much trouble. This flexibility is one of the desirable features of the current method.

Following the geometry of Figure 3.4, we can now determine the column densities for a given layer by calculating the path length of the line of sight within the layer and multiplying that length by the number density of each species to yield the column density of each species. For the layers between the lowest layer and the topmost "layer," the path length is given by

\[ l_j = 2(d_{j+1} - d_j) = 2 \left( \sqrt{r_{j+1}^2} - r_{\text{pca}}^2 \right) \left( \sqrt{r_j^2} - r_{\text{pca}}^2 \right), \quad (3.21) \]

where \( r_j \) is the radius of layer \( j \), \( r_{\text{pca}} \) is the radius of the point of closest approach of the line of sight, and \( d_j \) is as described in the caption to Figure 3.4. For the lowest layer, the path length is

\[ l_{\text{low}} = 2d_{\text{low}+1} = 2\sqrt{r_{\text{low}+1}^2} - r_{\text{pca}}^2, \quad (3.22) \]

The column density of species \( i \) in layer \( j \) is then given by

\[ N_{ij} = l_j n_{ij}, \quad (3.23) \]

where \( n_{ij} \) is the number density of species \( i \) in layer \( j \).

**Performing the Attenuation**

Once the column densities of each species in each layer have been determined, we can combine them with the cross section data to attenuate the fluxes. In doing
this, we have to keep two things in mind: any temperature-dependence of the cross sections and use of the coarse or fine wavelength grid.

Each atmospheric layer has a specified temperature. As with the number densities, we assume that the temperature within each layer is constant, a reasonable approximation if the layers are thin enough. Thus, we can include the effects of any temperature-dependence of the cross sections by generating cross sections for each species $i$ for each layer $j$ at the temperature of the given layer. There are three possible scenarios for this.

If we have no temperature-dependence information, we use the same cross sections for all the layers. If we have temperature-dependence information, but the temperature of a given layer falls outside the temperature range of the data, we use the cross sections at the temperature closest to that of the layer. We do not perform any extrapolation for such cases. Finally, if we have temperature-dependent cross sections and the temperature of the layer falls within the range for which this information exists, we use linear interpolation to generate the cross sections at the temperature of the layer. Regardless of the scenario, we designate the cross sections for species $i$ in layer $j$ as $[\sigma_{ca}(\lambda_{cgn})]_{ij}$ or $[\sigma_{ba}(\lambda_{fgn})]_{ij}$, where $ca$ indicates a "continuum" absorption cross section, $ba$ refers to a high-resolution band absorption cross section, and $\lambda_{cgn}$ specifies the bin-center wavelength of the $n^{th}$ coarse (cgn) or fine (fgn) wavelength grid bin.

Once the cross sections are set up, we loop through the coarse wavelength bins and attenuate the fluxes in each bin. Remember, the coarse wavelength bins represent the spectral "lines" that will be converted to a model attenuated spectrum. There are two possible cases to consider for each bin: "continuum" absorption only or "continuum" plus high-resolution band absorption.

In the case of "continuum" absorption only, we have a coarse wavelength bin in which no fine wavelength bins exist (i.e., no high-resolution band absorption over the given wavelength range). For each such bin, we can calculate the optical
The attenuated flux in this coarse bin is then calculated as

\[ F(\lambda_{cgn}) = F_0(\lambda_{cgn}) e^{-\tau(\lambda_{cgn})} , \tag{3.25} \]

where \( F_0(\lambda_{cgn}) \) is the unattenuated flux in the bin.

When we have "continuum" plus high-resolution band absorption, on the other hand, we have fine wavelength bins within the coarse bin. In this case, we calculate the optical depth for each fine wavelength bin within the given coarse bin as

\[ \tau(\lambda_{f_{gn}}) = \sum_{i} \sum_{j=\text{low}}^{j_{\text{num}}} \left\{ [\sigma_{\text{ca}}(\lambda_{cgn})]_{ij} + [\sigma_{\text{ba}}(\lambda_{f_{gn}})]_{ij} \right\} N_{ij} , \tag{3.26} \]

where we note that the "continuum" absorption cross sections, which are defined on the coarse wavelength grid, are the same for each fine wavelength bin within the given coarse bin. The attenuated flux in each fine wavelength bin is then calculated as

\[ F(\lambda_{f_{gn}}) = F_0(\lambda_{f_{gn}}) e^{-\tau(\lambda_{f_{gn}})} , \tag{3.27} \]

and the resulting flux in the coarse wavelength bin is just the sum of the attenuated fluxes in the fine wavelength bins within the coarse bin:

\[ F(\lambda_{cgn}) = \sum_{\text{finebins}} F(\lambda_{f_{gn}}) . \tag{3.28} \]
3.5.4 Modeling the Ratio Spectrum

The next phase in the method is to model the ratio spectrum for comparison against the data ratio spectrum. To do this, we model an attenuated spectrum using the fluxes from Section 3.5.3 and ratio this spectrum to a model reference spectrum.

In general, modeling a spectrum involves combining an input spectrum with the throughput of the instrument. What the throughput is depends on the instrument in question, but it is a function of the entrance slit, the optical path, and the sensitivity. We will refer to the function expressing the throughput as the "line shape" profile because, among other things, it represents the shape that an input spectral line will have in the recorded spectrum. No line recorded by a real instrument will be equal in shape to the actual line because of resolution limits to the optics. Thus, what we need to know is this "line shape" profile. Then, we simply apply it to each of the "lines" in our coarse wavelength grid and sum the results to produce our model spectrum.

The Voyager UVS "Line Shape" Profile

The base "line shape" profile for a Voyager UVS spectrum is given by the convolution of two triangular functions, in which the base of each triangle spans a defined number of spectral channels. The first triangular function includes effects owing to the optics. The base of this triangle is 4.20 for the occultation port (used for solar observations) and 5.42 for the airglow port (used for stellar observations). The second triangular function includes scattered light effects which are not removed by the descattering matrix. It has a base of 3.22 for both ports. After convolving the two triangular functions, we normalize the area under the profile to one in order to preserve the incoming flux. In the case of a stellar observation, this base profile is the final "line shape" profile. In the case of a solar observation, the base profile must be altered to account for the finite size of the sun.
The reason for this lies in the way in which the sun's image is recorded by the detector as opposed to a star's image. Figure 3.5 illustrates this difference. A star is a point source which falls onto a single spot on a given detector anode. The sun, on the other hand, has a finite size, and its image can span several detector anodes. The number of anodes spanned depends on the distance of the UVS from the sun. For the Titan solar occultation, the image spanned roughly two anodes.

Because each anode contains a different fraction of the sun's image, we need to weight the "line shape" profile in accordance with the distribution of the sun's light across the detector. In addition, the sun occupies a finite area in the entrance slit, and the variation of the input flux owing to the slit function (see Appendix A) must be considered in this weighting as well.

To calculate this weighting function, we visualize the incoming photon flux from the sun as forming a cylinder on the microchannel plates, where the base of the cylinder is the size of the sun's image. The cylinder has a constant height upon
entry to the UVS slit, but the slit function must be applied to the cylinder to get
the cylinder's height as a function of distance from the cylinder center in anode
(channel) units.

We next break this truncated cylinder up into slices, with each slice having
a width of $\frac{1}{20}$th of an anode and the edges of the slices parallel to the anode edges.
Using the height function we just determined, each slice is assigned a height equal
to the height of the truncated cylinder at the position of the slice center. Each slice
is then assumed to be a rectangular parallelepiped and its volume is calculated.
The volume for each slice is then ratioed to the total volume of the original, non-
truncated cylinder to yield the fraction of the input flux as a function of distance
from the cylinder (i.e., the sun's image) center. These are relative calculations, so
we can assume the cylinder has a height of one to begin with.

This fractional flux is the weighting function for the finite sun. It is con-
volved with the base profile to yield the final "line shape" profile. After the convolution,
we again normalize the area under the profile to one to preserve the incoming
flux. This negates the reduction effect of the slit function in terms of the total
incoming flux, but the "line shape" profile is used to distribute the light across
the spectral channels, not to account for the total flux recorded. Because this flux
reduction information is needed to model the spectra, however, we preserve it prior
to the normalization.

The Ratio Spectrum

Once we have the "line shape" profile, it is a straightforward procedure to model
the attenuated and reference spectra needed to generate the ratio spectrum. In
each case, we perform a series of operations on the "lines" represented by the bins
of the coarse wavelength grid. For the attenuated spectrum, the fluxes are those we
calculated in Section 3.5.3. For the reference spectrum, the fluxes are the original,
unattenuated fluxes.
For each "line," we first reduce its flux by the factor owing to the slit function of the UVS. For a stellar observation, this is just the value of the slit function at the position of the star in the slit. For a solar observation, this is the sum of the fractional volumes we calculated in determining the weighting function for the finite sun.

We next apply a calibration factor to the "line" flux to convert it from real flux units to the photoevent units of a processed UVS spectrum. In a perfect instrument (i.e., one with infinite resolution), this step would not be necessary because the calibration would divide out in the ratio. However, we have a "line shape" profile with a non-zero width, so our line "flux," although pertaining to a single wavelength, is spread out over several channels of the spectrum and combined with other wavelengths before the ratio step. Thus, the calibration factor must be applied.

With the "line" flux set to the proper value, we then position the "line" at the proper spectral location (in terms of channels) and apply the "line shape" profile to it. This means we center the profile at the "line" and integrate the profile over each channel to determine the fraction of the flux in the "line" that is recorded by the given channel. Once the fractions are determined, we multiply the "line" flux by each fraction and add the results to the proper channels of the model spectrum.

In positioning the "line," we treat the attenuated spectrum differently than the reference spectrum. The "lines" of the attenuated spectrum are positioned according to the spectral shift related to the actual position of the source in the slit as determined from its limit cycle value. For stars, this is the star's position; for the sun, this is the central position of the solar disk. The "lines" of the reference spectrum, however, are positioned according to the spectral shift related to the average limit cycle value of the spectra which were averaged to produce the corresponding reference data spectrum. In generating the data ratio spectra, we divided each attenuated data spectrum by a binned reference spectrum. The spectra which were averaged to yield this binned spectrum covered a range of limit cycle values and,
therefore, a range of spectral shifts. Thus, by using the average spectral shift of the data reference spectrum, we are better modeling the process applied to the data.

We repeat this process for each “line” of the coarse wavelength grid. When all the lines have been treated, we ratio the attenuated spectrum to the reference spectrum to generate the final model ratio spectrum for comparison to the data ratio spectrum.

3.5.5 Further Considerations of the Finite Sun

In addition to the differences in the “line shape” profile that are introduced by the finite size of the sun, we need to consider two other effects. The first is the projection of the solar disk in the atmosphere. If this is large in extent, then the attenuation will vary across the disk because it spans a large range of altitude and, therefore, density. The second is the variability of the solar flux across the disk of the sun. This, as well as the first effect, can influence the modeled spectrum because the flux on the detector is weighted more heavily in some regions than others. Both of these have plagued previous analysis methods and forced various assumptions about disk uniformity and variations in absorption with altitude. Fortunately, we can include these effects in our method without much trouble.

Both of these can be handled by dividing the sun into a series of segments and treating each segment as an individual source. This addresses the disk projection effect because each segment will experience attenuation along a different line of sight. The geometry information for the observation still pertains to the center of the solar disk, but we can easily relate this geometry to the segments. This also solves the flux variability problem because we can assign a fraction of the total flux to each segment according to whatever pattern we choose. Figure 3.6 illustrates the division of the sun into segments.

The impact on the modeling procedure of dividing the sun into segments is minimal. We simply perform the steps of Sections 3.5.3 and 3.5.4 for each segment.
Figure 3.6: Illustration of the division of the sun into multiple segments. Each segment has its own line of sight, which is determined by the angular separation of the center of the segment from the center of the sun, the point to which the nominal line of sight is referenced. Each segment also has its own weighting factor, which allows for the consideration of a non-uniform solar disk.

The "line shape" profile is determined in the same manner, replacing the total projected image of the sun with that of the particular segment. This makes the fractional volume calculations for the weighting function more complicated but not tremendously. The model attenuated and reference spectra are generated by summing the modeled spectra for each segment prior to ratioing. The ease with which this troublesome consideration is integrated into our occultation analysis method is further evidence of its robust nature.

3.5.6 Iterating to the Optimal Densities

The procedure described in the preceding sections takes us from a given model atmosphere to a model ratio spectrum, which we can compare to a data ratio spectrum. The key step now is to find the atmosphere that minimizes the mismatch between the data and model spectra. We cannot use the classic inversion techniques because we forward model the ratio spectrum from the atmosphere. We also cannot use minimization techniques that rely on the calculation of gradients because we do not phrase the problem through mathematical equations.
What we need is a multidimensional minimization method that is straightforward, robust, reasonably fast, and generally independent of the function to be minimized. The downhill simplex method developed originally by Nelder and Mead (1965) is one such method. Unlike most multidimensional minimization procedures which rely on calculations of derivatives or utilize one-dimensional minimization techniques as an integral part of the procedure, the downhill simplex method only requires function evaluations and uses simple, geometrically-conceived concepts of the parameter space to perform the minimization.

A simplex is a geometrical figure which consists of N+1 points in N dimensions, as well as all the lines and polygonal faces which connect the points together. We will refer to these points as the "vertices" of the simplex. A simplex is a line in one dimension, a triangle in two, a tetrahedron in three, and so on. Higher-order dimension simplexes are difficult to impossible to visualize, but the procedure works the same regardless of the number of dimensions involved. In the downhill simplex method, the simplex is represented by an array \( \mathbf{V} \) of N+1 vectors \( \mathbf{v} \) (the vertices) of N elements each. These N elements represent the N unknown parameters of the function to be minimized.

We begin the method by initializing the simplex array \( \mathbf{V} \). This means setting up the N+1 vertices of the simplex and evaluating the function at each one. We can think of one vertex as being our initial guess at the solution and the remaining vertices as spanning the possible solution space. If this initial guess is \( \mathbf{v}_o \), then the other vertices can be defined as

\[
\mathbf{v}_i = \mathbf{v}_o + \lambda \mathbf{e}_i,
\]  

(3.29)

where the \( \mathbf{e}_i \) are N unit vectors and \( \lambda \) is a characteristic length scale for the problem. The \( \lambda \) can be replaced with individual \( \lambda_i \)'s for each direction, or the other vertices can be determined randomly. The idea is to start the simplex near the solution to reduce the number of steps required to minimize the function. All that really
matters, however, is that we set up N+1 vertices and evaluate the function at each one.

Once the simplex array \( \mathbf{V} \) has been set up, we must compute the vector \( \mathbf{s} \), which contains sums taken across the elements of \( \mathbf{V} \). Each element of \( \mathbf{s} \) is given by

\[
s_i = \sum_{j=1}^{N+1} V_{ij}.
\]

Thus, the \( i^{th} \) element of \( \mathbf{s} \) is the sum of the \( i^{th} \) elements of the N+1 vectors \( \mathbf{v} \) in the array \( \mathbf{V} \) (i.e., the \( i^{th} \) elements of the N+1 vertices in the simplex). This vector is used in the calculation of new vertices in the simplex iteration procedure.

With the simplex array \( \mathbf{V} \) and the vector \( \mathbf{s} \) initialized, the method proceeds by taking a series of steps that guide the simplex through the complexity of the N-dimensional topography until it encounters a minimum. Each step consists of a series of possible actions. These are illustrated in Figure 3.7 for the case of \( N = 2 \), in which the simplex may be visualized as a triangle. In the following paragraphs, A–D refer to this figure.

The first action in every step is to "reflect" (A) the simplex away from the "worst" vertex, which is the one with the largest function value. This "reflection" establishes a new vertex and is expressed mathematically as

\[
\mathbf{v}_{\text{new}} = \left( \frac{1 - \alpha}{N} \right) \mathbf{s} - \left( \frac{1 - (N+1)\alpha}{N} \right) \mathbf{v}_{\text{worst}},
\]

where \( \alpha \) is a factor which varies with the action being taken. It is -1 for this "reflection," indicating that we are moving "away" (the minus sign) from the "worst" vertex. Once the new vertex is determined, we calculate the value of the function for that vertex.

If the new vertex has a function value smaller than that of the "worst" vertex, we replace the "worst" vertex with the new one and recalculate \( \mathbf{s} \). If, in
Beginning of step

A) Reflection

B) Reflection and expansion

C) Contraction

D) Multiple contraction

Figure 3.7: Illustration of a step in the simplex procedure. We use the case of two unknowns because the simplex is a triangle and the geometrical nature of the method is well illustrated. The top triangle represents the simplex at the start of the step. As described in the text, the simplex will end up in one of the four states A–D, depending on the “move” it makes in the current step. Note that the “best” vertex is always the same, though it is only labeled for the topmost triangle.
addition, the function value at this new vertex is smaller than that of the "best" vertex, which is the one with the minimum function value thus far, the simplex is "extended" in the direction of the new vertex by a factor of two (B). The rationale here is that we want to take larger steps in the directions which are most beneficial. This "extension" is also accomplished using equation 3.31, with $\alpha = 2$ and the new vertex replacing the original "worst" vector $\vec{v}_{\text{worst}}$. If this "extended" vertex (B) is even better than the vertex from the original "reflection" (A), we replace the vertex of A with the "extended" vertex of B and recalculate $\vec{s}$. If the "extended" vertex is not better, we throw it away and keep the "reflected" vertex of A.

If, on the other hand, the new vertex from the "reflection" (A) has a function value larger than that of the next-to-worst vertex, the "reflection" gained us nothing. The new vertex is still the "worst" one, regardless of whether it has a smaller or larger function value than the original "worst" vertex at the beginning of the step. In this case, the simplex "contracts" (C) away from the "worst" vertex, halfway toward the rest of the simplex. This "contraction" is accomplished using equation 3.31 as well, with $\alpha = 0.5$ and $\vec{v}_{\text{worst}}$ being the original "worst" vertex. By "contracting," the simplex tries to confine itself to a more favorable part of parameter space. We can think of the simplex as being in a "valley" — to either side are the "valley walls" which take us away from the minimum, so we want to confine ourselves to the "valley floor" and "move" along it.

If this "contracted" vertex is better than the original "worst" one, we keep it and recalculate $\vec{s}$. If the "contraction" results in a vertex that is still the worst in the simplex, no action is able to eliminate the "worst" vertex. In this case, the simplex performs a "multiple contraction" (D) about the "best" vertex by pulling in half the distance along the directions to each of the other vertices. We can think of the simplex as trying to squeeze itself together to pass through a particularly narrow "hole" in parameter space, much like threading a needle. This "multiple contraction" is performed by replacing each vector $\vec{v}$ in the simplex array $\mathbf{V}$ (excluding the "best" vector, of course) with the average of that vector and the "best"
vector. Once the new vectors are determined, the vector $s$ is recalculated.

At the end of a step, the simplex has “moved” into one of the four states represented by A–D. By performing a series of such steps, the simplex will eventually converge to a minimum function value and the procedure will terminate. The criterion for termination in a multidimensional minimization, however, can be tricky. Three possibilities exist for the downhill simplex method. One is to end the procedure when the vector distance “moved” in a given step is smaller in magnitude than a specified value. Another is to stop the procedure when the difference in function value between the “best” and “worst” vertices is smaller than a defined tolerance. The third is to limit the number of steps allowed. We use the latter two and terminate the procedure when either the normalized difference in function value between the “best” and “worst” vertices, defined by

$$
\Delta f = \left| \frac{f_{\text{worst}} - f_{\text{best}}}{|f_{\text{worst}}| + |f_{\text{best}}|} \right|
$$

is less than a specified value or the number of steps exceeds a set maximum.

As in any minimization routine, the procedure may have converged to a local rather than global minimum. Anomalous steps could also fool the termination criterion and cause a premature halt to the procedure at a point which is not a minimum at all. As such, it is a good idea to restart the minimization procedure at the supposed minimum and see if it converges to the same point. In the downhill simplex method, this means reinitializing $N$ of the vertices while keeping the one marking the minimum. If the procedure converges to the same point, it is likely a true minimum, though not necessarily a global one. If it converges to a different point, the procedure may have to be restarted again to distinguish between the two. Frequent restarts are wise in multidimensional situations because many local minima may exist depending on the problem. Such restarts should be reasonably inexpensive because the method has already converged to the restart point once and we are starting the procedure already there.
The downhill simplex method adapts well to the problem of absorptive occultation analysis. One advantage it has is that it is completely disconnected from the function to be minimized. All that the method knows is that for each set of N unknowns, the function can be evaluated. Thus, the function can be anything as long as it has a defined value for a given set of unknowns. For us, the “function” is the process of modeling a ratio spectrum, the function value is the mismatch between the model and data ratio spectra, and the N unknowns are the densities of the N species for the given atmospheric layer we are retrieving.

Another advantage of the method is its lack of mathematical detail. We are not constrained in the way we treat our “function” or its evaluation. We use a straightforward \( \chi^2 \)-style calculation in comparing the model and data ratio spectra defined by

\[
\Delta S = \sum_c \frac{[M(c) - D(c)]^2}{[\sigma_D(c)]^2},
\]  

(3.33)

where \( \Delta S \) is the spectral mismatch (i.e., our function value), the sum is taken over the \( c \) channels of the spectra, \( M(c) \) and \( D(c) \) are the values of the model and data ratio spectra for channel \( c \), and \( \sigma_D(c) \) is the uncertainty of the data ratio spectrum for channel \( c \), which we calculated in the data processing of Chapter 2. If we want, we can restrict the sum to a given set of channels, use arbitrary weightings for each channel instead of the uncertainties, or impose penalties if a given density is too small or too large. Other minimization methods allow these changes as well, but they often require extensive changes to the mathematical equations involved. Changes in the downhill simplex method of minimization are trivial in comparison.

The downhill simplex method we have implemented is based on the subroutine amoeba of Press et al. (1992). We have adapted the routine to replace the mathematical function they assume with the spectrum modeling “function” that we need.
3.5.7 Putting It All Together

With the modeling procedures of Sections 3.5.1–3.5.5 and the downhill simplex method of Section 3.5.6, we have all that we need to retrieve the atmospheric number densities from the occultation data. We will now run through the entire procedure to show how it all fits together.

We begin the retrieval with an input model atmosphere. Nominally, this is our best guess at what the atmosphere is; however, it may be anything we want as long as the atmospheric quantities are physically plausible (e.g., densities cannot be negative). The number densities in each layer are used to initialize the simplex procedure for that layer. The temperature of each layer is used to determine the proper photoabsorption cross sections to use in the event that we have information on the temperature-dependence of the cross sections. In addition, the temperature of the topmost, unbounded “layer” is used in calculating the distributions of the various species in the topmost “layer,” which we need in order to calculate the column densities in this “layer.”

Once the model atmosphere, the source spectrum, and the cross section data are set up, we loop through the data spectra one at a time from the top of the atmosphere down. For each spectrum, we establish the lowest layer intersected by the line of sight. There are four possible scenarios depending on the outcome.

If this is the first spectrum (i.e., the one whose line of sight is highest in the atmosphere), this layer becomes the topmost “layer” of the output model atmosphere because we cannot retrieve any layers higher than this one. As such, we truncate the model atmosphere at this layer and use the approximations of Section 3.5.3 for the topmost, unbounded “layer.” We then use the simplex procedure to iterate to the optimal number densities for this “layer.”

If the determined lowest layer is the same as the lowest layer of the previous spectrum, we run the simplex procedure as usual to find the nominal densities for
the layer. In this case, however, the densities in each iteration of the simplex procedure are averaged with the optimal densities already determined for the previous spectrum (or spectra) in this layer to yield an average density for the layer prior to the attenuation of the incoming fluxes. Thus, the densities determined by the simplex iteration on the current spectrum are those densities which yield the best average density for the layer. Such averaging will continue as long as the line of sight remains within the same lowest layer. Note that we do not store these running average densities for the layer but the running sums of the densities; thus, we are not continually averaging the previous average into a new one.

If the determined lowest layer is not the same as that of the previous spectrum, we “freeze” the number densities of the old lowest layer and do not vary them anymore. If there had been multiple lines of sight within the old layer, we perform a final averaging on the densities and “freeze” the averages. We then use the simplex procedure to find the number densities in this new lowest layer.

Finally, it is possible for the line of sight to skip a layer. In this case, we “freeze” the old lowest layer as above and use the simplex procedure as usual to determine the densities in the new lowest layer. At each step in the simplex procedure, however, we linearly interpolate in log(density)-altitude space between the current layer’s densities and the “frozen” densities of the old lowest layer to “fill in” any intervening atmospheric layers that may have been skipped. When the current lowest layer is “frozen,” these skipped layers are also “frozen” through a final linear interpolation.

In this manner, we determine the densities in the model atmosphere layers as the line of sight descends through the atmosphere. The procedure ends when we reach the planetary surface, the bottom layer of the input model atmosphere, or the final data spectrum.
To improve our determination of the density profiles, we perform the retrieval a number of times. Each retrieval begins with a different set of initial conditions, and the results from all the retrievals are averaged to yield the nominal profiles. At the same time, this enables us to generate uncertainties for the retrieved profiles using the normal standard deviation calculations. The benefit of this approach is that the "valley floor" on which the optimal densities for a given layer lie is potentially very broad, with any number of density sets yielding approximately the same mismatch between the model and data ratio spectra. By beginning the retrieval at many points and determining several of these "optimal" density sets, the average profiles and their corresponding uncertainties are more likely to reflect this inherently broad solution space than any single retrieval by itself.

3.5.8 Retrieving the Atmospheric Temperature

The procedure described in the previous section assumes that the temperature profile of the model atmosphere is specified. We need the temperature in the approximations we use to handle the topmost, unbounded "layer" of the atmosphere. We also need it to determine the proper photoabsorption cross sections to use when temperature-dependent cross sections are available. We now consider the possibility of retrieving the atmospheric temperature profile simultaneously with the atmospheric densities.

If we choose a species whose density is not dominated by photochemical production and loss (e.g., N$_2$ or CH$_4$), we may assume that the number density of this species locally follows an exponential distribution of the form

$$n = n_o \exp \left( -\frac{z - z_o}{H} \right),$$

(3.34)

where $n_o$ and $z_o$ are the number density and altitude at a reference level and $H$ is the density scale height. This scale height is related to the temperature through
the equation

\[ H = T \left( \frac{dT}{dz} + \frac{mg}{k} \right)^{-1} , \]  

(3.35)

where \( m \) is the mass of the species involved, \( g \) is the local gravity, and \( k \) is the Boltzmann constant. Thus, if we know the scale height \( H \) and the temperature gradient \( \frac{dT}{dz} \), we can solve for the temperature \( T \).

We can determine the scale height by fitting the distribution of equation 3.34 to the densities of the chosen species in the current layer and a few layers above it. The current layer serves as the reference level, and the fit is performed in log(density)-altitude space so that we can use the standard least-squares formulas for fitting a line to data (taken from Bevington and Robinson, 1992). The scale height is then obtained from the slope of the line.

We can determine the temperature gradient in a similar fashion by fitting a line to the temperatures in the same few layers above the current layer. The gradient is then obtained from the slope of the line. Note that we do not include the current layer in the fit because it is the temperature of this layer that we are trying to determine. The current layer is included in the scale height determination because we obtain the densities of the layer during the simplex procedure. We view the temperature as a dependent variable in this scheme and base its calculation upon the retrieved densities.

With the scale height and temperature gradient determined, we can solve for the temperature using equation 3.35. This assumes, however, that we know the densities and temperatures in the layers above the current one so that the fits can be performed. Because we work from the top of the atmosphere down, this is not a problem except that we begin the retrieval with the topmost, unbounded "layer," above which we have nothing.
To handle this, we "fake" extra layers in our atmosphere. These "fake layers" lie above our topmost, unbounded "layer" and have temperatures equal to that of the topmost "layer." This establishes the temperature gradient as zero to begin with, making the upper atmosphere isothermal (a reasonable starting condition). The densities in these "fake layers" are calculated from the exponential distribution of Section 3.5.1, which is evaluated using the temperature and densities of the topmost "layer," the temperature having been input and the densities having been obtained from the simplex procedure. We do not retrieve the temperature in the topmost "layer" but rather leave it at the input value and use it to "jump start" the temperature retrieval. As we move down through the atmosphere, we will determine the densities in subsequent layers through the simplex iteration, and fewer and fewer "fake layers" will be necessary in the calculation of the temperature. Eventually, the "fake layers" will no longer be used at all.

Because part of the reason for retrieving the temperature is to allow us to use the proper temperature-dependent cross sections when they exist, we need to be sure that the calculation is performed at a point in the simplex iteration which makes this possible. We use the following scheme to enable us to do this:

1. Guess the initial densities in the current layer (i.e., initialize the simplex) or adjust the densities in the current layer based on the comparison of step 4.
2. Perform the temperature calculation as outlined above, using the "fake layers" if necessary.
3. Set the cross sections properly according to the calculated temperature.
4. Model the ratio spectrum and compare it to the data spectrum.
5. Repeat steps 1–4 until convergence is achieved.

This scheme ensures that the temperature is calculated before we model the spectrum, so the temperature-dependence of any cross sections is included in the modeling. It also ensures that the temperature in the current layer is calculated using
the optimal densities when the simplex procedure terminates.

3.6 Testing the Method

To assess the method's ability to retrieve atmospheric number density profiles from occultation data, we performed the following test. First, we constructed a model atmosphere from the Yung et al. (1984)/Yung (1987) profiles for N₂, CH₄, C₂H₂, and C₂N₂. We multiplied the C₂H₂ and C₂N₂ profiles by factors of 10 and 100, respectively, to enhance their absorption signature. Above an altitude of 1200 km, the profiles were extrapolated as described in Section 4.3. Next, we generated two sets of model occultation data using this atmosphere and geometry information from the Titan ingress occultation. The first set is "noise-free," with the resulting model ratio spectra left untouched. The second set is "noisy," and the model ratio spectra have been perturbed using uncertainties from the Titan ingress data. Finally, we ran both sets of model occultation data through the retrieval procedure to see how well we could retrieve the original profiles. We used a tolerance of $10^{-8}$ and a maximum of twenty steps in the simplex procedure. Only one retrieval was performed in each case, so the resulting profiles have not been averaged.

The results of this test are shown in Figures 3.8 and 3.9. We can see that the retrieval has worked well overall, and the input profiles have been reproduced within the potential ranges. The presence of "noise" in the second set of model data has influenced the results to some extent, but the retrieved profiles are still excellent matches to the input profiles over much of the retrievable range. The primary difference between the "noise-free" and "noisy" cases is that portions of the retrieved profiles which are "ragged" in the "noise-free" case are even more so in the "noisy" one. As an example, the C₂N₂ profile between 850 and 1000 km is marginal in the "noise-free" case. In the "noisy" case, the retrieval in this region is worse as evidenced by the growth of the indicated "drop-out" feature. In the region between 500 and 850 km, however, the retrieved profile is approximately the same.
Figure 3.8: Retrieval of profiles in a "noise-free" test case. The smooth lines represent the input profiles used to generate the model occultation data, and the retrieved profiles are overlaid on these. The dashed lines bracket the altitude range over which the given species was potentially retrievable based on a visual assessment of their absorption signatures in the model ratio spectra. The matches between the retrieved and input profiles are quite good. The indicated cases of mismatch are discussed in the text.
Figure 3.9: Retrieval of profiles in a "noisy" test case. The description of this figure is the same as for Figure 3.8. The matches between the retrieved and input profiles are still quite good, despite the addition of noise. The differences between the "noise-free" and "noisy" cases are discussed in the text.
in the two cases. Similar examples exist for CH$_4$ and C$_2$H$_2$.

We can understand this difference by examining the model ratio spectra. In regions where the retrieved profile is an excellent match to the input profile and the addition of "noise" has minimal effect, the given species shows a strong absorption feature in the model spectra. In regions where the match between the retrieved and input profiles is poor and "noise" has a pronounced effect on the retrieval, the given species has weak absorption features. Thus, as we might expect, the retrieval works best when the absorption features that distinguish one species from another are strong. This also explains why one profile being "ragged" coincides with another being "ragged" (e.g., CH$_4$ and C$_2$H$_2$ between 1100–1300 km and C$_2$H$_2$ and C$_2$N$_2$ between 850–1000 km). When the absorption features are weak, it is difficult to distinguish among the various species and the retrieval procedure "trades" density from one species to another.

In addition to the effects of "noise" on the retrieved profiles and the problems of weak versus strong absorption features, there are three general features of the retrieved profiles that need explaining. The first of these, labelled "non-retrievable," is the large deviation of the retrieved N$_2$ profile from the input one. This begins at the altitude at which the ratio spectrum shows complete absorption below 1000 Å, the point at which the N$_2$ cross sections effectively drop to zero. We can only retrieve a profile for a given species if the cross sections for the species are non-zero. Once the wavelength range for which non-zero cross sections exist has been completely absorbed, there is no possible way for the species to be retrieved. In the simplex procedure, the densities of such species are pushed to larger and larger values in an attempt to produce an absorption signature. When this fails, the procedure more or less lets the densities wander, although the "profile" usually follows the general direction of the remaining profiles which can still be retrieved. The CH$_4$ profile also exhibits this behavior below 700 km, the point at which absorption over the wavelength range of its non-zero cross sections is total.

The second feature of interest in the retrieved profiles is the one labelled
"drop-out." This represents a point in the retrieved profile where it makes a sudden drop to lower densities before recovering to the nominal level. This behavior has been investigated and appears to be connected to the location of the line of sight within the atmospheric layer. This hints at a connection with the assumption of constant density within a given atmospheric layer, but further tests are needed. The presence of the "drop-outs" does not seem to adversely affect the retrieval procedure to a large degree, though they can influence the averaging procedure we use to generate the nominal retrieved profiles and their corresponding uncertainties.

The final thing to note about the retrieved profiles is the portion of the C$_2$N$_2$ profile labelled "upper limit." When a species has non-zero cross sections over a wavelength range that is not totally absorbed but there is no signature of the species in the spectrum, the simplex method drives the densities to values that are as large as possible without creating a noticeable absorption feature in the spectrum. As such, the profile may be taken as an upper limit to the number density of the species, albeit a conservative one. This aspect of our retrieval method is more disturbing than the other two because, without the "true" profile to compare against, we might not be able to distinguish an "upper limit" from a valid profile. However, other tests have shown that these profiles are usually characterized by a vertically-constant density structure before changing slope at the point at which the profile becomes valid. Thus, we can generally identify such portions of the retrieved profiles through interpretation of the results. Note that the entire profile could be an "upper limit" if a retrieved species never shows an absorption signature in the data, or that such "upper limit" portions can come and go in a given profile as absorption by the species fades in and out of the data.

With the above caveats, we can confidently use the method we have developed to retrieve number density profiles from the Titan solar occultation data, and we turn now to that task.
CHAPTER 4

TITAN'S UPPER ATMOSPHERIC STRUCTURE

4.1 Retrieving Titan's Atmosphere: The Specifics

Before we discuss the results of the retrieval, there are several issues we should address that are specific to the application of the method of Chapter 3 to the Titan solar occultation. These include the way we handle the “dip” artifact in the light curves, the input solar spectrum, the choice of species to retrieve, and considerations of the uncertainties in the data and subsequent retrieval.

“Dips” and Fits

The “dip” artifact in the longer wavelength light curves (see Section 2.4 and Figure 2.10) presents a difficulty in the retrieval procedure. We must somehow force the procedure to ignore the “dips” because they do not represent true absorption. However, the light curves have been attenuated somewhat during the “dip” range because the lower-altitude ends of the “dips” are at transmissions less than one.

The solution to this problem is to fit the light curves with a smooth function that joins the light curves across the “dips.” Actually, this is somewhat desirable because retrieval methods generally perform better when the light curves are smooth. As such, we fitted not only the longer wavelength light curves with “dips” in them but all the light curves.

The fitting function we used is a double exponential of the form
\[
\frac{I}{I_o}(x) = \exp \{- \exp \{-\alpha(x)\}\}, \tag{4.1}
\]

where

\[
\alpha(x) = \sum_{i=1}^{n-2} a(i) \left( \frac{x - a(n - 1)}{a(n)} \right)^{i-1}, \tag{4.2}
\]

the \(a\)'s are the parameters of the fit, \(n\) is the total number of parameters, and \(x\) is the time/space ordinate of the light curves (i.e., altitude or spectrum number). This function is constrained between the values of zero and one, so it is an ideal form for a light curve.

This form works well for the shorter wavelength light curves but runs into trouble at the longer wavelengths. In addition to the "dip" artifact, we had to deal with the two-level structure in these curves (see Figure 2.10). To overcome this obstacle, we fitted the longer wavelength light curves with a sum of two double exponentials:

\[
\frac{I}{I_o}(x) = a(n) \exp \{- \exp \{-\alpha_1(x)\}\} + [1 - a(n)] \exp \{- \exp \{-\alpha_2(x)\}\}, \tag{4.3}
\]

where

\[
\alpha_1(x) = \sum_{i=1}^{n-5} a(i) \left( \frac{x - a(n - 4)}{a(n - 3)} \right)^{i-1}, \tag{4.4}
\]

\[
\alpha_2(x) = \sum_{i=1}^{n-5} a \left( i + \frac{n - 5}{2} \right) \left( \frac{x - a(n - 2)}{a(n - 1)} \right)^{i-1}, \tag{4.5}
\]

and the other quantities are as before.
We performed the fits using the Marquardt-Levenberg minimization procedure as implemented by Press et al. (1992) in the routine \texttt{mrqmin}. To generate the best fit possible, we varied the total number of parameters over a defined range and fitted the light curve for each total. We then selected the fit with the smallest mismatch to the light curve data as the best fit. For curves fitted with equations 4.1 and 4.2, we varied the number of parameters from three to twelve. For curves fitted with equations 4.3, 4.4, and 4.5, we varied the number of parameters from seven to twenty-five. Generally, five parameters were needed in the first case and eleven in the second. In fitting across the "dips," we aided the fitting routine by replacing the "dips" with straight lines connecting the two sides of the "dip." However, the uncertainties of the actual data were retained.
The results of the fitting procedure are shown in Figure 4.1 for the three light curves we followed through the processing steps in Chapter 2, and the fits are seen to be quite good. This is borne out by the uncertainties in the fits, which we determined using a procedure known as the "bootstrap" method. Based on a Monte Carlo technique, the "bootstrap" method works by generating synthetic light curves using the fit to the data in combination with the data uncertainties. Each synthetic light curve is then fitted in the same manner as the data itself, with the resulting fits being stored. After a specified number of synthetic light curves have been fitted, the stored fits are analyzed and confidence interval curves are selected. We chose to run the procedure 200 times to determine the 10% and 90% confidence limits of our best fits to the light curves. Plotted on the scale of Figure 4.1, these limits are indistinguishable from the best fit for the first two channels and only somewhat different than the fit to channel 111. This is true for nearly all the channels of the spectrum, with only a few fitted a bit worse.

The Solar Spectrum

As an input source spectrum in the retrievals, we use the SC#21REFW reference spectrum of Hinteregger et al. (1981), adjusted to represent the solar spectrum for November 12, 1980, using their model and the appropriate factors. The reference spectrum and adjustment factors were provided by K. Fukui (personal communication, 1996). Conveniently, the Titan solar occultations occurred on a date which falls within the time range for which their model is valid.

The reference spectrum is specified as a series of lines and corresponding fluxes. We have plotted the adjusted spectrum for November 12, 1980, in the top panel of Figure 4.2, while the bottom panel shows the corresponding model Voyager UVS spectrum for the case of the sun being in the center of the slit. Note that in addition to adjusting the reference spectrum to the proper date, we have reduced the fluxes to account for the distance Titan is from the sun (the reference spectrum
Figure 4.2: Model solar spectrum used in the retrieval procedure. It is the SC#21REFW reference spectrum of Hinteregger et al. (1981), modified to the date of the Titan solar occultations. The top panel shows the spectrum as input to the retrieval method, and the lower panel shows the same spectrum as it would be measured by the Voyager UVS. Note that the fluxes have been reduced for the 9.5 AU distance between the sun and Titan.
is applicable to 1 AU). Also note that the continuum level between 1100–1250 Å is an estimate. The reference spectrum has gaps in this wavelength range, but we need something to input to the modeling procedure. Thus, we fill the gaps with a continuum level equal to the minimum value of the spectrum near 700 Å. This should have a negligible effect on the retrievals because the input spectrum is only critical in situations where input spectral lines match up with strong absorption lines. This is not the case for the given wavelength range.

Which Species to Retrieve?

Ideally, we want to retrieve as much information from the occultation data as we can. Thus, we want to include as many species as possible in the retrieval procedure. On the other hand, the more species we include, the larger the uncertainties in the resulting profiles generally are, particularly if the data have large uncertainties. As such, we have to make a trade-off between how many species we can retrieve and how well we want to know the resulting profiles. We have taken several steps to narrow down the species whose density profiles we retrieve from the data.

The first step was to examine the photochemical models. Although we should never force data to fit a particular model, models can be used as guides to what to look for in the data. A species which is prevalent in all three of the photochemical models we have for Titan is a potential candidate for retrieval. Based on this examination, we selected the following species: N$_2$, CH$_4$, C$_2$H$_2$, C$_2$H$_4$, C$_2$H$_6$, C$_4$H$_2$, C$_4$N$_2$, C$_4$N$_2$, HCN, HC$_3$N, H$_2$, N, and H.

Once we had selected these species, we modeled the Titan occultations using atmospheres based on each of the photochemical models. Above the maximum altitude of each photochemical model, we linearly extrapolated the mixing ratio profiles for all but a few species, whose profiles were increasing with height at such a rate that the resulting densities extrapolated to near constant values. For these species, we simply set the mixing ratio above the maximum altitude to that at the
maximum altitude.

We next did two things with these model occultations. First, we ran the model occultations through the retrieval procedure to see how well the input profiles were recovered. By comparing the input and retrieved profiles, we could determine which species might be masked by absorption from other species and, therefore, less likely to provide a useful retrieval. Second, we compared the model spectra to the data spectra to identify features in the model spectra that were clearly not in the data. Based on these two different comparisons, we were able to eliminate $\text{H}_2$, $\text{N}$, and $\text{H}$ as being "non-retrievable" because their absorption is probably masked by that of $\text{N}_2$ and $\text{CH}_4$. We also eliminated $\text{C}_4\text{N}_2$ because it produced an absorption signature that is not observed in the data.

Finally, we did some "quick" models of occultation spectra, in which we varied the total column densities of several species and modeled the resulting spectra. By comparing these against the data spectra, we could determine whether or not a given species produced an absorption signature we see in the data. This test complemented the above one comparing spectra based on the photochemical models because we varied the species included and their density profiles (via the column densities), thereby covering a wider range of possible atmospheres. The conclusions from this test were similar to those based on the photochemical models.

Based on the above tests, we selected nine species for retrieval: $\text{N}_2$, $\text{CH}_4$, $\text{C}_2\text{H}_2$, $\text{C}_2\text{H}_4$, $\text{C}_2\text{H}_6$, $\text{C}_4\text{H}_2$, $\text{C}_2\text{N}_2$, $\text{HCN}$, and $\text{HC}_3\text{N}$.

**What Wavelengths to Use?**

Normally, we would use the entire measured spectrum in the retrieval procedure. Unfortunately, the cross sections in the $\text{N}_2$ band region, which roughly covers 650–1000 Å, are not well known. We examine this in more detail in Section 4.3, but the cross sections tend to yield $\text{N}_2$ densities that are too small. Thus, we must avoid the band region of the spectrum.
The end of the N$_2$ band region at 1000 Å represents the end of the N$_2$ cross sections. Rayleigh scattering cross sections exist longward of 1000 Å, but they are many orders of magnitude smaller and do not come into play. This limits the N$_2$ retrieval to the continuum region shortward of 650 Å, where the cross sections are better defined. This presents a problem, however, because the remaining species have continuum absorption cross sections shortward of 650 Å as well, and they are on the order of the N$_2$ cross sections. Because continua are generally featureless, separating the contributions of each species is difficult unless another region of the spectrum involves band absorption or a significant change in the continuum absorption cross section magnitudes (e.g., the strong edge in the CH$_4$ continuum at 1350 Å). With only the continuum region available for N$_2$, we might be in trouble; however, the structure of Titan’s atmosphere comes to our rescue.

As luck would have it, it appears that there is no significant absorption from CH$_4$ until the N$_2$ continuum region is completely absorbed. This conclusion is reached by comparing the absorption at wavelengths shorter than 650 Å to that at wavelengths between 1000 and 1100 Å. The CH$_4$ cross section has nearly identical values in these two regions, implying that the level of CH$_4$ absorption is equal in the two regions. Because there is no significant absorption in the range 1000–1100 Å before the absorption below 650 Å is complete, we can conclude that the absorption at wavelengths less than 650 Å is due to N$_2$ only. This assumes that there are no other species as abundant as CH$_4$ at these altitudes, which is reasonable.

Thus, we retrieve the N$_2$ density profile from the spectral channels short of 650 Å. The remaining species are retrieved using the channels longward of 1000 Å. We do use the N$_2$ band region between 650–1000 Å in the spectral comparisons of Section 4.3, but it is not used in the retrievals. We also exclude the first and last five channels of the spectrum because of possible edge effects in the processing.
How Uncertain Are Things?

The Titan data are "messy," having required a great deal of processing. Despite a careful consideration of the uncertainties involved, it is possible that they are underestimated. As such, we take a conservative approach to the density retrieval.

To determine the density profiles of the nine species we have selected, we perform a series of twenty retrievals, each with a different starting atmosphere. Each retrieval is run with a simplex tolerance of \(10^{-8}\), a maximum of fifty simplex steps, and a coarse wavelength spacing of 0.5 Å. We then average the twenty retrieved profiles for each of the species to generate the final, nominal profiles. We also determine uncertainties at the 65% level (i.e., roughly the 1-\(\sigma\) level) for each of the average profiles using standard confidence interval methods.

Normally, the starting atmospheres for the retrievals would be reasonable guesses at the actual Titanian atmosphere; however, we have chosen to input atmospheres in which all the number densities are constant with altitude. The reason for this is that it forces the simplex procedure to move away from the initial guess, avoiding any possibility that the simplex goes nowhere because the initial guess is "good enough." Each input atmosphere has a different constant value, but all the profiles within a given atmosphere are the same. These twenty constant values span the range of \(1.0 \times 10^5\) to \(5.0 \times 10^6\) cm\(^{-3}\) in approximately equal intervals.

Solar Disk Considerations

Retrievals performed with a segmented solar disk, both uniform and non-uniform, yielded insignificant differences from those done with a single-segment, uniform disk. The often large uncertainties in the data and correspondingly large variations in the retrieved profiles have likely masked any differential absorption effects in the data. However, the sun's projection in Titan's atmosphere subtended only 6–8 km during the ingress occultation and 15–17 km during the egress. The corresponding image
on the UVS detector spanned only two channels, so differential absorption effects are probably immeasurable in any event. In light of this, all the retrievals presented in the following sections assumed a single-segment, uniform sun.

**Photoabsorption Cross Sections**

An extensive literature search was conducted to find the most up-to-date photoabsorption cross sections available. All the cross sections used in the retrievals are described in Appendix D and illustrated in the figures therein.

### 4.2 The Retrieved Atmosphere

Using the specifics of the Titan solar occultations outlined in the previous section, we ran the retrieval procedure on the Titan data. We present the results of those retrievals and discuss their implications in this section and the next. The two sections are tied together closely, and frequent references are made to one another. To simplify the various literature references we make, we abbreviate them as follows:

- **Y84/87** : Yung et al. (1984)/Yung (1987)
- **T95** : Toublanc et al. (1995)
- **L96** : Lara et al. (1996)
- **S82** : G. R. Smith et al. (1982)
- **Y94** : Yelle et al. (1994)

Note that the retrieved profiles presented in this section have had any obviously "non-retrievable" portions of their curves removed for clarity. The profiles most affected by this are the N\textsubscript{2}, CH\textsubscript{4}, and C\textsubscript{2}H\textsubscript{6} profiles because these species have distinct cut-offs in their cross sections in the wavelength range of the Voyager UVS
spectrinim. In addition, we have removed the uppermost portions of some profiles in which the retrieval was clearly an "upper limit." This is justified because the remaining profile illustrates the trend in the density, and the elimination of these portions allows us to plot the profiles at the highest possible altitude resolution.

In all the figures, the error bars on the density profiles represent the 65% confidence intervals for the retrieved densities. Because these are plotted on a log scale, they appear somewhat "skewed" to the low-density side of the profiles.

4.2.1 N\textsubscript{2} Profiles

In Figure 4.3 we compare the N\textsubscript{2} profiles retrieved from the ingress and egress occultations against the N\textsubscript{2} profiles from the engineering models of S82 and Y94. The S82 profile was computed using the equations and parameters specified in their paper. The Y94 data was provided by D. F. Strobel (personal communication, 1997) and only extends to 1300 km altitude. The measured N\textsubscript{2} density range at 1265 km altitude quoted by S82 is also shown in Figure 4.3 by the black bars.

The immediate observation is that the retrieved N\textsubscript{2} densities are larger than those of S82, though only marginally so for the ingress occultation. Although a more rigorous processing method has been applied to the Titan data to generate the light curves under analysis in this work, the differences between the retrieved profiles and the S82 measurements are likely tied to the portion of the spectrum involved in the retrieval. S82 used a single spectral channel near 725 Å, which falls into the N\textsubscript{2} band absorption region. We confined our retrieval to the continuum region shortward of 650 Å and used several channels of the spectrum. As we discuss in Section 4.3, there is evidence that the N\textsubscript{2} band absorption cross sections are not known well enough to retrieve the N\textsubscript{2} density accurately from that region of the spectrum and that densities so retrieved will be too small. Given that the measured densities from S82 were used in generating their engineering model, the differences between the retrieved profiles and the model are easy to understand.
Figure 4.3: Retrieved N₂ profiles compared against the model of S82 and the recommended engineering model for Cassini of Y94. The bar at z = 1265 km represents the range of N₂ densities measured by S82.
The differences between the retrieved profiles and the Y94 profile are similarly easy to understand. This profile was derived using the S82 measurements (among a number of other constraints), which biases their model to be lower than our retrieved profiles. The densities we have retrieved are 50% (ingress) to 80% (egress) larger than the Y94 profile, but we believe it should be possible to generate a new model which is consistent with the retrieved profiles.

Although it appears as if they are missing, the error bars are plotted in Figure 4.3. They happen to be on the same scale as the “point” symbols and, hence, are not visible. The confidence intervals are tiny for the N$_2$ profiles because we retrieved them assuming only one absorbing species and using a limited range of channels. With little spectral variation and only one species to which to attribute the absorption, the retrieval procedure converged to the same general point in every run. As such, the N$_2$ profiles would seem to be extremely well determined; however, the point-to-point variations in the profiles make this difficult to believe.

We can potentially understand these point-to-point variations through a consideration of the data light curves and their corresponding uncertainties. Because we fitted them with smooth functions prior to the retrieval, the light curves are quite smooth as a function of altitude. The corresponding uncertainties, however, vary in magnitude from spectrum to spectrum and channel to channel. Thus, it is possible that certain channels are weighted more or less heavily in the retrieval as a function of altitude. As the most heavily weighted channel (or channels) varies from spectrum to spectrum, the retrieved density will vary if the channels, taken individually, would yield different densities.

To make this clear, let’s consider a hypothetical situation in which we have two spectral channels, A and B. We assume these “data” are such that channel A would yield densities lower than the actual values if it were the only channel in the retrieval while channel B would yield densities higher than the actual values. For a given spectrum, let’s assume that the uncertainty of channel A is much larger than that of B. In this case, channel B will dominate the retrieval (remember, the
mismatch in equation 3.33 is inversely related to the uncertainty of the data) and the density will be high. Let’s now assume that in the next spectrum the situation is reversed and A dominates the retrieval, yielding a low density. If this sequence repeats itself, the retrieved density can “bounce” between low and high values. In this case, the average through the points is likely a good representation of the actual density profile, but the individual points themselves will be high or low.

There are three instances in which this “high-low” variation might not be observed for a single species retrieval. The first occurs when the uncertainties are approximately equal such that no one channel dominates the retrieval. In this case, the retrieved density profile will be derived roughly from the average of the channels and should be a reasonable approximation to the actual profile. The second instance occurs when the light curves are roughly the same. In this case, it does not matter which, if any, channel dominates the retrieval because all the channels yield approximately the same densities. Note that we are assuming continuum (i.e., relatively featureless) absorption in this example. The final case occurs when many channels are used in the retrieval because it becomes less likely that a channel or few will dominate the retrieval.

If we now try to understand the retrieved Na profiles, we find good agreement between our situation and the hypothetical one outlined above. The ingress light curves show variations across the spectral range used in the retrieval, and their uncertainties show a moderate range of variation from spectrum to spectrum and channel to channel. These variations are generally consistent with the point-to-point variations in the retrieved ingress profile. Near 1275 km altitude, at which point the retrieved profile shows much less variation, the channel-to-channel variation in the magnitudes of the uncertainties is smaller and and the point-to-point variations are damped out. The same is generally true for the egress occultation; however, there is less variation in both the light curves and their uncertainties, consistent with the smaller point-to-point variations in the retrieved egress profile.
4.2.2 CH₄ Profiles

In Figure 4.4 we compare the CH₄ profiles retrieved from the ingress and egress occultations against the CH₄ profiles from the three photochemical models of Chapter 1 (Y84/87, T95, L96) and the recommended engineering model for Cassini of Y94. To facilitate estimation of the CH₄ mixing ratio, we have included an N₂ profile for each occultation. Each profile is the N₂ profile of Y94 scaled to match the levels of the retrieved N₂ profiles. The ingress profile has been scaled by 50% and the egress profile by 80%. The measured CH₄ density ranges quoted by S82 are also shown in Figure 4.4 by the black bars.

There are two things which stand out in this figure. The first is the difference between our measurements and those of S82. This is most likely a result of the improved data processing. We pointed out in Section 1.4 that the optical depth profiles derived by S82 were inconsistent with each other (see Figure 1.3). The newer processing has removed this inconsistency. At the same time, we have considered more species than S82, who limited their analysis to CH₄ and C₂H₂ in the long wavelength channels. Some of the absorption they attributed to CH₄ is probably absorption by other species.

That this might be the case is related to the second feature of Figure 4.4, the decrease of the retrieved profiles relative to the N₂ profiles at the higher altitudes. Methane is lighter than N₂, and it should have a larger scale height if the two species are in diffusive equilibrium or the same scale height if they are well mixed. It is difficult to imagine a scenario in which the CH₄ density actually decreases relative to N₂ this high in the atmosphere. Chemistry is a possibility, but a mechanism is not evident. “Blow-off” or escape of CH₄ is unlikely. The logical reason for the decrease is that the retrieval has assigned some of the absorption due to CH₄ to other species.

We investigated this possibility and found that it is likely the case for the higher altitudes. Above 1150 km, there is very little absorption in the main
Figure 4.4: Retrieved CH$_4$ profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models. Also shown are the recommended CH$_4$ profile of the Y94 Cassini engineering model and the range of density measured by S82. The N$_2$ profiles are scaled versions of the Y94 profile (described in the text).
CH₄ channels of the spectrum (between 1000 and 1100 Å), but there is potentially absorption at longer wavelengths. In the retrieval procedure, the simplex method tries to fit the nominal spectrum, but because CH₄ does not produce the best spectral fit, the absorption is assigned to other species even though CH₄ could provide some of the absorption within the uncertainties. In this case, the other species are C₂H₄, C₂H₆, and C₄H₂, whose retrieved densities near 1150 km are on a par with CH₄'s. The retrieved CH₄ density eventually exceeds those of these species around 1000–1150 km. At these altitudes, the signature of CH₄ is clearly evident in the spectra (see Section 4.3), and the retrieved CH₄ profile is better defined than at higher altitudes. It is above this altitude that the retrieved CH₄ profiles begin to decrease with altitude.

Thus, we see that the retrieval method assigned larger densities to these other species at higher altitudes on the basis of the nominal spectral shape although the absorption could have been attributed to CH₄. This illustrates an important point about occultation analysis procedures: by fitting the spectrum as well as possible, we might produce a physically implausible result even though a physically plausible one is possible within the uncertainties. It also illustrates the importance of understanding the limitations of any method used in scientific analysis and demonstrates the danger of blind acceptance of any result.

Through the above investigation, we can conclude that the CH₄ profile below 1000 km is well retrieved and that the profile above this level should probably be increased to consistent levels. Correspondingly, the C₂H₄, C₂H₆, and C₄H₂ densities should be decreased somewhat, which we will address momentarily. Regardless of this, however, the retrieved CH₄ density will still be less than that of S82, which has implications for the photochemical models and the airglow investigations.

The photochemical models are affected because the CH₄ density throughout the mesosphere must decrease. In addition, the retrieved CH₄ profiles track the N₂ profiles closely, indicating that the two species are well mixed to high altitudes. Unlike the case of a giant planet atmosphere, in which the CH₄ scale height differs
from the background H₂ scale height by a factor of eight, the CH₄ scale height is within a factor of two of the N₂ scale height. Thus, we expect the signature of diffusive separation at the homopause to be more subtle. Based on the retrieved profiles in Figure 4.4, the homopause is not clearly evident but it likely to be at least as high as 1000 km if not higher. This strongly supports the conclusion of Strobel et al. (1992), who found that the homopause must be high in the atmosphere and favored a level near 1025 km, while the photochemical models have placed the homopause lower in the atmosphere. Finally, we note that the retrieved egress profile implies there is less CH₄ at the morning terminator than at the evening terminator, perhaps indicating a diurnal variation in density that is not addressed in the current photochemical models.

The airglow investigations are affected by the new results because less CH₄ means less absorption of the N₂ emissions. This also supports the conclusions of Strobel et al. (1992), who found that the levels of CH₄ consistent with the S82 data were too high to reproduce the airglow observations.

### 4.2.3 C₂H₂ Profiles

In Figure 4.5 we compare the C₂H₂ profiles retrieved for the ingress and egress occultations against the C₂H₂ profiles of the three photochemical models. The measured C₂H₂ density ranges quoted by S82 are also shown in Figure 4.5 by the black bars.

The most important implication of the retrieved C₂H₂ profiles in Figure 4.5 is that they indicate there is much less C₂H₂ in Titan's upper atmosphere than S82 determined. The primary reason for this is the lack of an absorption feature at 1480–1520 Å in our spectra (see Section 4.3). One of the strongest C₂H₂ absorption features is at these wavelengths, and its absence greatly reduces the amount of C₂H₂ we find in Titan's atmosphere.

Why we find no feature at these wavelengths while S82 did may be due
Figure 4.5: Retrieved C$_2$H$_2$ profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models. Also shown are the ranges of density measured by S82.
to several things. First, our more detailed data processing should have yielded better results for the long wavelength channels of the spectra. Second, we used reference spectra taken outside the attenuation region and at the proper spectral shift. S82 used a single reference spectrum for this region, taken from just after the gain change. The effects of absorption, although minimal, were already seen in this spectrum, which means they divided attenuated spectra by an attenuated spectrum. At the same time, the limit cycle motion (see Figure 2.4) was varying rapidly during this phase of both occultations. The corresponding spectral shifts in the attenuated spectra did not match that of the single reference spectrum, and this probably led to the superposition of different absorption features in the ratioed spectra. Given the features we see in our spectra to either side of this wavelength range, it is also possible that they were misinterpreted as C₂H₂ absorption. Finally, because S82 limited their investigation to CH₄ and C₂H₂ in this region, all the absorption that occurred in these long wavelength channels had to be due to these species only.

Whatever the origin of the difference, the effect on the photochemical models is clearly evident: they all overestimate the amount of C₂H₂. Given that the S82 results provided the only constraint for these models in the upper atmosphere, this is understandable. However, it has been difficult for the photochemical models to produce the S82 levels of C₂H₂. Only Y84/87 had any success in reproducing the S82 structure, but their levels fell short. T95 was able to produce a profile consistent with the level but not the structure. Finally, L96 reproduced neither. Y84/87 commented that the most likely explanation for the mismatch is that S82 attributed absorption due to other species to C₂H₂, a strong possibility given that C₂H₂ was the only species besides CH₄ that S82 considered in the relevant wavelength range. T95 and L96 followed Y84/87's example and claimed the same reason for the mismatch. Given our results, this explanation appears to be true, but it is unclear whether the models which couldn't reproduce the high levels of C₂H₂ of S82 can now match the lower levels we find here.
4.2.4 $C_2H_4$ Profiles

In Figure 4.6 we compare the $C_2H_4$ profiles retrieved for the ingress and egress occultations against the $C_2H_4$ profiles of the three photochemical models. There are no previous measurements of the $C_2H_4$ density at these altitudes.

Above 800 km, the three photochemical models have similar structure, though their absolute levels are quite different. The retrieved egress profile is consistent with the photochemical models in terms of structure, and the densities are a particularly good match to those of L96. The retrieved ingress profile, on the other hand, does not match the photochemical models as well, falling off more slowly at higher altitudes. However, we have commented (see the discussion of CH$_4$ above) that the densities at these altitudes are probably overestimated and should be reduced. Such a reduction will "pull" the densities down into a structure consistent with that of the models and the egress profile. As with the egress profile, the L96 model is likely to provide the best overall match to this "reduced" ingress profile.

From 550–800 km, the model profiles possess moderately different structure. In this region, the Y84/87 profile is the best match to the retrieved profiles, having a structure that is approximately vertical. There is, however, a slight hint at some curvature in the retrieved profiles over this altitude range. This might be consistent with the T95 model, but the evidence is weak and the Y84/87 profile has a similar, if abrupt, curvature to it. In addition, the Y84/87 model reproduces the density levels better than the other two models.

Below 550 km, the retrieved profiles begin to increase rapidly. This is more evident in the ingress profile, but the egress shows the turn-up as well. Although the plotted altitude range cuts off the model profiles at 400 km, all three models show a similar turn-up in the $C_2H_4$ profile at lower altitudes. The Y84/87 model starts to increase near 350 km, the T95 model at 250 km, and the L96 model at 300 km. Thus, the increase in the Y84/87 model is closest in altitude to those in the retrieved profiles, providing further support for the Y84/87 model below 800 km.
Figure 4.6: Retrieved C$_2$H$_4$ profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models.
4.2.5 C$_2$H$_6$ Profiles

In Figure 4.7 we compare the C$_2$H$_6$ profiles retrieved for the ingress and egress occultations against the C$_2$H$_6$ profiles of the three photochemical models. There are no previous measurements of the C$_2$H$_6$ density at these altitudes.

At the higher altitudes, the Y84/87 and L96 models tend to bracket the retrieved C$_2$H$_6$ densities in the egress occultation. The same is probably true for the ingress occultation, which is another case where CH$_4$ absorption is potentially assigned to C$_2$H$_6$ and the profile should be “pulled down” to some extent (see Section 4.2.2). Within the uncertainties, both the Y84/87 and the L96 photochemical models are generally acceptable. The T95 model clearly underestimates the C$_2$H$_6$ density at these altitudes; however, it matches both retrieved profiles well at the lower altitudes until the retrieved profiles begin to deviate a little around 500 km.

Near 800 km, both retrieved profiles exhibit a local maximum in the C$_2$H$_6$ density. The ingress profile appears to show a local minimum just prior to the maximum, but this is probably a function of the densities above this level being too high. These maxima are somewhat unexpected given that all three model profiles show a general fall-off with altitude and no features, and they might be indicative of some interesting chemistry in the atmosphere.

Alternatively, the maxima could represent an adjustment of the C$_2$H$_6$ profiles related to the CH$_4$ retrieval. The retrieved CH$_4$ profiles end near 800 km, at which point the CH$_4$ absorption is complete. C$_2$H$_6$ and CH$_4$ have similar cross sections (see Figure 3.1), but CH$_4$ is generally more abundant so the C$_2$H$_6$ absorption is usually masked to some extent by CH$_4$ absorption. When CH$_4$ can no longer be retrieved, it is possible that the C$_2$H$_6$ signature is more obvious and the retrieval adjusts itself to reflect this. Given that the C$_2$H$_6$ profiles appear continuous across the region of the local maxima, however, it is difficult to conclude that this is actually the case.
Figure 4.7: Retrieved C$_2$H$_6$ profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models.
4.2.6 C₄H₂ Profiles

In Figure 4.8 we compare the C₄H₂ profiles retrieved for the ingress and egress occultations against the C₄H₂ profiles of the three photochemical models. There are no previous measurements of the C₄H₂ density at these altitudes.

The Y84/87 profile provides an excellent match to the structure and level of the retrieved ingress profile at high altitudes. At lower altitudes, the Y84/87 model is still a reasonable match to the structure of the retrieved ingress profile, but the densities themselves are more than an order of magnitude too high. Between 600 and 800 km, the T95 and L96 models are close to the retrieved ingress profile, but they are generally poor matches overall.

The situation is similar for the retrieved egress profile at the lower altitudes, with the Y84/87 model providing a reasonable structural match. However, the egress profile is nearly vertical at the higher altitudes. This hints at a possible "upper limit" in the profile at these altitudes, and it also represents another potential source of incorrectly assigned CH₄ absorption (see Section 4.2.2).

There is, however, a second possibility related to this "upper limit." From spectral evidence we discuss in Section 4.3, it is possible that the C₄H₂ profile is underestimated at low altitudes and overestimated at high altitudes. This is another instance in which the spectral match might be better for one species than another even though the first species could provide an acceptable match within the uncertainties. In this case the other species is C₂N₂. Replacing some of the retrieved C₄H₂ density at high altitudes with C₂N₂ and some of the C₂N₂ at low altitudes with C₄H₂ might provide a better match to the T95 and L96 models for both species while still providing an acceptable spectral match; however, it is unlikely to solve the entire problem. Given that the retrieved ingress profile is already a reasonable match to the Y84/87 model and that the spectral evidence is weaker for the ingress occultation, only the retrieved egress profile is likely to "benefit" from such a density "swap;" however, the ingress profile could be altered as well.
Figure 4.8: Retrieved C₄H₂ profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models.
4.2.7 C$_2$N$_2$ Profiles

In Figure 4.9 we compare the C$_2$N$_2$ profiles retrieved for the ingress and egress occultations against the C$_2$N$_2$ profiles of the three photochemical models. There are no previous measurements of the C$_2$N$_2$ density at these altitudes.

Of the nine species we retrieved, the C$_2$N$_2$ profiles represent perhaps the worst matches between the model and retrieved profiles. The primary reason for this is not related to the retrieval itself but instead is connected to the relevant reactions in the photochemical models. As noted by Yung (1987), our understanding of the rates for reactions involving carbon-nitrogen species such as C$_2$N$_2$ and C$_4$N$_2$ is poor, and the uncertainty in these rates is often large. The most widely accepted rates (i.e., the "nominal" rates) for these reactions yield more C$_4$N$_2$ than C$_2$N$_2$, but different assumptions about the chemistry lead to rates which yield more C$_2$N$_2$ than C$_4$N$_2$.

Given the uncertainty in the rates, Yung presented models for two different sets of reaction rates, the "nominal" one and a secondary set which reversed the yield of C$_2$N$_2$ and C$_4$N$_2$. Because tests (see Section 4.1) showed no sign of C$_4$N$_2$ absorption in the data, we have plotted the Y84/87 profile for the secondary set of rates, the one which yielded the most C$_2$N$_2$. The models of T95 and L96, however, used the "nominal" rates only; therefore, their profiles are somewhat lower in comparison.

As we see in Figure 4.9, the T95 and L96 models are very poor matches to the retrieved profiles. The Y84/87 model, on the other hand, does a good job of matching the overall structure of the retrieved profiles, particularly for the ingress occultation. The egress profile is a slightly worse match, but this is exaggerated somewhat by the portion of the retrieved profile above 950 km, which tends to be vertical and is probably another instance of an "upper limit." Overall, the reasonably good agreement in shape between the Y84/87 profile and the retrieved profiles supports Yung's conclusions about possibly "non-nominal" reaction rates
Figure 4.9: Retrieved C$_2$N$_2$ profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models.
for the carbon-nitrogen species.

Finally, as we mentioned in the discussion of the $C_4H_2$ profiles (see Section 4.2.6), it is possible for some of the $C_2N_2$ and $C_4H_2$ absorption to be incorrectly assigned (spectral evidence is presented in the Section 4.3). However, any correction that might be necessary will not reduce the $C_2N_2$ densities to the levels predicted by the T95 and L96 models. A “corrected” profile will still be on the order of the Y84/87 profile, and the conclusion regarding the reaction rates is unchanged.

4.2.8 HCN Profiles

In Figure 4.10 we compare the HCN profiles retrieved for the ingress and egress occultations against the HCN profiles of the three photochemical models. Measurements of the HCN density at the low end of the altitude range of the retrieved profiles have been made by Tanguy et al. (1990) and Hidayat et al. (1997), and these are compared to the retrieved profiles in Figure 4.11.

Of the three photochemical models, the Y84/87 and T95 models provide fair matches to the retrieved HCN profiles. The overall shape of the Y84/87 profile appears to be more in line with that of the retrieved profiles, but the T95 model is within the uncertainties over much of the altitude range. The L96 model generally underestimates the HCN densities except for the lower altitudes of the retrieved egress profile. We note, however, that the slope of the L96 profile is in good agreement with that of the retrieved profile for the ingress occultation below 650 km.

The Y84/87 model best matches the retrieved profiles at the high and low altitudes, particularly for the egress occultation. The largest deviations occur at the middle altitudes between 700–900 km. It is interesting to note that the deviations are in opposite directions for the two occultations, but this is partly a function of the altitude at which the retrieved HCN profiles show the “zig-zag” — between 700–800 km for the ingress and 800–900 km for the egress. This is also the altitude range over which the $C_2H_6$ profiles showed the local maxima (see Figure 4.7). This
Figure 4.10: Retrieved HCN profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models.
Figure 4.11: Retrieved HCN profiles compared against the profiles of the Tanguy et al. (1990) and Hidayat et al. (1997). The dashed and dotted lines represent the uncertainty in the Hidayat et al. and Tanguy et al. data, respectively.
may be coincidence, but the chemical relationships between the two species should be investigated to see if there is a connection. Finally, we note that the HCN profile of Y84/87 is the one Yung (1987) computed using the secondary reaction rate set, but the differences between the HCN profiles calculated with the two sets are much smaller than in the case of the \( \text{C}_2\text{N}_2 \) profiles.

In comparing the retrieved HCN profiles to the measured profiles in Figure 4.11, we see that the retrieved profiles fall in between the two nominal measurements. In the ingress occultation, the retrieved profile tends toward the nominal Tanguy et al. profile, while the egress profile closely follows the Tanguy et al. lower limit. If the ingress profile increased less dramatically at the lowest altitudes, it would also tend to follow the Tanguy et al. lower limit. This is potentially the case because the spectral evidence for HCN at these low altitudes is weak in the ingress occultation, and the density profile might increase in this range as it becomes "non-retrievable" (see Section 3.6). This is interesting to note because this lower limit is generally an extension of the measured HCN profiles below 200 km. Both the Tanguy et al. and Hidayat et al. measurements make an abrupt change of direction at this altitude, and we must wonder whether or not this change actually occurs.

4.2.9 \( \text{HC}_3\text{N} \) Profiles

In Figure 4.12 we compare the \( \text{HC}_3\text{N} \) profiles retrieved for the ingress and egress occultations against the \( \text{HC}_3\text{N} \) profiles of the three photochemical models. As with HCN, the Y84/87 profile was computed using the secondary reaction rate set, but the differences are small. There are no previous measurements of the \( \text{HC}_3\text{N} \) density at these altitudes.

None of the model profiles provides a good match to the retrieved \( \text{HC}_3\text{N} \) profiles. It is possible that the retrieved profiles are actually "upper limits" at the high altitudes because the spectral evidence for its presence is not strong. At the lower altitudes, where the spectral evidence is perhaps stronger, the densities could
Figure 4.12: Retrieved HC$_3$N profiles compared against the profiles of the Y84/87, T95, and L96 photochemical models.
be underestimated owing to overestimation higher in the atmosphere. The \textit{total} column density is what drives the retrieval, so a substantial overestimation of the densities in the high altitudes might lead to an underestimation of the densities at the lower altitudes. This would have the effect of skewing the retrieved profile to the vertical, a structure the retrieved HC$_3$N profiles tend to exhibit. As long as the "upper limit" portions of the retrieved profile are limited in extent, this underestimation should not be a problem.

The general "verticality" of the retrieved profiles suggests that the HC$_3$N densities are not particularly well retrieved. If we limited the extent of the overestimation by forcing the densities to lower values at the higher altitudes, we might see the profile in the lower altitudes shift to higher densities, which would be more in line with the photochemical models. However, it seems unlikely that any such correction would bring the retrieved profiles up to the levels required by models.

4.2.10 The Thermospheric Temperature

The temperature retrieval procedure we described in Section 3.5.8 failed to yield a realistic temperature profile. We discuss this further in Sections 4.4 and 5.2. While this has a minimal effect on the density retrievals, it primarily leaves us without any temperature information. We can, however, determine the thermospheric temperature directly from the retrieved N$_2$ profiles without developing a new method of retrieval.

To do this, we generate a series of model density profiles using equations 3.15 and 3.16 and varying the temperature from 130 to 200 K. We then determine which of these profiles best fits each of the retrieved N$_2$ profiles using a straightforward rms calculation. The temperatures corresponding to these best-fit profiles are the thermospheric temperatures for the two occultations.

To generate the model profiles, we make several assumptions. First, we assume Titan's thermosphere is isothermal because the above equations were derived
for an isothermal atmosphere. Second, we assume the atmosphere is in diffusive
equilibrium because the homopause is probably near the 1000–1100 km altitude
level (see Section 4.2.2) and the retrieved N₂ profiles go no lower than 1200 km.
Thus, the mass \( m \) in equation 3.16 is that of N₂ only. Finally, we assume the
"critical level" occurs at the \( \tau = 1 \) level for the N₂ continuum absorption from
which the N₂ profiles were retrieved. This is at 1265 km for the ingress occultation
and 1280 km for the egress. This choice is somewhat arbitrary, but it is acceptable
because we only need to be close to the actual level for the equations to be valid.

The results of this procedure are displayed in Figure 4.13. For each occultation,
the retrieved N₂ profile is shown along with the best-fit model profile and two
limiting profiles, which were determined visually as bracketing the range of accept-
able fits to the retrieved profiles. The temperatures corresponding to each of the
model profiles are indicated, with \( T = 150 \pm 10 \) K for the ingress and \( T = 155 \pm 10 \) K
for the egress. These are significantly lower than those calculated by S82, who found
\( T = 176 \pm 20 \) K for the ingress and \( T = 196 \pm 20 \) K for the egress. Consistent with the
S82 analysis, we find that the ingress and egress temperatures are slightly different;
however, we find a difference of only 5 K instead of 20 K. Given the closeness of
our two temperatures and that they are well within the uncertainties, we conclude
that a temperature asymmetry is unlikely.

Because the thermospheric temperatures of S82 have been used in models
of the mesospheric temperature profile as well as the photochemical models, the dif-
ferences between their temperatures and ours have far-reaching implications. HCN
rotational line cooling is relatively efficient on Titan, so it may be a simple matter
to bring the radiative transfer models in line with the lower temperatures. However,
we note that the HCN profile determines the level of HCN cooling, and prior to our
analysis the profile was only available from models. In addition, the hydrocarbons
are also sources of cooling, and our analysis has provided new information on their
profiles. Thus, detailed modeling is necessary to determine whether the retrieved
profiles and temperatures yield a consistent model of the middle atmosphere.
Figure 4.13: Model $N_2$ profiles for various temperatures compared to the retrieved $N_2$ profiles. The middle (solid) profile in each case is the best-fit to the retrieved profile. The other two (dashed) profiles represent the limits of the models which provide a moderate fit to the retrieved profile. The temperature of each model profile is indicated.
4.3 Comparisons of Data and Model Spectra

In this section, we compare data spectra at several altitudes to the corresponding spectra modeled using the retrieved atmosphere and the three photochemical models. The purpose of this comparison is to establish the spectral evidence for various species as well as to point out the shortcomings of the photochemical models. In addition, we examine features that could lead to a misassignment of absorption such as that we have potentially identified for C$_2$N$_2$ and C$_4$H$_2$.

In each comparison figure, the left column of plots pertains to the ingress occultation and the right column to the egress occultation. There are six altitudes at which we compare the spectra, so the comparison between the data and a given model spans two figures. Note that we have chosen the altitudes to illustrate the changes in absorption rather than spacing them at regular intervals.

In all cases, the data are represented by the circles, the data uncertainties by the vertical lines, and the model spectrum by the solid line. The data spectra shown are actually the fits to the data as described in Section 4.1; however, the uncertainties are the true data uncertainties determined in the processing of Chapter 2. With the exception of the 1141/1142 km spectra, which fall into the "dip" region of the light curves, the fitted spectra are approximately the same as the actual data spectra owing to the high quality of the fits. We plot the fitted spectra because they are what we actually used in the retrievals.

To model spectra using the photochemical models, the profiles in these models had to be extended beyond their published upper limits. We used linear extrapolation in log(density)-altitude space to accomplish this for each species with the exception of those whose density increases relative to N$_2$ with altitude (CH$_4$, H$_2$, N, H). These species extrapolated to nearly constant densities, so we instead set the mixing ratio constant above the highest altitude of the models, allowing the densities to fall off with the N$_2$ scale height. We note that this leads to an underestimation of the column densities of these species when we model the occultation spectra;
however, because the models already provide too much absorption, using more accurate profiles would only exacerbate this problem.

In comparing the various spectra, we break the spectrum up into three regions. The first covers approximately 600–1000 Å, the second 1000–1400 Å, and the third 1400–1670 Å. This breaks the spectrum up into roughly an N₂ region, a CH₄ region, and an “everything else” region. There are overlaps, of course, but these are the dominant absorbers in each case. It helps to refer to Figure 3.1 in the following discussions.

4.3.1 Data and Retrieved Atmosphere Model Spectra

Figures 4.14 and 4.15 compare the data spectra to spectra modeled using the retrieved atmosphere profiles shown in Figures 4.3–4.10 and 4.12.

1318/1319 km

In the first pair of plots, we are primarily concerned with N₂ absorption. N₂ continuum absorption covers the range 600–650 Å, and N₂ band absorption covers the range 650–1000 Å. This can be seen in Figures 3.1 and D.1, which display the N₂ cross sections. The continuum region actually extends to shorter wavelengths, but we did not use the first five channels of the spectrum in the retrieval (see Section 4.1) and have eliminated them from the plots.

As we can see in Figure 4.14, neither of the model spectra match the 600–1000 Å region of the data spectra well. While the overall structure is generally in agreement with the data (the band features near 750, 875, and 950 Å are seen in the data though they are a bit washed out compared to the models), the level of the models is lower than the data over most of the region. The band feature near 675 Å is less obvious, but it falls in the range with the greatest uncertainties.
Figure 4.14: Comparison of data and model spectra: retrieved atmosphere. In this figure and the following ones, the data spectra are plotted as circles, the 1-σ uncertainties as vertical lines, and the model spectra as solid lines. The altitudes correspond to the point of closest approach of the line of sight.
Figure 4.15: Comparison of data and model spectra: retrieved atmosphere (continued).
The reason for this mismatch is the same as the reason we did not use the \( N_2 \) band absorption region in the retrieval: we don't know the \( N_2 \) band absorption cross sections adequately. If we look at Figure D.1, the inset shows an example of the high-resolution \( N_2 \) band absorption cross sections, which are generally high peaks separated by regions of near-zero absorption. When these band systems are measured at low resolution, the various lines are blended together, lowering the peak absorption and filling in the regions between them. In addition, instrumental line shape functions get blended into the measured cross section data. In fact, the cross sections in the inset are actually sharper than shown because the instrumental function has not been deconvolved from them. The net result of the measurement process is that the cross sections in the band absorption region are "short and squat," as can be seen in a comparison of the inset of Figure D.1 to the main plot of that figure. When we model the absorption spectrum with such cross sections, we end up with too much absorption in the band region and the model spectrum is lower than the data spectrum.

The continuum cross sections, on the other hand, are easier to measure and are better defined because of the lack of any sharp line structure. As such, we limited ourselves to the continuum region from 600–650 Å in retrieving the \( N_2 \) density profiles. As we can see in the first set of plots in Figure 4.14, the model spectra match the data spectra well over this range, indicating that the retrieved \( N_2 \) densities are good. A slight mismatch between the data and model does exist in the ingress plot, but it likely occurs because the model spectra are generated using the full retrieved atmosphere. The retrieval of the species other than \( N_2 \) began at an altitude of roughly 1150 km, so these profiles had to be extrapolated to the higher altitudes. If the extrapolation is a bit off, we could easily generate more absorption than is necessary. This suspicion is supported by the absorption near 1000–1100 Å, a region in which the cross sections for the non-\( N_2 \) species are similar in value to their cross sections in the 600–650 Å region. The 1000–1100 Å absorption is unnecessary within the large uncertainties, which hints that the extrapolated density profiles are perhaps not optimal. The mismatch in the ingress \( N_2 \) continuum region is consistent
with the level of absorption near 1000–1100 Å, and elimination of the absorption near 1000–1100 Å by adjustment of the extrapolated density profiles would probably eliminate the mismatch at the same time.

Our choice of the continuum rather than the band absorption region for the N₂ retrieval explains why the N₂ densities we retrieve are larger than those of S82 (see Figure 4.3). They used a single spectral channel near 725 Å to retrieve N₂ and this wavelength falls into the band region. From the plots, we can see that we’d need less N₂ to match that wavelength of the spectrum in the ingress occultation, which is the one that S82 primarily used for their analysis. However, reducing the N₂ density to a level such that the band region of the data spectrum is matched by the model spectrum results in a serious mismatch in the continuum region. Because the continuum cross sections are better understood, this is unacceptable, and we are confident in our results. We note that the situation is not as clear for the egress occultation, but this region of the egress data spectrum is unreliable and a valid comparison cannot be made. We discuss this problem in detail for the 1142 km spectrum, in which it is most pronounced. Finally, we note that the uncertainties in the data spectra are larger in the region used by S82, making that particular wavelength range a poor choice for retrieving the N₂ density.

With the subject of N₂ absorption settled, we now consider the rest of the spectrum. As we commented in Section 4.1, there is no significant absorption between 1000–1100 Å within the uncertainties. This is why we determined that the N₂ and CH₄ densities could be retrieved separately even though there is overlap of the cross sections in the N₂ continuum region. What little absorption does exist between 1000–1100 Å in the model spectra probably results from the potentially non-optimal extrapolation of the retrieved density profiles for the non-N₂ species.

Past 1100 Å, there are a number of possible absorptions that are not matched by the model spectra. In this wavelength region, the absorptions are due to species other than N₂. As we discussed above, the retrieval of these species began near 1150 km and the profiles were extrapolated to the higher altitudes. The lack of
features in the model spectra is, perhaps, further indication that this extrapolation could be improved because several species could generate the features observed in the data. However, in doing so, they would also generate features at other wavelengths that are not observed. Alternatively, the features in the data spectra are generally weak given the uncertainties and may not be real. Only the feature near 1350 Å in the egress spectrum falls below the model spectrum level when the uncertainties are considered. Given the persistence of the features in the spectra at lower altitudes, however, their reality seems to be confirmed. As such, the probable explanation is that the extrapolated density profiles need to be adjusted to match features which are potentially reduced within the levels of the uncertainties.

1141/1142 km

By 1141/1142 km altitude, the N₂ continuum region is completely absorbed (complete absorption actually occurs closer to 1200 km). The region below 750 Å is effectively completely absorbed as well. This does not appear to be the case for the egress occultation, however, because of anomalous data. The egress occultation light curves for the spectral channels covering the 650–750 Å range take an unrealistic turn at the gain change and decrease very slowly from that point on. The structure of the light curves is clearly unrelated to the structure of the N₂ band absorption, regardless of the problems we mentioned with those cross sections. No explanation for this anomalous behavior has been found, but from experience we know that the light curves are in error and have chosen to ignore them. Because we do not use them in the retrievals anyway, this has no effect on the density profiles.

Between 750–1000 Å, the model spectra continue to be low relative to the data. This is primarily because of the band absorption cross section problems we discussed above, but absorption by other species is making its presence known now as well. We can see this in the structure of both data and model spectra longward of 1000 Å. All the species under consideration have non-zero cross sections below
1000 Å, so they will contribute some amount to the absorption at those wavelengths. Because these species exhibit continuum absorption below 1000 Å, their contribution to the region is less suspect, and the N₂ band absorption is still the problem.

Longward of 1000 Å, the structure in the data spectra is more apparent than in the plots for 1318/1319 km. We can now see where features lie and indicate which species might be involved. A possible feature covering 1000–1100 Å does not fit the change in the CH₄ cross section but is consistent with C₂H₄ and C₂N₂. A series of broad features covers the range from 1150–1400 Å and might be caused by a combination of any of the retrieved species except N₂, CH₄, and C₂H₆. N₂ doesn't absorb at this wavelength, and the cross sections for the other two are too flat. Given the lack of a strong feature near 1500 Å, we can also rule out C₂H₂. A feature centered on 1450 Å could be due to C₄H₂, HCN, or HC₃N. The last two features, covering 1525–1650 Å, must be due to either C₄H₂ or C₄N₂.

The model spectra are fair matches to the data at these altitudes, but they could be improved. This might be a function of the photoabsorption cross sections, many of which represent band absorption and could be invalid at the temperatures in Titan's atmosphere. It might also be related to the retrieval procedure, which generally finds the best numerical rather than physical match to the data. Within the uncertainties, we could potentially match the overall shape of the data spectra better with different atmospheres, yielding a slightly worse numerical match in the process. The features are still weak enough, however, that a serious discussion of changes is not warranted.

1021/1022 km

As we move deeper in the atmosphere, we continue to have the mismatch in the N₂ band region. This is still primarily a function of the problems with the N₂ band absorption cross sections, but other species are definitely contributing to the absorption and might be involved in the mismatch to some extent.
CH$_4$ dominates the absorption from 1000–1400 Å in the ingress occultation as evident from the large "bite" taken out of the spectra. Because the CH$_4$ cross sections peak between 800–1000 Å, it has a substantial effect in that range as well. A CH$_4$ "bite" is also present in the egress spectra, but it is smaller than in the ingress occultation. This is the primary reason that the retrieved CH$_4$ densities for the egress occultation are lower than in the ingress occultation.

A problem common to both occultations is the peak near 1100 Å. This is most pronounced in the egress spectrum, but it is present in the ingress as well. We can see in the plots that the model spectrum is not a particularly good match to this peak. The CH$_4$ cross sections are generally flat at these wavelengths, so the presence of the peak indicates that a species other than CH$_4$ plays a major role in the absorption in this region. An examination of the photoabsorption cross sections in Appendix D fails to reveal a good candidate, which leads to several possibilities. The peak could be due to a combination of species, with C$_2$H$_4$ and C$_2$N$_2$ being potential candidates. We might need to consider an additional species, though it is not obvious what this would be. The photochemical models yield a small peak at these wavelengths (cf. Figure 4.18), so it is possible for a rearrangement of the densities to yield a better match. The uncertainties in the data are larger in this region, so the peak may also be somewhat reduced in reality. Whatever its origin, the peak remains an outstanding problem in matching the data spectra.

Turning to wavelengths longward of 1400 Å, we see that the features we observed in the previous plots have deepened over the intervening altitudes, which allows us to discuss the model spectra in greater detail. We can now see why we believe the C$_4$H$_2$ densities might be overestimated at high altitudes and the C$_2$N$_2$ densities underestimated (see Section 4.2), particularly in the egress plot. The features from 1525–1650 Å must be due to either C$_4$H$_2$ or C$_2$N$_2$, the only species with the proper structure in their cross sections. However, C$_4$H$_2$ also has large cross sections at 1400 and 1450 Å. Comparing the model egress spectrum to the cross section data in Figure 3.1, we can see that C$_4$H$_2$ is primarily responsible for the
structure in the egress model spectrum. This has led to the poor match at 1400 Å in the egress plot.

If we reduced the amount of C₄H₂ and upped the amount of C₂N₂, we would probably have a better match in this region of the spectrum. Increasing C₂N₂ might also help with the mismatch at the 1100 Å peak. On the other hand, C₂N₂ provides no absorption feature near 1450 Å, requiring something else to provide the feature there. HCN and HC₃N are the only other candidates besides C₄H₂ for this, but the HCN feature is weak and the HC₃N feature is broad. This feature is the most difficult one to match in the data and hints at the possibility of an unknown species or, perhaps more likely, the possibility of poorly known cross sections for C₄H₂, HCN, and/or HC₃N at these wavelengths.

It is also possible (and likely) that any changes we make in the densities of these species will change the spectrum at other wavelengths such that the overall match to the data is worse. We cannot make changes in one wavelength region without assessing the changes they introduce elsewhere. The goal is to find the best overall match to the spectrum, and this necessarily involves trade-offs.

935/936 km

By 935/936 km, we see complete absorption of the N₂ band region in the ingress spectrum, though there is still some amount of transmission in this region of the egress spectrum. This is probably a result of the lower CH₄ densities in the egress occultation, though the mismatch between the data and model egress spectra is still caused by the N₂ cross section problem.

Between 1000–1400 Å, CH₄ continues to dominate the attenuation in both occultations, and the ingress levels remain higher than those in the egress. Whereas they had pronounced signatures in previous spectra, the other species now seem to provide small perturbations to an overall CH₄ absorption spectrum at these wavelengths. In fact, the absorption features we attributed to these species seem less
prevalent in these spectra. This might be a visual effect caused by the smaller uncertainties in the data spectrum, but the retrieved profiles for the species responsible for these features tend to turn down to lower density levels by this point, indicating that the features actually have lessened somewhat.

Longward of 1400 Å, the absorption features seem to have "bottomed out" in that they are not increasing in depth as they were previously. Instead, the overall level from 1400–1670 Å appears to be decreasing while the features remain at the same depths relative to the overall level. The model spectra match the data in this wavelength region about the same as in the 1021/1022 km plots, though the mismatch in the ingress spectrum near 1400 Å is more pronounced at this altitude. The evidence still indicates a possible excess of C₄H₂ relative to C₂N₂, but the entire spectrum has to be considered and, in general, the rest of the spectrum is a good match structurally.

698/698 km

By 698 km, the data spectra are completely absorbed short of the CH₄ edge near 1350–1400 Å and we can no longer determine the CH₄ density. In addition, this begins to limit our ability to separate the contributions to the absorption from the other species because the wavelength range over which various features can be compared has been reduced substantially. Nevertheless, the remaining features are strong enough to allow our retrieval to proceed to even lower altitudes with good results.

The overall match of the model and data spectra is now excellent over the entire available wavelength range. A primary factor in this is the change in the structure near 1400 Å, which we are now able to match. Why the data spectra changed in that wavelength region is difficult to determine, but two possibilities come to mind. The first is that the atmosphere has changed such that the feature is simply gone. The second is that the "dip" artifact in the long wavelengths came
into play at previous altitudes. The 698 km spectra are well beyond the “dip” feature in the light curves, so the fitted light curves used in the retrievals are no longer a “guess” at the true attenuation but are representative of it. However, the 935/936 km spectra are also from the “post-dip” part of the light curves (though closer to it), so the disappearance of the feature in the data spectra is unlikely to be due only to an avoidance of the “dip.”

The strongest absorption signature in the data is that of C₄H₂, which provides the features between 1550–1650 Å as well as some of the features short of that range. The presence of other species is more difficult to see in the spectra, but from the profiles we know that several of them contribute at this altitude. These include C₂N₂, which can make up some of the 1550–1650 Å features, and HCN and HC₃N, both of which have absorption features in the 1400–1500 Å range. Finally, the absorption edge at 1400 Å is pushed to the right a little relative to the CH₄ edge, indicating that C₂H₆ is at work.

469/470 km

The final set of plots shows we are still getting a fair amount of flux through the atmosphere even at relatively deep levels. The feature at 1550–1650 Å is still observed though it is somewhat weaker in the ingress occultation. The C₂H₆ absorption edge continues to shrink the wavelength range on the left and has more or less erased the absorption features short of 1550 Å. As the remaining wavelength region continues to shrink, our ability to infer densities from the data is correspondingly reduced. We can still see the absorption features that we have followed throughout the atmosphere, but the ability of the retrieval procedure to identify the correct species is gradually being weakened at the lower altitudes. Despite these difficulties, however, the match to the data is remarkably good at these altitudes, and the retrieved densities should be reasonably well determined.
4.3.2 Data and Photochemical Model Spectra

In the previous section we saw how well the retrieved atmosphere matched the data. We now turn to the photochemical models to see where they succeed and where they fail in matching the data. Figures 4.16–4.21 compare the data spectra to spectra modeled using the Y84/87, T95, and L96 models.

1318/1319 km

Given that all three models used N₂ profiles derived from the S82 analysis, we would expect the model spectra to show less absorption in the N₂ continuum region than the data spectra because the S82 analysis yielded smaller N₂ densities than we have determined. Instead, we see just the opposite in the ingress spectra for the three photochemical models, while the egress spectra are all reasonably good matches. Taking CH₄ absorption into account, however, provides an answer to this. The three models used CH₄ profiles which were also derived from the analysis of S82, who determined larger CH₄ densities than we have. Thus, in the ingress spectra, the lower N₂ density has been offset by the larger CH₄ density such that the model spectra show more absorption than the data. In the egress spectra, this same offset occurs, but the differences between the S82 and our N₂ densities are larger (we find more N₂ in the egress occultation than in the ingress), and the CH₄ absorption only brings the spectrum level down to that of the data rather than below it.

As with the retrieved atmosphere model spectra, none of the photochemical model spectra matches the N₂ band region, but this is expected on the basis of the problems with the cross sections. The larger CH₄ densities in the photochemical models have simply exaggerated the mismatch.

Beyond the N₂ band region, we continue to see the effects of too much CH₄. The absorption between 1000–1400 Å is due solely to CH₄ in the photochemical models. While the model levels are on a par with some of the data points, the...
Figure 4.16: Comparison of data and model spectra: Y84/87.
Figure 4.17: Comparison of data and model spectra: Y84/87 (continued).
Figure 4.18: Comparison of data and model spectra: T95.
Figure 4.19: Comparison of data and model spectra: T95 (continued).
Figure 4.20: Comparison of data and model spectra: L96.
Figure 4.21: Comparison of data and model spectra: L96 (continued).
overall level of absorption is too high in the model spectra, indicating that their CH$_4$ densities are too high. Besides the CH$_4$ absorption, there does not appear to be any significant absorption beyond 1000 Å. This is marginally consistent with the data at these altitudes given their large uncertainties, though an adjustment of the photochemical models at these altitudes could possibly yield a match to some of the potential features.

1141/1142 km

At 1141/1142 km, we see that the photochemical models continue to have too much CH$_4$ absorption, as evidenced by the magnitude of the CH$_4$ “bite” in the model spectra relative to that in the data. At the same time, other species are beginning to make their presence known. The C$_2$H$_2$ feature centered near 1500 Å is clearly observed in the Y84/87 spectra and is present in the T95 and L96 spectra to a lesser degree. Beyond this, however, we cannot specifically identify the signature of another species, though “wiggles” in the model spectra suggest they are there. In particular, we note the presence of the “bump” feature near the 1100 Å peak in the data. Understanding this “bump” might provide a clue to the origin of the peak, which we were unable to match in the retrieval procedure (see previous section).

1021/1022 km

As we move deeper in the atmosphere, the CH$_4$ density in the photochemical models remains too high, though not to the same degree as before. For example, the L96 model is only moderately off for the ingress data. In fact, we might even state that the structure of the model spectra between 1000 and 1400 Å is slightly better than that of the spectra modeled using the retrieved atmosphere. This observation supports the argument that the retrieval procedure finds the best numerical rather than physical match.
At the longer wavelengths, the photochemical models continue to fit the data poorly. The C$_2$H$_2$ feature is becoming increasingly large; however, this is simply a result of trying to match the S82 measurements. The L96 model shows the smallest C$_2$H$_2$ feature, but we have already shown (in Section 4.2.3) that they either couldn’t reproduce the S82 results or chose not to. There are hints of absorption at other wavelengths beyond 1400 Å in the model spectra, but none of them comes close to matching the features in the data spectra.

935/936 km

By 935/936 km, the story with the CH$_4$ density has changed. All three models have too much CH$_4$ to match the egress occultation, but the L96 model now has too little CH$_4$ to match the ingress occultation. The T95 model has close to the right amount, though it still slightly overestimates the density. We should note, however, that these two models fail to reproduce the structure in the longer wavelengths, meaning they need more absorption by other species. The increased densities for these species would likely push the model spectra below the data in the 1000-1400 Å region, making any conclusions regarding the CH$_4$ density less valid.

The overall structure in the 1000-1400 Å range is generally good for all three models. In the 1400–1670 Å range, it continues to be poor. The Y84/87 does the best at matching the structure of the 1525–1650 Å feature, but the level of absorption is too high in this model. The T95 and L96 models do a better job with the level, but they do not provide nearly enough absorption beyond 1525 Å. None of the models matches the 1400 Å feature, but we have commented on our inability to match this with the retrieved atmosphere and this feature remains somewhat of a mystery. All three models continue to have too much C$_2$H$_2$ absorption.

As a final note on these spectra, we noticed that if the Y84/87 spectra were shifted to the left by 40–50 Å, that model would appear to produce the structure in the longer wavelengths quite well. Thinking we might have made an error in
the spectral shifting during the modeling process, a thorough check of this was performed, and we determined that the shifting has been handled properly. The seeming match in the Y84/87 spectrum on shifting is therefore coincidental, though it might provide clues to the origins of the long wavelength features that hitherto we may have been unaware of.

698/698 km

At 698 km altitude, we see one of the biggest shortcomings of the photochemical models: they all produce too much absorption at the lower altitudes. The T95 spectra are completely absorbed by this point. The Y84/87 spectra are close to complete absorption, though the structural match to the data is reasonably good. The L96 spectra show the highest levels, and they show a decent match to the structure of the 1525-1650 Å feature now. Below 1500 Å, however, they still exhibit a poor structural match.

Looking back at the profile comparisons of Section 4.2, it is easy to understand why the photochemical models are almost opaque at these altitudes. The model profiles are generally higher than the retrieved profiles, particularly for C₂H₂, C₄H₂, and HC₃N. The situation is actually worse than this, however, because we only included the most abundant species of the photochemical models in modeling these spectra. If we included all of the species they have predicted, the atmospheres would be even more absorbing than they already are. This is a serious problem and one that the models must address.

469/470 km

By these altitudes, the T95 and L96 model spectra are completely absorbed. The Y84/87 spectra are almost so, but a small amount of transmission is observed.
4.4 Some Remarks on the Retrievals and Comparisons

At the end of any scientific endeavor, one should always step back and look at the results with a critical eye to judge what is and isn't significant, to see where the methods might have failed, and to understand the limitations of the conclusions. In closing this chapter, we make a few remarks on the above retrieval and subsequent comparisons between the data and models.

First, we must remember that the photochemical models are just that: models. Our knowledge of the pertinent chemical reactions is often limited, and a comparison of the three models referenced here shows that there is often disagreement in the proper estimates to use. We have seen that the photochemical models fail to match the S82 C$_2$H$_2$ measurements, a problem which Y84/87 attributed to a misassignment to C$_2$H$_2$ of opacity due to other species. We have found in this work that the C$_2$H$_2$ density is substantially lower than the value determined by S82, perhaps confirming the Y84/87 conclusion. However, the net sum of the other species in all three models provides too much opacity in any event, regardless of the source, and indicates that they are not correct on some level. It remains to be seen how well revisions of these models can reproduce the profiles retrieved here.

We should note that, in some sense, it is unfair to compare the Y84/87 model to those of T95 and L96 because they have benefitted from an extra decade of laboratory work and refined analyses of the Voyager IRIS and radio-occultation data. On the other hand, the generally better match between the retrieved profiles and the Y84/87 model is, perhaps, proof that a well thought out model can go a long way toward offsetting the gains of time. We must keep in mind, however, that any agreement between the photochemical models and the retrieved profiles may be somewhat illusory. The model profiles were generated from base profiles for N$_2$ and CH$_4$ which are different from the ones retrieved here. As such, the models might undergo substantial changes if redone using our retrieved profiles, and we may find that these newer models are better or even worse matches than the current ones.
In regard to our retrieval method, we discovered a few items of note as well. Our method for retrieving the temperature profile simultaneously with the density profiles failed miserably. This is primarily a result of the large uncertainties in the retrieved profiles, which made fitting a locally exponential distribution to the profiles impossible. The retrieved temperature profiles were literally "jumping all over the place," and we have spared the reader by not including any figures of them.

Our attempt at retrieving the temperature may also have another implication. We "jump start" the temperature retrieval by inputting the temperature of the topmost, unbounded "layer." This temperature is used in equation 3.15 to establish the distribution of each species in the topmost "layer," and it is not changed during the retrieval procedure. Thus, the densities and, therefore, column densities of the topmost "layer" are dependent on this input temperature. Should we input a value far from the true one, we could potentially skew our distributions such that we under or overestimate the densities at the base of the topmost "layer." The retrieval procedure generally compensates for this by over or underestimating the corresponding densities in the next few layers to offset the incorrect results, but there might be a residual bias in the profiles.

This problem of incorrectly estimating the densities in the topmost "layer" has no net effect on any of the retrieved profiles we have presented with the possible exception of the N₂ profiles. Owing to their large layer-to-layer variations, most of the profiles effectively absorb any miscalculation of the topmost "layer" density. The N₂ profiles, however, show little variation because they represent a one-species retrieval. In this case, an erroneous temperature could potentially bias the N₂ profiles. We examined this effect and found that the bias is less than 5%, so we have not considered it to be significant. The bias is small because the input temperature (175 K) was reasonably close to the retrieved thermospheric temperatures (150 K ingress, 155 K egress). A further iteration starting with a smaller temperature, perhaps 160–165 K, would probably provide slightly more accurate N₂ profiles.

Finally, the temperature retrieval problem has a minor effect on the cross
sections employed in the retrieval. Because the cross sections are temperature-dependent, the choice of which cross sections to use relied on the derived temperatures for the layers. If the temperature was wrong, the cross sections were wrong. Fortunately, the excursions in the temperature rarely came into play because almost all of the cross section data used in the retrievals are for temperatures greater than 195 K, a value the retrieved temperature exceeded a few times only, and most are at room temperature (295 K). Even when an incorrect cross section was used, however, the effect was insignificant because the available cross section data shows little actual dependence on temperature.
CHAPTER 5

CONCLUSIONS AND FUTURE WORK

5.1 Summary of Conclusions

In the preceding chapters and accompanying appendices, we have presented detailed discussions of the various aspects of the research in this dissertation. Here, we highlight the major points and summarize the conclusions we have reached from our analysis of the Titan solar occultation data.

First, the Monte Carlo model we developed for the UVS detector assembly represents a major improvement in our ability to process raw UVS data into analyzable spectra. We have successfully used the model to understand post-flight changes in gain and current limiting. For the first time, we have been able to correct UVS spectra for the even channel problem, recovering the full spectral resolution of the instrument. The inclusion of the model in an iterative linearization scheme allows us to reproduce the statistical fluctuations in real spectra and eliminate the averaging inherent in previous methods.

Second, a detailed consideration of the Titan solar occultation data coupled with the new linearization scheme has allowed us to generate light curves of excellent quality despite the problems associated with the gain change at mid-occultation, the inexplicable anomalies of the egress reference spectra, and the near-zero counting rates in the HVL 2 gain state for many of the channels. Perhaps the best evidence of the success achieved is seen in the data spectra of Figure 4.14, which clearly show the presence of the N₂ band absorption features.
Third, we have developed a robust, highly flexible occultation analysis method which incorporates many features, including the ability to handle multiple species, temperature-dependent cross sections, and a finite, non-uniform source. The procedure has worked well on application to the Titan solar occultation data, and we have retrieved profiles for nine species. The uncertainties on the profiles for the non-N$_2$ species are moderately large, but the profiles are well constrained by them. Given the nature of multiple-species retrievals and of the Titan solar occultation data, this was our primary goal in retrieving the profiles, and we have achieved that goal.

Fourth, we note several differences between our results and those of G. R. Smith et al. (1982). Our N$_2$ densities appear to be slightly higher than those determined by S82, which we attribute to their use of a band absorption region of the spectrum. Our CH$_4$ densities are smaller than those of S82, though the magnitude of the difference is a bit unclear given the downturn in our CH$_4$ profiles at the level of the S82 results. Our C$_2$H$_2$ densities are significantly lower than those of S82 owing to the lack of the strongest C$_2$H$_2$ absorption feature in our spectra. Absorptions do exist to either side of this feature and may have been interpreted as due to C$_2$H$_2$ by S82 because they considered C$_2$H$_2$ only, but it is also possible that the changes in data processing have led to changes in the resulting spectral shape. Finally, our determined thermospheric temperatures are roughly 25–40 K cooler than those of S82, which has implications for the radiative transfer models of Titan’s middle atmosphere.

Fifth, there is good agreement between the retrieved profiles and the photochemical models for some of the species and not-so-good agreement with others. All the models overestimate the CH$_4$ density at high altitudes, though this is understandable in light of the results of S82. The CH$_4$ densities might be underestimated in the T95 and L96 models at low altitudes, but this is probably a function of the densities of other species in these models being too low. All the models overestimate the C$_2$H$_2$ density, but this is again because the previous measurements of S82 were
too high. The Y84/87 profile is the best match to the structure of the retrieved C$_2$H$_2$ profile. The T95 and L96 models are reasonable matches to the retrieved C$_2$H$_4$ profile at high altitudes, while the Y84/87 model is a better match at low altitudes. As with the C$_2$H$_2$ profile, the Y84/87 model provides the best structural match to the overall C$_2$H$_4$ profile. The retrieved C$_2$H$_6$ profile is reasonably matched by the Y84/87 and L96 models above 700 km, but the T95 profile is the best match below that altitude. The Y84/87 and T95 models are fair matches to the HCN profiles, with the Y84/87 profile being better structurally, while the L96 model is too low over most of the altitude range of the retrieval. The remaining profiles — C$_4$H$_2$, C$_2$N$_2$, and HC$_3$N — are all poorly matched by the models. The Y84/87 model provides a moderate structural match to the C$_4$H$_2$ and C$_2$H$_2$ profiles, but that isn’t saying much in this case. The difference between the Y84/87 and the other two models regarding the C$_2$N$_2$ profile may provide important information about the reaction rates involved. Finally, it is unclear what effect the use of different temperature profiles might have on these comparisons. The Y84/87 model used a constant temperature above the stratosphere, while the T95 and L96 models used the more physically realistic profiles of Lellouch and Hunten (1987) and Yelle et al. (1994), respectively.

Sixth, the spectral comparisons support the conclusion that the retrieval method works well. The matches between the data spectra and spectra modeled with the retrieved atmosphere link the retrieved profiles to the data spectra and illustrate where problems might exist. These problems involve a possible misassignment of C$_4$H$_2$ and C$_2$N$_2$, but the situation is not resolved and the entire spectral match needs to be considered. These comparisons also turned up two absorptions — one centered near 1050 Å and the other near 1450 Å — that are difficult to match, indicating potential cross section problems, the presence of an additional species, or possible artifacts in the data processing.

Finally, the spectral comparisons demonstrate some of the problems with the photochemical models, particularly their inability to match the long wavelength
features. The comparisons do, however, reveal some good matches in structure between the model and data spectra at several altitudes. More than anything, though, the comparisons illustrate that the photochemical models lead to too much absorption at the lower altitudes. This is a serious problem, and there is more to be said on the matter.

Figure 5.1 shows the data light curves for spectral channel 119 of both the ingress and the egress occultations. As we can see, the light curves flatten out a second time between 400–450 km and are not fully absorbed until roughly 325 km in the ingress occultation and 305 km in the egress occultation. Over this range of altitude, about 4% of the light is still transmitted, which means that the photochemical models must be able to transmit some light down to the top of the low-altitude haze layer. This "second step" in the light curves happens for wavelengths covering roughly 1500 to 1670 Å (channels 103–121) in the UVS spectra, and the cut-off is abrupt in each spectral channel.

We did not retrieve any density information from this region because we did not attempt to fit the light curves here (our fits went to zero between 375 and 425 km), and there is little meaningful spectral information other than total flux to be had. The altitude at which the cut-off occurs is consistent with that for the detached haze layer seen in the Voyager images (cf. Rages and Pollack, 1983) but is slightly lower than that noted by Hubbard et al. (1993) in their analysis of the 28 Sgr occultation data. This is probably a result of seasonal effects as the Voyager observations took place nine years prior to the 28 Sgr occultation. The difference in the altitudes of the cut-offs for the two occultations, however, is consistent with the conclusion of Hubbard et al. that Titan’s atmosphere is not spherically symmetric and shows latitudinal asymmetries.
Figure 5.1: Light curves illustrating the cut-off at low altitudes. The upper curve is from the ingress occultation, and the cut-off occurs at roughly $z = 325$ km. The lower curve is from the egress occultation, and the cut-off altitude is around $z = 305$ km. The level of the signal prior to the cut-off indicates that approximately 4% of the incoming solar light in this spectral channel (119 in both occultations) is transmitted through the atmosphere until the cut-off. Similar cut-offs exist in channels 103–121, covering the wavelength range of roughly 1500–1670 Å.
5.2 Future Work

The scientific endeavor is an ongoing process, and the study of Titan’s atmosphere is no exception. This work provides researchers with a better picture of the structure of Titan’s upper atmosphere than has previously been available. Even so, it has mainly concentrated on the aspects of retrieving the atmospheric structure from the Voyager UVS data and less so on the scientific implications of those results, leaving the door wide open for future work. We mention some possibilities here.

First, the retrieval method needs some refinement. Although it performs well in retrieving density information, it has some minor problems that need to be addressed. In Section 4.4, we noted that the temperature retrieval failed and might have some influence on the density retrieval. We need to develop an alternate method of extracting the temperature information and fully assess the possible influence this may have had on the density profiles. We should also investigate ways to prevent the method from yielding physically unrealistic results (e.g., the “drop-outs” noted in Figures 3.8 and 3.9). Because the method was designed with minimal assumptions about the physical structure of the atmosphere, it is easily adapted to different situations, and it should be possible to develop a system of weights and penalties to avoid problems of this kind.

From the scientific perspective, the opportunities for future work are many. In Chapter 1, we demonstrated the wide-ranging application of the original analysis of G. R. Smith et al. (1982). Our work has eliminated the inconsistencies of that analysis and extended the breadth of the results tremendously. Tighter constraints exist for photochemical models, and improvements in these will lead to better models of the ionosphere, atmospheric escape processes (which impact on models of the hydrogen torus), and the temperature structure of the middle atmosphere.

At the same time, we need to remember that the retrieved density profiles are the ones which yield the best numerical fits to the UVS spectra. We have commented that it is possible for different profiles to provide acceptable fits to the
data within the uncertainties. In fact, the downturn in the CH\textsubscript{4} profiles is a good example of an unlikely exchange of CH\textsubscript{4} opacity for that due to another species, in this case C\textsubscript{2}H\textsubscript{4}, C\textsubscript{2}H\textsubscript{6}, and/or C\textsubscript{4}H\textsubscript{2}. Part of the purpose in comparing the photochemical models to the retrieved atmosphere was to demonstrate that there are instances where the models give good matches to the UVS spectra despite the mismatches in the density profiles.

In addition to improving the retrieval method to yield better profiles, we should also pursue an approach in which different photochemical models are compared to the data. Such an approach would provide a complementary view of the atmosphere because it would match the spectra on physical grounds rather than numerical minimization, which is the driving factor behind the retrieved profiles. Given the uncertainties associated with the relevant chemical reactions, however, this approach should always be used in conjunction with a retrieval procedure such as that presented here. The goal in this dual procedure would be to find the most consistent atmosphere on both numerical and physical grounds, but we should never let a model dictate the result when the data might actually be telling a different story.

With the launch of Cassini scheduled for later this year, the future looks bright for continued studies of Titan's atmosphere. Further analysis of the results presented here will allow scientists to develop a model of Titan's atmosphere on which Cassini observations can be based. Should Cassini find a somewhat different atmosphere on Titan, the current work will provide information on possible seasonal or other changes.

William Somerset Maugham once said, "It is bad enough to know the past; it would be intolerable to know the future." Indeed, science would be rather boring if we already knew the answers. With that in mind, we continue our investigations of Titan's atmosphere, never knowing what mysteries it might yet reveal.
APPENDIX A

THE VOYAGER UVS

An understanding of the operation of the Voyager UVS is integral to any attempt to analyze UVS data. We present a brief discussion of this operation here. Broadfoot et al. (1977) and Broadfoot et al. (1981b) describe the Voyager UVS in greater detail. Note that while the following general description applies equally well to either the Voyager 1 or Voyager 2 UVS, there are slight differences between the two instruments in actual operation (e.g., wavelength coverage, detector gain, sensitivity).

A.1 Optical Configuration

The Voyager UVS is a compact, Wadsworth-mounted, objective grating spectrometer covering the wavelength range of approximately 500 to 1700 Å. The objective grating design is commonly used to observe point sources, but the Voyager UVS has been adapted to observe extended sources as well through the use of a mechanical collimator which restricts the field of view. Figure A.1 illustrates the basic design of the UVS. The actual Voyager UVS instrument is shown in Figure A.2.

Radiation from the observed source enters the UVS through one of two ports and then passes through a series of thirteen mechanical baffles which comprise the collimator. The airglow port is used to observe extended and stellar sources, while the occultation port is used to observe the sun. The field of view in the dispersion direction of the grating is restricted by the collimator to 0.1° (FWHM) for the airglow port and 0.25° (FWHM) for the occultation port. The field of view
in the cross-dispersion direction is open but is defined by the angular width of the detector in the image plane to be 0.87° for both ports. Radiation does not enter the occultation port directly but is reflected into the port by a platinum overcoat mirror offset 20° from the airglow port line of sight. The offset of the occultation port is necessary so that other Voyager instruments boresighted with the UVS airglow port are not pointed at the sun. Neither port has a dark slide, so radiation "leaks" in from the port not directly in use. This leakage is generally negligible, particularly for solar observations, but must be kept in mind in the event the unused port is pointed at a second source by chance.

Use of the mechanical collimator leads to the reduction of the incoming radiation as the source moves off-axis. This reduction is described by the "slit function" of the port, which represents the fraction of light entering the slit that ultimately gets collimated and reaches the grating.

Slit functions for the airglow port of both the Voyager 1 and Voyager 2 UVS are well-known. Slit functions for the occultation ports, on the other hand, have not been determined previously, primarily because stars are rarely observed in the occultation port.
We have determined the slit function for the Voyager 2 occultation port from a special series of observations in which the occultation port was slewed across a bright star (α Vir) four times and then positioned on the star for an extended period of time. The four slews yielded the overall shape of the slit function for the entire slit. The extended observation with the star near the center of the slit yielded more detail near the peak of the slit function. The resulting slit function is shown in Figure A.3. A similar set of observations was obtained for the Voyager 1 occultation port, but poor transmission or reception rendered the data set completely useless and we have been forced to use the Voyager 2 slit function for Voyager 1. This is reasonable given that the airglow port slit functions for the two spacecraft are similar.
Figure A.3: Slit function determined for the Voyager 2 occultation port. The slit function was generated by binning the α Vir observations according to position in the slit and averaging the binned observations. The resulting average was then mirrored about the central axis of the slit and averaged again to produce a symmetrical slit function.

Once the incoming radiation has been collimated, it undergoes a single normal incidence reflection from the concave diffraction grating, which simultaneously focusses and disperses the radiation onto the detector assembly. The grating is a platinum replica blazed at 800 Å and has a ruling of 540 lines/mm, giving a plate dispersion of 93 Å/mm.

At the detector assembly, the diffracted and focussed photons form an image of the source at each wavelength, but the use of the collimator and imperfections in the grating result in some photons being scattered. These scattered photons are not properly focussed by the grating and result in radiation of wavelength X contaminating the image for wavelength Y and vice versa for all wavelengths. These
instrumentally scattered photons are referred to as "scattered light" and must be
removed in processing UVS spectra (see Section C.2.2).

The use of an objective grating results in two important considerations for
Voyager UVS spectra. First, the UVS has distinctly different spectral resolutions for
point and extended sources. For extended sources, the resolution is roughly 30 Å. For
point sources, the resolution is roughly 18 Å. The sun, which is a finite source
(i.e., one which is too large to be considered a point source but which does not fill the
slit and is therefore not an extended source), has a spectral resolution that falls in
between these values. Second, the wavelength range actually recorded by the UVS
varies for a point source depending upon its position in the UVS slit. The nominal
wavelength ranges for the two spacecraft are 534.83–1701.59 Å for Voyager 1 and
513.45–1680.21 Å for Voyager 2. As the source moves off-axis, these wavelength
ranges change as the position of a given wavelength on the detector assembly shifts
because of a change in the incidence angle of the incoming light at the grating.
Because the detector assembly is fixed in position, the recorded wavelength range
changes as new wavelengths move "onto" the detector and others move "off". The
magnitude of the wavelength shift is 3.24 Å per 0.01° that the source is off-axis. This
effect is pertinent for both point and finite sources and must be considered when
modeling an occultation by an atmosphere because of the wavelength dependence of
the absorption coefficients of the atmospheric constituents. The wavelength range
for spectra of extended sources is unaffected because such sources completely fill
the slit.

A.2 Detector Assembly

All photons reaching the active area of the detector assembly undergo a three-
stage process to convert the photon energy to detector counts. Each of these stages
corresponds to a part of the detector assembly, which was developed for the Voyager
UVS and is described in detail by Broadfoot and Sandel (1977). The detector itself
is a self-scanned anode array with 126 active elements (there are 128 anodes total but the final two are unused), each spanning a wavelength interval of 9.26 Å.

The first stage is the conversion of photons to charge. This is accomplished through the use of a dual microchannel plate (MCP) electron multiplier and a semi-transparent photocathode. The two MCPs are in a chevron configuration. Photons of wavelength 500 to 1250 Å fall directly onto the MCP surface and generate a photoelectron in the MCP according to the MCP quantum efficiency. Each photoelectron initiates a charge cascade of electrons, which ultimately exits the back of the MCPs and falls onto the detector anodes. Photons of wavelength 1250 to 1700 Å fall onto a CuI photocathode deposited onto a MgF₂ filter plate on top of the MCP. The photocathode is included because it has a higher quantum efficiency than the MCP in this wavelength region. Photons falling onto the photocathode generate photoelectrons per the quantum efficiency. These photoelectrons are then guided onto the MCP by an electric field and generate charge cascades in the MCPs as in the shorter wavelength region not covered by the photocathode.

At this point, it is important to distinguish between a photon and a photoevent. Photons refer to the physical radiation quanta which emanate from the observed source and are dispersed onto the detector assembly by the grating. Photoevent refers to any photon which generates a photoelectron in the MCPs or photocathode. Because the quantum efficiency of the MCPs and the photocathode is less than one, there are always more photons than photoevents.

The magnitude of the charge cascades in the MCPs depends upon the gain of the MCPs. The Voyager UVS can operate in several different gain states to enable it to observe sources over a wide range of intensities. The higher the gain, the larger the number of electrons in the charge cascade and, ultimately, the larger the recorded signal. Gain states are referred to by "HVL x", where HVL is short for high-voltage level and x is a number identifying the gain state. The identification number increases with the gain (e.g., HVL 3 is higher than HVL 2).
The second stage is the collection of charge by the detector anodes. The electron charge cascade which exits the back of the MCPs moves down onto the detector anodes under the guidance of an electric field. This electron "cloud" will spread as it moves from the MCPs to the detector anodes and end up on several anodes because of both a distribution of directions on exiting the MCP and mutual electron repulsion. The anodes are read out with each scan of the detector, and the electron charge on each anode is converted to detector counts in the third stage. The distribution of charge on the detector anodes is two-dimensional, but the detector is linear such that all charge on a given anode is converted to a single count value.

The third and final stage is the conversion of the charge on the anodes to detector counts. The charge from each anode is passed through a 3-bit A-to-D converter. The first threshold level of the converter varies for each of the detector anodes because of fabrication differences across the anode array. The remaining threshold levels are equally spaced above the first and span a range of $1.25 \times 10^5$ electrons each. The charge on each anode is compared against the thresholds and converted to detector counts. This conversion is done for every anode during each scan of the detector, and the resulting counts on each anode are summed over the number of scans corresponding to the integration time (which depends on the data mode of the spacecraft) to produce the final spectrum.

The A-to-D converter operates in one of two modes. The first mode is a pulse counting mode (henceforth referred to as "count mode") in which a single count is recorded for any charge that exceeds the first threshold level of the converter, no matter how large the charge may actually be. The second mode is referred to as "pulse height mode." In this mode, the charge on an anode is converted to counts using the full thresholding capability of the converter, resulting in a range of zero to seven counts depending on the amount of charge. Count mode is used for observations of stars and diffuse sources, while pulse height mode is used when observing bright sources such as the sun. It is important to note that a detector anode is saturated when the resulting count in each scan is seven, indicating that
the true flux at the wavelength recorded by the given anode cannot be ascertained.

One final note on UVS terminology is the distinction between anodes and channels. There is a one-to-one correspondence between the anodes of the detector and the channels of a spectrum. The charge collected on anode X is recorded in channel X of the spectrum, so the distinction is purely one of convenience. Generally, anode is used when discussing the elements of the detector array, while channel is used when referring to UVS spectra. However, there are often cases in which the two are used interchangeably, and the distinction is made here to avoid any confusion which may arise.
APPENDIX B

THE DETECTOR ASSEMBLY MODEL

B.1 Model Overview

To better understand the performance of the Voyager UVS, we have constructed a Monte Carlo model of the detector assembly. The model predicts the detected signal at the anode array caused by an arbitrary distribution of photoevents at the front of the microchannel plates. The model has three separate stages: 1) generation of photoevents; 2) generation of a charge for each photoevent; and 3) conversion of each charge to counts. Figure B.1 is a schematic of the detector assembly model.

For the purposes of this model, it is convenient to visualize the boundaries of the anodes in the detector array as extending vertically to the front of the microchannel plates. The illuminating spectrum from which the photoevent rates are determined is always equivalent to a Voyager UVS spectrum, which has 126 channels that correspond to the 126 anodes of the detector. Indeed, the primary motivation for developing this model is to be able to convert detector counts in a UVS spectrum to photoevents during the spectrum processing procedure (see Section C.2.1), which yields a photoevents spectrum with 126 channels. The convenience of defining the boundaries of the anode array at the front of the microchannel plates is that it allows us to position the photoevents of the illuminating spectrum on the MCPs in a meaningful fashion.

The first stage in the modeling procedure is to determine the number of photoevents occurring in a given scan of the detector. The Voyager UVS detector obeys Poisson statistics, so we simply choose a random number of photoevents from
Figure B.1: Schematic representation of the detector assembly model. The charge falling on any given anode is parameterized as a function of the distance $d$ between the center of the charge spreading and the center of the anode.

a Poisson distribution with a specified average rate. The average rate is allowed to vary from anode to anode (where "anode" refers to the defined boundaries at the front of the MCPs) according to the spectral shape of the incoming radiation and is given by the number of photoevents on an anode divided by the number of scans per the integration time of the spectrum. Once we have the number of photoevents, we assign each photoevent a location on the microchannel plates by randomly locating the photoevent within the "anode" of its origination.

The second stage in the modeling procedure is to assign a charge to each of the photoevents. Each charge is chosen randomly from an exponential distribution fitted to laboratory measurements and represents the total number of electrons in the pulse generated in the microchannel plates due to a particular photoevent. The
exponential distribution is directly proportional to the gain of the MCPs. These charges will then spread as they travel from the microchannel plates to the anode array to form the two-dimensional charge distribution on the anodes.

The final stage of the modeling procedure is to convert this charge into detector counts. The detected signal on any anode is a function of the amount of charge that spreads onto that anode. We have developed a parameterized function to determine the fraction of the generated charge that falls onto a given anode (see Section B.4). We first multiply the total charge associated with the photoevent by the fraction on each affected anode to find the charge on that anode. We then convert the charge on each anode to detected counts via a scheme that mimics the A-to-D converters in the instrument. Finally, we sum the resulting counts on each anode from each scan to produce the final model spectrum.

In order to implement the Monte Carlo model, we must know several key pieces of information related to the Voyager UVS. The remainder of Appendix B is devoted to describing these pieces of information and the methods by which they were determined. Because this dissertation is concerned with the Voyager 1 solar occultation by Titan, we limit the following descriptions to the Voyager 1 UVS except in cases where it is convenient to discuss the Voyager 2 UVS as well.

### B.2 Detector Thresholds

We need the detector thresholds to convert the charge collected on each anode to detector counts. There are seven counting thresholds for each anode owing to the 3-bit A-to-D converters. The first threshold level for each anode originates in the geometry of the anode array. The remaining six thresholds are defined relative to the first and have a uniform spacing of \(1.25 \times 10^5\) electrons.

Figure B.2 is a plot of the lab-measured first threshold level for each of the anodes with the exception of anodes 3 and 4 (see below). The nominal level is
Figure B.2: First threshold levels for the Voyager 1 UVS. The dashed line represents the nominal threshold level of $2.5 \times 10^5$ electrons. The 16-anode periodicity of low thresholds is due to the fabrication process. Anodes 3 and 4 are anomalously high for unknown reasons.

$2.5 \times 10^5$, but nonuniformities in the fabrication process have led to the threshold varying from anode to anode. In particular, a periodicity exists in which every fifteenth and sixteenth anode (starting with anodes 1 and 2) has a low threshold level. The mask used to fabricate the anode array consisted of 16-anode sections, and these low threshold levels correspond to the junctions between the sections. Because the threshold levels are linked to the fabrication of the anode array, they are not expected to vary substantially with time, and we have chosen to use the lab-measured values in the detector assembly model.

Figure B.2 also shows that anodes 3 and 4 have anomalously high threshold levels. The reason for this is not known, but a fabrication-related cause is suspected because the problem occurs in both the Voyager 1 and Voyager 2 UVS instruments. The threshold levels shown for anodes 3 and 4 are not the lab-measured values.
Spectra processed using the lab-measured values showed anomalously low values in channels 3 and 4, indicating that the threshold levels were too high. As such, the threshold levels for anodes 3 and 4 were determined in-flight by adjusting the levels until processed spectra had a smooth profile across this region of the spectrum.

B.3 Scan Rates

The scan rate is a critical parameter in any attempt to model the Voyager UVS detector's response or to linearize a spectrum. Therefore, we must know the number as accurately as possible. Previous analyses of Voyager UVS occultation data generally used the nominal value of 3125 scans per second, but Voyager UVS spectra of the sun appear to saturate at a level which would indicate fewer scans per second if saturation occurs at a count level of seven counts per scan in pulse height mode.

The nominal value of 3125 scans per second is based upon an anode clock time of 5 μsec per anode (or 200 kHz). Because the anodes are read out in pairs, it takes $64 \times 5$ μsec to perform one scan of the detector, or 320 μsec per scan. This time per scan leads to the nominal value of 3125 scans per second. If the anode clock time were something other than the nominal value of 5 μsec per anode, the number of scans per second would differ from 3125. Thus, we searched the Voyager UVS lab test information to determine whether the anode clock time was measured to be other than 5 μsec per anode.

This search yielded lab-measured anode clock frequencies of 194.8 kHz for Voyager 1 and 194.187 kHz for Voyager 2. The corresponding anode clock rates and number of scans per second are $\approx 5.13$ μsec per anode and 3043.75 scans per second for Voyager 1 and $\approx 5.15$ μsec per anode and 3034.17 scans per second for Voyager 2, respectively.

The non-integer nature of these estimates is real because it is possible to
have a non-integral number of scans in a second. The anodes are read out continuously, but a spectrum has a set duration. Thus, it is normally the case that a spectrum will be “completed” before the current anode read-out (the current scan) has reached the end of the anode array. The next spectrum will then begin at that point (i.e., in the middle of a scan). Because it is not possible to determine where in the anode array a spectrum’s integration begins and ends, the fractional part of these numbers of scans per second is generally neglected or rounded to the nearest integer value. Given that we are dealing with one scan in no fewer than $\approx 1000$ (a 0.32 second spectrum, which is the shortest integration time of the Voyager UVS), and that the data undergo a compression which leads to a loss of significance anyway, it is reasonable to neglect the fractional part or round it off to the nearest integer value.

The question remains, however, of whether or not the Voyager UVS scan rates are the same in-flight as they were in the lab. To test this, we examined saturated Voyager spectra and estimated the number of scans per second. Two assumptions are made in this estimation. First, we assume the spectrum is actually saturated. The H Lyman $\alpha$ line is the strongest solar line in this wavelength range, so it is the best indicator of saturation. We can be reasonably sure that the spectrum is saturated if the counts levels in the peak H Lyman $\alpha$ channels are equal, particularly in the odd channels. If the even H Lyman $\alpha$ channels are the same as the odd ones, or if the counts level in channels away from the H Lyman $\alpha$ channels is the same as that in the H Lyman $\alpha$ channels, we are confident that we have a saturated spectrum. Figure B.3 illustrates a spectrum with saturated channels.

The second assumption is that we have seven counts per scan in each scan of a saturated spectrum. If there were a mixture of sixes and sevens, then we would not be able to determine the number of scans producing the given saturated spectrum. Modeling a saturated spectrum for any reasonable instrument gain and photoevents level shows that this assumption is good to better than 0.02%, and we may assume seven counts per scan.
Figure B.3: Example of a spectrum with saturated channels. The dashed line is at 7000 counts, the level we would expect the spectrum to saturate at if the number of scans per second were the nominal value of 3125. The saturated channels fail to reach this level, indicating that the number of scans per second is less than the nominal value.

Under these assumptions, the number of scans per second is determined by taking the saturated counts level, dividing it by seven, and then dividing by the spectrum duration. If the spectrum was overflowed (see Section 2.2), we corrected for this first. In addition, we determined the range of counts and the corresponding range of number of scans per second that we can expect given the compression of the spectral data. The results of this test are summarized in Table B.1.

A comparison of the scan rate estimated from the saturated spectra with the predicted number based upon the measured true anode clock time (frequency) shows that the predicted number falls within the range of uncertainty introduced by the data compression for the 0.32 second spectra. However, this is not true for the 3.84 second spectra. For these spectra, the predicted number of scans per second is less than the minimum value estimated from the saturated spectra. It is worth
Table B.1: Comparison of In-Flight and Lab-Measured Scan Rates

<table>
<thead>
<tr>
<th>Spectrum Description</th>
<th>Range of In-Flight Count Levels</th>
<th>Range of In-Flight Scans per Second</th>
<th>Predicted Count Levels</th>
<th>Lab-Measured Scans per Second</th>
</tr>
</thead>
<tbody>
<tr>
<td>Voyager 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>974239.5, 1978/207</td>
<td>16384 (81919)†</td>
<td>3047.58</td>
<td>16281 (81816)</td>
<td>3043.75</td>
</tr>
<tr>
<td>3.84 seconds</td>
<td>16511.5 (82046.5)</td>
<td>3052.33</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HVL 2</td>
<td>16639 (82174)</td>
<td>3057.07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Voyager 1</td>
<td>3492127, 1980/317</td>
<td>6784</td>
<td>3028.57</td>
<td>6818</td>
</tr>
<tr>
<td>0.32 seconds</td>
<td>6815.5</td>
<td>3042.63</td>
<td>6818</td>
<td>3043.75</td>
</tr>
<tr>
<td>HVL 3</td>
<td>6847</td>
<td>3056.70</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Voyager 1</td>
<td>3680012, 1981/13</td>
<td>6784</td>
<td>3028.57</td>
<td>6818</td>
</tr>
<tr>
<td>0.32 seconds</td>
<td>6815.5</td>
<td>3042.63</td>
<td>6818</td>
<td>3043.75</td>
</tr>
<tr>
<td>HVL 3</td>
<td>6847</td>
<td>3056.70</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Voyager 2</td>
<td>1024956.3, 1978/208</td>
<td>16128 (81663)</td>
<td>3038.06</td>
<td>16023 (81558)</td>
</tr>
<tr>
<td>3.84 seconds</td>
<td>16191.5 (81726.5)</td>
<td>3040.42</td>
<td>3034.17</td>
<td></td>
</tr>
<tr>
<td>HVL 3</td>
<td>16255 (81790)</td>
<td>3042.78</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Voyager 2</td>
<td>2069020.147, 1979/191</td>
<td>6784</td>
<td>3028.57</td>
<td>6797</td>
</tr>
<tr>
<td>0.32 seconds</td>
<td>6818.5</td>
<td>3042.63</td>
<td></td>
<td>3034.17</td>
</tr>
<tr>
<td>HVL 3</td>
<td>6847</td>
<td>3056.70</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

† The () indicate values after correction for overflow.
noting that the predicted number is less than the minimum estimated number by roughly 4 scans per second for both spacecraft. This may indicate that the difference is connected with the extended integration time. Alternatively, it may be due to the fact that the 3.84 second spectra were taken at earlier dates than the 0.32 second spectra and thermal effects due to a closer proximity to the sun may play a role. It is also possible that the overflow associated with these spectra may play a role when coupled with the data compression.

Based upon the study performed here, we find it likely that the lab-measured anode clock frequencies are representative of the in-flight anode clock frequencies. Thus, we adopt the scan rates corresponding to the lab-measured clock frequencies as the true scan rates. These are 3043.75 scans per second for Voyager 1 and 3034.17 scans per second for Voyager 2, respectively.

In practice, it is often inconvenient to work with a non-integral number of scans. Thus, we use these scan rates to determine the number of scans per duration of the spectrum involved and then round off the resulting number to the nearest integer value (e.g., a 0.32 second Voyager 2 spectrum has $3034.17 \times 0.32 = 970.93 \Rightarrow 971$ scans in it). The significance of this fractional part was discussed above, and little is lost to the rounding.

### B.4 Charge Spreading Parameterization

A major element of the detector assembly model is the parameterization of the spreading of the electron cloud as it travels from the microchannel plates to the anode array. This parameterization determines the fraction of the total charge which is deposited on each anode and is therefore intimately linked to the detected signal in each channel of the model spectrum.

It is crucial that we have as accurate a parameterization of this spreading as possible to validate the use of the detector assembly model; however, this is difficult
to achieve in practice. The spreading of the cloud is caused by both a distribution of electron trajectories as the charge cascade exits the back of the microchannel plates and mutual repulsion of the electrons within the cloud itself. Such details are difficult, perhaps impossible, to reproduce and any implementation would be extremely computer-intensive. Because millions of these calculations are involved in modeling a single UVS spectrum of the sun and thousands of such spectra must be processed in a solar occultation, the problem of exact modeling of the electron spreading becomes intractable. At the same time, lab measurements of the electron spreading are sparse, making determination of parameters in such a detailed model difficult.

Given the above, the use of a detailed parameterization is not justified and we make two gross simplifications in all the charge spreading models which follow. First, we assume that the charge spread is axially symmetric and that the axis is perpendicular to both the microchannel plates and the anode array. This cannot be strictly true because the microchannels are not perfectly vertical (there is $\approx 8^\circ$ of tilt relative to the vertical), but the deviation is considered to be negligible given that the charge spread is unlikely to be axially symmetric in the first place. Second, we assume that the radius of the charge spreading at the anode array is dependent on the total charge in the electron cloud. The first assumption eliminates the need to know the distribution of electron trajectories, and the second one eliminates the need to model the mutual repulsion of the electrons.

B.4.1 Model Descriptions

There are four models that we have developed to represent the charge spread from the microchannel plates to the detector anodes. Here, we describe each model and derive the equations that represent the model.
Model 1: Right Circular Cone Model

In model 1 the charge spread takes the form of a right circular cone. The apex of the cone originates at the microchannel plates, and the circular base lies on the detector anodes. The pertinent geometrical parameters of model 1 are illustrated in Figure B.4.

The quantity we need to calculate is the fraction of the electron cloud that falls onto a given anode. A straightforward way to do this is to calculate the partial volume of the cone that overlies the anode and ratio this volume to the total volume of the cone, which is given by

\[ V_{\text{cone}} = \frac{1}{3}\pi HR^2. \]  

The quantity we need to calculate is the fraction of the electron cloud that falls onto a given anode. A straightforward way to do this is to calculate the partial volume of the cone that overlies the anode and ratio this volume to the total volume of the cone, which is given by

\[ V_{\text{cone}} = \frac{1}{3}\pi HR^2. \]  

In Figure B.5, we see that the volume of the cone falling on a given anode may be expressed as the difference between two partial volumes of the cone. These partial volumes are represented in cross-section by the hatched areas of the figure, where the cross-section is taken through the axis of the cone. The parameters \( d_L \)

![Figure B.4: Geometry of the right circular cone model. The various quantities are described in the text.](image)
Figure B.5: Illustration of the volume calculation procedure for the right circular cone model. There are three cases for the calculation as discussed in the text. The flat U-shaped object is the anode over which the volume is to be determined. The distances $d_L$ and $d_R$ are those between the charge spread axis and the left and right anode edges, respectively.

and $d_R$ are the distances from the axis to the left and right edges of the anode, respectively.

As we can see in Figure B.5, there are three cases to consider, depending on the position of the anode relative to the photoevent location (i.e., the cone axis). Cases 1 and 2 are simply mirror images of one another, and the volume of the cone over the anode is found by subtracting the smaller of the two volumes from the larger. Case 3 is different in that the anode edges bracket the photoevent location. In this case, we calculate the volumes to the left and right of the anode and subtract their sum from the total volume of the cone to get the volume on the anode.
Regardless of the case we have, we need to calculate the volume of the cone between the surface of the cone and a plane through the cone at the distance \( d_L \) and \( d_R \), where the intersection of the plane and the base of the cone is a line representing one edge of the anode and the plane is perpendicular to the base of the cone. Assuming the geometry of Figure B.4, this volume is the integral of the cone’s height over the area of the base lying between the cone surface and the plane and is expressed as

\[
V = \int_{\theta_L}^{\theta_R} \int_{r(\theta')}^R h \ r' \ dr' \ d\theta'.
\]  

(B.2)

From Figure B.4, we can see that similar triangles gives

\[
\frac{H}{R} = \frac{h}{R - r'},
\]  

(B.3)

where \( H \) is the maximum height of the cone on the axis and \( R \) is the radius of the base of the cone. From Figure B.4, we can also see that \( r(\theta) \) is given by

\[
r(\theta) = \frac{R \cos \theta_o}{\cos \theta'}.
\]  

(B.4)

Using equation B.3 and equation B.4, we can rewrite equation B.2 as

\[
V = 2H \int_{0}^{\theta_o} \int_{\frac{R \cos \theta_o}{\cos \theta'}}^{R} \left( r' - \frac{(r')^2}{R} \right) \ dr' \ d\theta',
\]  

(B.5)

which upon evaluation gives

\[
V = 2HR^2 \left[ \frac{\theta_o}{6} - \frac{1}{3} \cos \theta_o \sin \theta_o + \frac{\cos^3 \theta_o}{6} \ln \left( \tan \left( \frac{\pi}{4} + \frac{\theta_o}{2} \right) \right) \right].
\]  

(B.6)

Equation B.6 represents the volume of the cone corresponding to one of the hatched cross-sections in Figure B.5. We use this equation to calculate the two volumes that
we need to determine the fraction of the cone’s volume that lies on any given anode. Note that the only parameter in this model is the radius $R$ of the base of the cone because the height $H$ drops out when the partial volume overlying the anode is ratioed to the total volume of the cone.

**Model 2: Two-Triangle Fractional Volume Model**

The right circular cone of model 1 is a simple representation of the spreading of the electron cloud from the microchannel plates to the detector anodes. It is unlikely, however, that the electron cloud is actually a cone. Rather than replace the cone with some other defined cloud shape, we chose to model the partial volumes associated with $d_L$ and $d_R$ directly. The reason for this is two-fold. First, it is difficult to find a solid of revolution similar to the cone that is easily integrated. We tried exponential, inverse power law, and gaussian-based solids, but the complications of integrating the revolution of such curves about the central axis made them intractable. Second, modeling the partial volumes directly avoids the need to know what the electron cloud looks like. We simply calculate parameterized volumes equivalent to those obtained using equation B.6 and subtract them appropriately using the scheme outlined in Figure B.5. The parameterization of the partial volumes is defined such that they are fractional volumes (i.e., the volumes indicated in Figure B.5 are less than or equal to 0.5), eliminating the need to ratio the resulting volume to a total volume.

Model 2 is illustrated in Figure B.6. The $x$-axis is the distance $d$ between the axis of the electron cloud and the edge of the anode for which we want the charge fraction. This distance is equivalent to the $d_L$ and $d_R$ of Figure B.5. The $y$-axis represents the fractional volume equivalent to the volume between the plane and the surface of the cone in model 1. Because we model a fractional volume directly, the $y$-axis runs from 0 (when the edge of the anode is at the radius of the electron cloud) to 0.5 (when the edge of the anode is at the axis of the electron cloud).
Figure B.6: Illustration of the fractional volume model. The solid line represents the fractional volume curve. The dashed lines represent extensions of the two lines composing the curve. $R$ is the maximum radius of the charge spread, and $d$ is the distance between the charge spread axis and the pertinent anode edge. Parameter $A$ is a value between 0 and 1, and $AR$ marks the x-axis intercept of the triangle 1 line. Parameter $B$ is a value between 0 and 0.5 and is the y-axis intercept of the triangle 2 line. In this illustration, $R = 1.0$, $A = 0.6$, and $B = 0.3$.

Figure B.6 illustrates why we refer to this model as a "two-triangle" model. The first triangle is the right triangle with vertices at the origin, $(0,0.5)$, and $(AR,0)$, where $R$ is the radius of the charge spread and $A$ is a model parameter that is between 0 and 1. The second triangle is the right triangle with vertices at the origin, $(0,B)$, and $(R,0)$, where $B$ is a model parameter that is between 0 and 0.5. The fractional volume is calculated by determining to which side of the intersection point $(x_i,y_i)$ our distance $d$ lies and then using the equation of the line representing the hypotenuse of the proper triangle to get the fractional volume. Thus, we need to know the equations for these hypotenuse lines and the value of $x_i$ against which we will compare $d$. 
The equations for the hypotenuse lines are easily obtained from the generic line equation

\[ y = mx + b, \quad (B.7) \]

where \( m \) is the slope of the line and \( b \) is the \( y \)-intercept. For triangle 1, we have

\[ f_\nu = \left( \frac{0.5 - 0}{0 - AR} \right) d + 0.5 = \left( \frac{-0.5}{AR} \right) d + 0.5. \tag{B.8} \]

For triangle 2, we have

\[ f_\nu = \left( \frac{B - 0}{0 - R} \right) d + B = -\left( \frac{B}{R} \right) d + B. \tag{B.9} \]

At the point \((x_i, y_i)\), equations B.8 and B.9 are equal to each other. We can substitute \( x_i \) for \( x \) in each equation, set them equal to each other, and solve for \( x_i \). This yields

\[ x_i = AR \left( \frac{0.5 - B}{0.5 - AB} \right). \tag{B.10} \]

The calculation of the fractional volume is now straightforward. The distance \( d \) is compared to \( x_i \). If it is less than \( x_i \), we use equation B.8 to calculate the fractional volume; if it is greater than \( x_i \), we use equation B.9. If \( d \) equals \( x_i \), we may use either equation, and we arbitrarily choose to use equation B.9. This fractional volume is calculated twice (once for each anode edge), and the resulting volumes are subtracted appropriately according to the three cases of Figure B.5 to yield the total fraction of the charge that is deposited on the given anode. Note that for case 3, the total volume of this model is considered to be 1.
Model 3: Two-Triangle Total Charge Fraction Model

Model 3 is a simplification of models 1 and 2 in which we directly model the charge fraction on an anode as a function of the distance $d$ between the anode's center and the location of the photoevent. This reduces the number of calculations that we have to perform by eliminating the need to calculate two volumes which are then subtracted and ratioed to the total volume.

Figure B.7 illustrates the model. As with model 2, we have chosen a two triangle approach. Note, however, that because we are not calculating a volume anymore, the maximum x-axis value is now $R + 0.5$ instead of $R$. This is because

![Diagram of the two-triangle total charge fraction model](image)

Figure B.7: Illustration of the two-triangle total charge fraction model. The solid line represents the total charge fraction curve. The dashed lines represent extensions of the two lines composing the curve. $R$ is the maximum radius of the charge spread, $d$ is the distance between the charge spread axis and the center of the anode, and $I_1$ and $I_2$ are the y-axis intercept points of the two lines making up triangles 1 and 2, respectively. Parameters $A$ and $B$ are the $x$ and $y$ values of the intersection point, respectively. In this illustration, $R = 1.5$, $A = 1.0$, and $B = 0.3$. 
the distance \( d \) is between the photoevent location and the anode's center, giving us an extra one-half anode upon which to have charge. In calculating the volumes of models 1 and 2, we had a maximum \( d \) of \( R \) because the distance represented that from the photoevent location to the edge of the detector anode. It's a difference in what \( d \) represents.

It is important to note that we have changed the meaning of \( A \) and \( B \) in this model as well. These two parameters now specify the intersection point, with \( A = x_i \) and \( B = y_i \). The reason we have changed the meaning of these two parameters is directly related to a major difference between this model and model 2. In model 2, we know that the fractional volume is 0.5 when \( d = 0 \). This allows us to specify \( B \) as anything between 0 and 0.5; in other words, we know the maximum \( B \) value that is allowed. We also know that the first triangle will start at 0.5 on the y-axis and go through the \( AR \) point on the x-axis. Thus, the meanings and values of \( A \) and \( B \) depend on knowing that the fractional volume cannot exceed 0.5. This is not the case with model 3. Because we are now modeling the total fraction of the charge on the anode directly, we do not know the maximum fraction \emph{a priori}. This makes it difficult to specify \( A \) and \( B \) as before without specifying an additional parameter in place of the 0.5 of model 2. We wish to avoid more parameters.

We also have another constraint in model 3 that was not imposed in model 2. The distance \( d \) is symmetrical in the sense that we can have a positive or negative distance depending on whether the photoevent location is to the left or right of the anode center. Thus, our function as shown only represents one-half of the true function, which is symmetric about the origin. Because we must account for all the charge with our full function, the integral under the function must be one. This means the function we actually use to calculate the charge fraction must have an integral of 0.5 under its full extent. This is another reason for changing the meanings of \( A \) and \( B \). In model 2, we did not have the 0.5 integral area constraint. We only had to start at 0.5 and continually decrease until we reached zero. Thus, we could specify \( A \) and \( B \) to be anything we wanted within the size limits. If model 3 was set
up in the manner of model 2, we would have one triangle of known size (that formed by \( B, R + 0.5 \), and the origin) and one of unknown size (that formed by \( AR \), the origin, and the unknown maximum fraction along the \( y \)-axis). We could determine the maximum value by making use of the 0.5 integral area constraint, but we might end up with a case in which the first triangle already exceeds the 0.5 area, forcing a "negative" triangle. At this point, the model breaks down and is meaningless. This is also the downfall of specifying the maximum value as another parameter. The 0.5 integral area constraint would only be satisfied if the three parameters and the radius \( R \) were chosen to make it work. This is too limiting.

By specifying the intersection point instead, we can avoid these problems. We can find the equations for the two triangle lines from the values of \( R, A, \) and \( B \) and the 0.5 integral area constraint without any problem. As with the case of model 2, we must choose our \( A \) and \( B \) with some logic. \( A \) cannot be greater than \( R + 0.5 \), and \( B \) cannot be greater than 1 (in reality we expect it to be much smaller than 1, but 1 is a mathematical limit).

The astute reader will note that it is possible to end up with a maximum fraction value along the \( y \)-axis (when \( d = 0 \)) that is less than the value of \( B \). In this case, the "two-triangle" nature of the function breaks down and the function is simply two lines — one that slopes up to the intersection point from the \( y \)-axis "maximum" and one that slopes down from there to the maximum distance point. This is acceptable as long as the "maximum" \( y \)-axis stays positive. What the function would represent here is a case in which the charge is depleted in the region near the photoevent location due to electron repulsion or a similar effect. While we don't expect this to be the case, it is a physical possibility and the math allows for it. In general, we will have a true "two-triangle" situation in which the charge falls off from the photoevent location in a continually decreasing manner.

With all this in mind, we can now proceed to determine the equations for the two triangles. From triangle 1 and the equation for a line we have
\[ 0 = S_1(R + 0.5) + I_1 . \] (B.11)

At the intersection point

\[ B = S_1A + I_1 . \] (B.12)

Solving equation B.11 for \( I_1 \) yields

\[ I_1 = -S_1(R + 0.5) . \] (B.13)

We can substitute this into equation B.12 and solve for \( S_1 \) to get

\[ S_1 = \frac{B}{A - (R + 0.5)} . \] (B.14)

Next, we rephrase equation B.12 in terms of the second triangle as

\[ B = S_2A + I_2 \] (B.15)

and solve for \( S_2 \) to get

\[ S_2 = \frac{B - I_2}{A} . \] (B.16)

To solve for \( I_2 \), we bring in the 0.5 integral area constraint. We can divide the area under the function into three separate sections. These are the two smaller triangles shown in Figure B.7 and the rectangle with sides of \( A \) and \( B \). The sum of the areas for these three sections must equal 0.5; therefore,

\[ 0.5 = AB + \frac{1}{2}B(R + 0.5 - A) + \frac{1}{2}(I_2 - B)A . \] (B.17)
Solving this equation for $I_2$ yields

$$I_2 = \frac{1 - B(R + 0.5)}{A}.$$  \hspace{1cm} (B.18)

We can now substitute the equations for $S_1$, $I_1$, $I_2$, and $S_2$ into the equation for a line and simplify the expressions to get the following equations for the total charge fractions:

$$f_{\text{charge}} = \frac{B}{A - (R + 0.5)}(d - (R + 0.5)) \quad d \geq A$$  \hspace{1cm} (B.19)

$$f_{\text{charge}} = \frac{B}{A}d + \left(1 - \frac{d}{A}\right)\left(\frac{1 - B(R + 0.5)}{A}\right) \quad d < A.$$  \hspace{1cm} (B.20)

**Model 4: One-Triangle Total Charge Fraction Model**

Model 4 is a simplification of model 3 in which we limit the number of parameters from three ($A$, $B$, and $R$) to just one ($R$). The two triangles of model 3 are replaced with a single triangle that runs from some value on the $y$-axis to the $R + 0.5$ point on the $x$-axis as shown in Figure B.8.

In this model, the only parameter is the radius $R$ of the charge spread. The slope and intercept of the triangle line can be determined from the radius and the 0.5 integral area constraint. We start with the equation for the hypotenuse line, which is

$$f_{\text{charge}} = Sd + I.$$  \hspace{1cm} (B.21)

When $d = R + 0.5$, we have
Figure B.8: Illustration of the one-triangle total charge fraction model. \( R \) is the maximum radius of the charge spread, \( d \) is the distance between the charge spread axis and the center of the anode, and \( I \) is the y-axis intercept of the line.

\[
0 = S(R + 0.5) + I , \tag{B.22}
\]

from which we can solve for \( S \) to get

\[
S = \frac{-I}{R + 0.5} . \tag{B.23}
\]

With the 0.5 integral area constraint, we can say that

\[
0.5 = \frac{1}{2} I(R + 0.5) . \tag{B.24}
\]

Solving this for \( I \) and substituting into equation B.23 yields \( S \) as
Thus, our equation for the line is

\[ f_{\text{charge}} = -\frac{1}{(R + 0.5)^2} d + \frac{1}{R + 0.5} \]  

(B.26)

**B.4.2 Parameter Searches**

Lab measurements exist which constrain the spreading of the electron cloud in a relatively straightforward manner. These data are illustrated in Figure B.9, in which the width (in anodes) of a detected photoevent is related to the total charge associated with the photoevent. The solid line represents the average of all the measurements, while the dotted lines represent the minimum and maximum charges associated with events of the given width.

There are two interpretations of the increase in the width of the detected photoevents with increasing total charge. The first is that the radius of the charge spread on the anodes increases as the total charge does. This would most likely be the result of the mutual repulsion of the electrons, the repulsion being larger when there are more electrons. The second possibility is that the radius of the charge spread on the anodes is constant, but as the total charge in the photoevent increases, the charge on the anodes correspondingly increases such that more anodes register counts.

We cannot distinguish between these two interpretations *a priori*. Thus, we tried both a constant radius and a charge-varying radius in our charge spreading models. The charge-varying radius is defined by

\[ R = R_0 + \left( \frac{q}{\alpha} \right)^\beta \]  

(B.27)
Figure B.9: Illustration of the lab-measured charge spreading and best-fit model. The solid line is the average of all charge measurements at a given event width. The dotted lines represent the minimum and maximum charges at each event width. The dashed line is the best-fit model corresponding to equation B.28. The inset is an expanded view of the plot at small event widths.

where $R_o$, $\alpha$, and $\beta$ are constants to be determined and $q$ is the total charge associated with the photoevent. $R_o$ is included because there should be a minimum radius that the charge spread covers for small charges owing to the distribution of initial electron trajectories and mutual repulsion of the electrons.

To determine the parameters of the four models defined in Section B.4.1, we performed an exhaustive search of parameter space. The parameters searched for were $R$ for models 1 and 4 and $R$, $A$, and $B$ for models 2 and 3. Both the constant $R$ and the charge-varying $R$ as defined by equation B.27 were tried for each model. The resulting best match to the lab data was for model 4 with a charge-varying radius given by
\[ R = 1.3 + \left( \frac{q}{16} \right)^{0.85}. \] (B.28)

This match is shown in Figure B.9 by the dotted line. No acceptable match was found for a constant radius in any of the models. Acceptable matches for the other three models were found with a charge-varying radius, but they were of poorer quality than that for model 4.

Note that the dotted line in Figure B.9 extends down to zero width. This is because some photoevents have charges that are too small to exceed the first threshold level on any anode. We can keep track of these in the model, so they are shown in the figure here.

Note also that the detector gains did not need to be known to determine the charge spreading parameters. The gains are used in the detector assembly model to determine the charges associated with photoevents. In the charge spreading parameter search, we only had to generate charges consistent with the exponential charge distribution (see Section A.2) and cover the range of charges in Figure B.9. Thus, we are able to determine the charge spreading parameters independent of the gains.

## B.5 Detector Gains

The detector gain controls the amount of charge which is associated with any photoevent. As such, it is important to know the gains as well as possible. While a single gain applicable to all regions of the microchannel plates was measured in the lab for each of the various gain states of the UVS, there are several factors which indicate that the lab-measured gains are no longer applicable and that new gains for the UVS must be determined in-flight.

First, the microchannel plates have a finite lifetime (cf. Sandel et al., 1977). The ability of the MCPs to provide charge to each photoevent decreases as
a function of total charge extracted from the plates. This implies that the gain has most likely decreased across the MCPs as a whole and that a single gain is unlikely to be applicable to the entire MCP. Regions of the MCPs exposed to more intense radiation should have lower gains than regions exposed to less radiation.

Second, gain-diagnostic spectra taken in-flight (see Section B.5.1) show that the gain in the region of the MCPs covered by the photocathode is higher than that in the region of the bare MCPs. The cause of this is not fully understood. A contributing factor may be a smaller lifetime decrease in the gain relative to the rest of the MCPs because the low sensitivity of this region has resulted in less charge being extracted over time. This cannot be the sole cause, however, because evidence points to a higher relative gain in this region of the detector in lab measurements prior to flight (see Section C.2.2). Regardless of the mechanism, the gains across the detector cannot be represented by a single value.

Finally, the Voyager 1 UVS suffered from exposure to the high radiation levels of the jovian magnetosphere during the Jupiter encounter. This adversely affected the gain of the instrument and makes an in-flight determination of the gains of the Voyager 1 UVS critical.

Fortunately, there is a means of determining the detector gains in-flight using the ratio of a pulse height mode spectrum to a count mode spectrum of the same source (see Section A.2 for a discussion of the two modes). The only difference between the two modes is the thresholding of the collected charge in the A-to-D converters. Because the pulse height mode converts charge to detector counts using the full thresholding capabilities of the converters, the ratio of a pulse height mode spectrum to a count mode spectrum will run from one (i.e., if one mode gets a count, the other will as well) to seven, depending on the magnitude of the collected charge. Because the amount of charge generated by a photoevent is dependent on the gain, the ratio of pulse height mode to count mode is diagnostic of the gain.

Figure B.10 illustrates models of the ratio of pulse height mode to count
Figure B.10: Dependence of the pulse height-to-count mode ratios on gain and photoevent rate. The curves were generated using the best-fit charge spreading parameterization of Section B.4 and the lab-measured thresholds for Voyager 1. Each point is an average of the 126 channels in the model pulse height-to-count mode ratio spectra. The gains are specified in units of electrons.

mode as a function of the photoevent rate for three gains. We can see that the ratio at a given photoevent rate increases with increasing gain. Thus, if we know the photoevent rate on an anode, we can determine the gain for a given pulse height-to-count mode ratio.

B.5.1 HVL 3 Gains

Because count mode is generally used to observe stars and pulse height mode is almost exclusively used when observing the sun, it is rare for the same source to be observed in both modes. On May 23, 1983, however, the Voyager 1 UVS did make such an observation of the star Beta Centauri. No other such observation exists for the Voyager 1 UVS (a second observation was requested by us in 1994 but was
During the Beta Centauri observations, the Voyager 1 UVS was fixed on
the star, and several hundred spectra were obtained in each mode. As is normally
the case with stellar spectra, the gain state of the UVS was HVL 3, the airglow port
was used to make the observations, and the spectrum duration was 3.84 seconds.
Because the spacecraft is continually making minor attitude adjustments, the star
moved around in the UVS slit according to the limit cycle motion of the spacecraft
(see Section 2.2 for a more detailed discussion of limit cycle motion). We binned the
spectra in each mode according to the limit cycle and normalized the binned spectra
to the duration of a single spectrum. We then determined the absolute position of
the star in the slit in each case and ratioed the pulse height mode spectra to the
count mode spectra for the overlapping bins. The pulse height-to-count mode ratio
was constant over roughly 80% of the overlapping region, with a drop-off occurring
when the spectra were acquired far from the center of the slit, most likely due to
poor signal-to-noise.

Despite the constancy of the ratio across most of the overlapping region, we
only used the spectrum taken in the center of the slit to determine the gains. The
reason for this is two-fold. First, spectra in the center of the slit have the highest
signal-to-noise ratio. Second, because the star is a point source, the spectrum shifts
on the detector depending on the position of the star in the slit (see Section A.1).
As such, the photoevent rate on a given anode changes with the change in the
incoming radiation. Because the knowledge of the photoevent rate is necessary to
determine the gain (see Figure B.10), we do not want to mix photoevent rates by
averaging the spectra over the constant region.

The pulse height-to-count mode ratio spectrum at the center of the UVS
slit is shown in Figure B.11 by the thin line. There are three general regions
in the ratio spectrum. The first covers channels 1-40 and is a region in which
the ratio slowly creeps up as the channel number decreases. This is the region
of the stellar spectra where there is effectively no signal owing to absorption by
Figure B.11: Comparison of the Voyager 1 Beta Centauri pulse height-to-count mode ratio spectrum (thin line) and the corresponding best-fit model (thick line). The poor match near channels 1–6 is due to the uncertain threshold values for anodes 3 and 4.

interstellar hydrogen. Because of the correspondingly low photoevent rate, the exponential charge distribution of the microchannel plates is unlikely to be fully sampled. Therefore, an unusually high charge may skew the pulse height-to-count mode ratio to a higher value than in the case of a fully-sampled distribution. In fact, tests indicate that the curves of Figure B.10 would turn up at the low photoevent rate end if the charge distribution was not statistically sampled. Figure B.10 was generated with a fully-sampled distribution.

The second region of the ratio spectrum covers channels 40-75. In this region the ratio climbs to a higher value and then tapers off again. The initial climb in the ratio corresponds to the edge of the hydrogen continuum absorption region, and a rapid rise occurs in the incoming stellar radiation. Because the stellar signal is highest in this region of the spectrum, we expect the photoevent rates to be high
and the charge distribution to be fully sampled. The detector sensitivity decreases across this region of the spectrum, so the decrease in the ratio after it peaks is most likely due to a decrease in the photoevent rate. Because the photoevent rate changes cause a change in the pulse height-to-count mode ratio, this region of the spectrum corresponds to the photoevent rates of the turn-up in the curves of Figure B.10.

The third and final region of the ratio spectrum covers channels 75-126. In this region, the detector sensitivity is lower than in the second region by more than an order of magnitude. The incoming stellar radiation does not increase such that the sensitivity decrease is offset; therefore, the photoevent rates are lower in this region than in the second. The ratio, however, is much higher, indicating that we must have a higher gain in this region of the detector. As discussed above, this may result from a smaller lifetime gain decrease in this region of the MCPs.

To infer the gains across the detector from the pulse height-to-count mode spectrum, we must know the photoevent rate on each of the anodes. Knowing the photoevent rates, however, relies on knowing the gains. Therefore, we employed the following iterative process:

1. Guess the detector gains.

2. Convert the pulse height mode spectrum to photoevents using the scheme discussed in Section C.2.1.

3. Use the determined photoevents spectrum to get the photoevent rates on each of the anodes and model both a pulse height mode and a count mode spectrum.

4. Ratio the model spectra and compare the result to the ratio of the data spectra.

5. Adjust the detector gains according to the mismatch in the model and data.

6. Repeat steps 2–5 until convergence is achieved.
The gains resulting from this process are shown in Figure B.12. The lab-measured HVL 3 gain for the Voyager 1 UVS was $12 \times 10^5$ electrons, so the in-flight gains are roughly 45% of the lab gain for anodes 1-40, 30% for anodes 41-80, and 75% for anodes 81-126. This variation of the gains across the MCPs is qualitatively consistent with what we'd expect given the observations made by the Voyager 1 UVS between its launch in 1977 and the Beta Centauri observation in 1983. During this time, the Voyager 1 UVS recorded numerous solar and stellar spectra. Solar count rates are high across much of the first and second regions, which hints that these observations are likely the primary source of charge depletion in these regions. The reduction of the second region relative to the first is probably a consequence of the stellar observations. Stellar count rates usually peak in the second region but are almost nonexistent in the first because the stellar flux is absorbed by the interstellar medium. Both solar and stellar count rates drop dramatically in the third region because of the low sensitivity of the MCPs. This is consistent with a
lower overall level of charge depletion and, hence, a smaller gain reduction.

Several consistency checks were performed to ensure that the determined gains are valid. First, the modeled pulse height mode and count mode spectra were compared against the data spectra. Both model spectra were excellent matches to the corresponding data spectra, ensuring that matching the ratio was not just a coincidence.

Second, once the current limiting function was determined (see Section B.6 below), we checked to be sure that the current limiting did not apply to the stellar spectrum. If it had, we would have had to redo the iterative process and include a step between steps 1 and 2 in which we computed a current limiting function. This would have been time-consuming, but fortunately it was not necessary because the stellar observation was not current-limited.

Third, we checked to see if the even channel problem (see Section B.7 below) was of consequence. It is possible that the even channels were affected during the observation, but the degree to which this occurred was minimal and the resulting effect was on the order of the channel-to-channel noise in the ratio spectrum. We therefore neglected any even channel effects.

Finally, because the Voyager 1 solar occultation by Titan occurred in November of 1980, we need to be sure that the gains determined using a ratio spectrum from May of 1983 are valid at the time of the occultation. To check this, we found an observation of Beta Centauri from mid-1980 and binned and normalized the spectra, which were in count mode, as we did the 1983 observation. We then compared the 1980 spectra to the 1983 spectra at the same position in the UVS slit. The spectra matched to well within 5%; therefore, assuming that the flux from Beta Centauri did not coincidentally change to offset a further gain decrease, the 1983 gains should be valid in 1980.

This result is reasonably expected if we evaluate the two most important causes of gain degradation for the Voyager 1 UVS. The first of these is the harsh
environment of the jovian magnetosphere, which affected the Voyager 1 UVS during the Jupiter encounter in 1979. The second is the sun. Solar observations are far and away the most intense the UVS makes. During the years from launch in 1977 to the 1980 Beta Centauri observation, the sun was observed numerous times. The sun was also observed between the 1980 and 1983 Beta Centauri observations; however, other than the solar occultations at Saturn and Titan, there were only a few solar observations of short duration. Because the flux from a source falls off as the square of the distance, the solar radiation was much more intense during the earlier observations. Additionally, the image of the sun's disk on the detector was larger when the spacecraft was closer to the sun, so a larger area of the detector was affected during the earlier observations. While further gain degradation most likely occurred after the 1980 Beta Centauri observation, the magnitude of the degradation is likely to have been small compared to previous degradation.

**B.5.2 HVL 2 Gains**

Because the gain in the HVL 2 state is approximately an order of magnitude lower than that in HVL 3, the sun is the only source that is bright enough to be observed in the HVL 2 gain state. Unfortunately, the sun is too bright to be observed in count mode (all the channels are 1), so we are not able to generate a meaningful pulse height-to-count mode ratio spectrum for HVL 2.

The lab-measured gain for HVL 2 for the Voyager 1 UVS is $1.4 \times 10^5$ electrons, which is a factor of 8.6 lower than the lab-measured gain for HVL 3. Because the gains in the two gain states should decrease in roughly the same proportion, it is reasonable to assume that the in-flight HVL 2 gains are roughly in the same ratio to the HVL 3 gains as in the lab. We assumed this at the start of the current limiting determination (see Section B.6), but eventually had to increase the factor to 10 to obtain a self-consistent result. Thus, the final HVL 2 gains are a factor of 10 lower than the HVL 3 gains shown in Figure B.12.
B.6 Current Limiting

At very high photoevent rates, the ability of the microchannel plates to replenish electrons to the illuminated region of the MCPs is exceeded because electrons are removed faster than they can be replaced. This results in an effective reduction in the gain of the MCPs. This phenomenon is referred to as current limiting because the current which restores electrons to the MCPs is the limiting factor. The size of the illuminated region of the MCPs plays an important role in the current limiting process as well. The larger the region, the greater the current limiting effects.

The current limiting characteristics of the Voyager UVS instruments were measured in the lab prior to launch. A functional representation was developed in which a gain reduction factor could be determined as a function of the product of the nominal gain and the photoevent rate. The nominal gain of the instrument would then be divided by this factor to yield the effective gain.

The lab-measured current limiting function was developed using an aperture such that the projected image of the source on the MCPs was equivalent in size to the imaged disk of the sun at Jupiter’s orbit. It was also developed from measurements made with the instrument when the MCPs had not suffered any in-flight gain degradation. Neither of these was true during the Voyager 1 solar occultation by Titan, so the lab-measured current limiting function is not valid for our purposes. Current limiting definitely plays a role in the high photoevent rates encountered when observing the sun, so a new function must be developed.

Approximately two months after the Titan encounter, the Voyager 1 UVS executed two “suncals”. A suncal is an observation in which the UVS slit is slewed across the sun. Because the Titan and Saturn solar occultations employed both the HVL 2 and HVL 3 gain states, one suncal was in HVL 2 and the other was in HVL 3. These two suncals provide the information we need to determine an in-flight current limiting function applicable to the time of the Titan solar occultation.
The following iterative procedure was used to determine the current limiting function:

1. Generate a current limiting function.
2. Generate an even channel correction factor grid (see Section B.7).
3. Convert both the HVL 2 and HVL 3 suncals from counts to photoevents using the scheme discussed in Section C.2.1.
4. Sum the 126 channels of each spectrum to produce a total number of photoevents for each spectrum.
5. Compare the profile of photoevents for the HVL 2 suncal against the HVL 3 profile.
6. Adjust the current limiting function according to the mismatch in the profiles.
7. Repeat steps 2–6 until convergence is achieved.

Because the parameterization of the charge spreading and the determination of the detector gains (under the caveat mentioned in Section B.5.1) do not depend on the current limiting function, we may be reasonably assured that the above procedure results in a valid current limiting function. The determination of the current limiting function is linked to the even channel correction factor grid; however, this correction depends on the gains, charge spreading parameterization, and current limiting function and not vice versa (see Section B.7).

As a check on this procedure, two tests were performed once the procedure converged to a solution. We selected several pairs of HVL 2 and HVL 3 spectra. Each HVL 2 spectrum was taken at the same position in the UVS slit as the HVL 3 spectrum in the pair, and the chosen pairs spanned the entire slit function. In the first test we compared the HVL 2 and HVL 3 photoevents spectra of step 3 above to be sure that the spectral shapes matched as well as the sum of the 126
channels. Because the same solar spectrum gave rise to each data spectrum, the photoevents spectra should be the same regardless of the gain state. In the second test we generated model counts spectra from the photoevents spectra and compared these against the data counts spectra of the same gain state (i.e., model HVL 2 was compared against data HVL 2).

In both comparisons, the match was fair. Of the various detector model parameters thus far determined, the HVL 2 gains are the most uncertain. Therefore, we enclosed the entire iterative procedure in a new loop that searched for the optimal HVL 2 gains. The resulting HVL 2 gains were a factor of 10 smaller than the HVL 3 gains, and the comparison tests then yielded acceptable matches.

The final current limiting function is plotted in Figure B.13. Note that the function is constant at 1 until a certain value of the gain-photoevent rate product. This is because current limiting only occurs when the photoevent rate is high.

Figure B.13: Plot of the best-fit current limiting function for Voyager 1. The solid line represents the determined function, while the dashed line is an extrapolation at the end of the measured range. The intersection of the curve with the x-axis indicates the point below which the gain/photoevent rate product is small enough that current limiting does not occur.
Figure B.14: Comparison of the HVL 2 and HVL 3 sunsels processed with the best-fit current limiting function. The mismatch at negative slit locations is explained in the text.

The profiles of summed photoevents for the HVL 2 and HVL 3 sunsels corresponding to the current limiting function of Figure B.13 are shown in Figure B.14. The poorer match of the profiles at negative slit locations is due to the H Lyman α line shifting onto the photocathode. When this happens, the photoevent rates associated with the H Lyman α line increase, and this increase is substantial enough to push the detected signal in the HVL 3 gain state into saturation. We cannot determine the true photoevent rate for a saturated signal, so the inferred rate is too low (see Section C.2.1). This does not represent a problem for us in any event because the Titan occultation is confined to positive slit locations where the match is excellent.
B.7 Even Channel Correction Factor

When the counting rate is high, a second phenomenon occurs in the Voyager UVS in addition to current limiting: the even-numbered anodes of the detector do not function correctly. Examples of this are shown in Figures B.3 and B.16, in which we see that the even channels of the spectrum are significantly lower than the odd channels to either side. We refer to this phenomenon as the "even channel problem".

While current limiting is expected to occur, the failure of the even anodes to work correctly is puzzling. The problem was never observed in the lab; indeed, when trying to determine the cause, we used the Voyager UVS prototype to observe a source of adequately high intensity and the even anodes functioned properly. It is only after launch that the problem began to be observed, and it affects both the Voyager 1 and 2 UVS instruments. A problem with the even anodes in both flight instruments is too coincidental and hints at a fabrication origin, but this does not explain why the prototype is unaffected or why the flight units did not exhibit the problem in the lab. We should note, however, that the proper conditions for observing the problem may not have been achieved in the pre-flight tests.

We know that the even anodes are the problem because the even and odd channels of a spectrum are similar in intensity until the counting rates are high, at which point the even channels begin to lag the odd channels. Further evidence of an origin in the even anodes is that all the even channels of an affected spectrum, even those at much different signal levels, begin to suffer at the same time. The anode array is fabricated such that all the even anodes are read-out through a common system that is separate from the common read-out system of the odd anodes. The simultaneous occurrence of the problem in all the even channels strongly points to an origin in the read-out system of the even anodes.

Regardless of the origin, to achieve full spectral resolution we must correct for the effect when we process the spectra of the Titan solar occultation because any observation of the sun, regardless of the gain state, results in high enough counting
rates to cause the even channel problem. At first, this may seem to be a daunting problem, but two characteristics of the problem hint at a possible solution. The first is that all the even channels are affected simultaneously, regardless of the local intensity on a given anode. This suggests that the anodes are affected when the overall signal on all the even anodes reaches a certain level. The second is that the magnitude of the problem increases as the overall signal increases. A given even channel may lag behind the adjacent odd channels by 10% at one level but by 20% when the overall signal level increases.

With these two characteristics in mind, we hypothesized that the charge collected by the even anodes was somehow being "lost" when the total charge on all the even anodes exceeded a certain level. If charge were lost, the number of counts caused by the charge on the even anodes would be smaller than it should have been. If more charge were lost as the total charge increased, the counts level would be reduced even more. There are a number of scenarios involving the readout electronics in which this would be the effective result, but none of them is easily proven and we do not go into details. Instead, we assume that this is the case. Then, we only have to develop a relationship for the amount of charge lost as a function of the total charge on the even anodes.

Figure B.15 illustrates our solution to the problem. The fraction of charge that is retained on each even anode is plotted as a function of the total number of counts in the odd channels of the spectrum and the ratio of the total number of even-channel counts to the total number of odd-channel counts. The relationship plotted in this figure was developed empirically by modeling spectra for a wide range of photoevent rates (to cover all possible values of odd-channel totals) while the charge fraction retained was varied from 0.05 to 1 (to cover all possible values of even-channel totals). For each model spectrum, we calculated the total number of counts on the odd channels and the ratio of the total even-channel counts to total odd-channel counts and related the results to the charge fraction retained for that spectrum. In this manner, we mapped out the entire "space" of count totals that
Figure B.15: Plot of the even channel correction factor grid for Voyager 1. The grid flattens out as the even-to-odd channel ratio approaches one. The abrupt edge at small values of odd channel totals is caused by poor statistics, but this region of the grid represents one that is never accessed by real data.

can be accessed by UVS spectra. The points resulting from this mapping procedure were irregularly spaced, so we interpolated them onto a regular grid. Now, when converting an observed spectrum from counts to photoevents (see Section C.2.1), we simply sum the number of counts in the even and odd channels of the spectrum, interpolate the fraction of charge retained on the even anodes using this grid, and apply that fraction as a correction factor during the linearization procedure. Because the grid relates charge retained to recorded counts, it is not dependent on the gain state and may be used equally well for both HVL 2 and HVL 3 spectra.

Figure B.16 shows how well this simple correction works. The top panel shows an observed solar spectrum which suffers from the even channel problem. The bottom panel shows the photoevents spectrum inferred using the method of
Figure B.16: Illustration of the effectiveness of the even channel correction factor grid. The upper panel shows a data counts spectrum (thin line) and the corresponding model counts spectrum (thick line). The lower panel shows the photoevents spectrum resulting from processing the data counts spectrum using the methods of Appendix C. The match between the spectra in the upper panel is excellent, and the processed spectrum in the lower panel shows no residual even channel problem.
Section C.2.1 and the even channel correction factor grid of Figure B.15. Finally, the top panel also shows the inferred photoevents spectrum converted back to counts, illustrating that a simple charge loss can be used to adequately model the even channel problem.

It should be noted that the even channel correction factor grid was developed for use in processing Voyager UVS spectra. Thus, the quantities needed to use the correction factor grid are those obtainable from an observed spectrum. If we wish to model a counts spectrum from a given photoevents spectrum, perhaps for prediction purposes, we cannot use the grid directly because we do not know how many counts the photoevents spectrum will yield. We can, however, perform an iterative method in which a fraction is guessed, the counts spectrum modeled, and the resulting counts used to infer a new fraction, repeating these steps until convergence is achieved.
APPENDIX C

PROCESSING VOYAGER UVS SPECTRA

Before Voyager UVS spectra can be analyzed, they must be processed to remove a number of instrumental effects. The manner in which this is done depends on the source that is observed and the operating mode of the detector. There are four possible categories into which spectra are thus divided: 1) count mode spectra of stellar or extended sources; 2) pulse height mode spectra of the sun; 3) pulse height mode spectra of stellar or extended sources; and 4) count mode spectra of the sun.

Practically every Voyager UVS spectrum falls into one of the first two categories. Because of this, standard practice when discussing UVS spectra is to adopt a naming convention in which count mode and stellar or extended source spectra are synonymous and in which pulse height mode and solar spectra are synonymous. That convention is followed here.

We will not discuss the remaining two categories. Category 3 spectra are extremely rare, and while they can be processed, the procedure is a special one. Category 4 spectra exist only because of mistakes in the UVS command sequencing. They are useless because the high intensity of the sun causes almost all of the detector anodes to register a count, generating a nearly flat, featureless spectrum.

C.1 Stellar or Extended Source Spectra

Stellar or extended source spectra (count mode spectra) are the most common type of Voyager UVS spectra, and the processing procedure is well established. Because
this work is primarily concerned with the Voyager 1 solar occultation by Titan, we provide only a brief summary of the procedure here. A more detailed discussion may be found in Holberg and Watkins (1992).

Count mode spectra are first corrected for the anode-to-anode variations in the detector thresholds via application of a correction spectrum. This is known as the fixed pattern noise (FPN) correction and is equivalent to the flat-fielding often performed on astronomical images. The FPN-correction spectrum also includes a factor relating detector counts to photoevents and application of the correction implicitly makes this conversion.

A background spectrum is next subtracted from the FPN-corrected spectrum. This background spectrum is due primarily to the radioisotope thermoelectric generators (RTGs) on the spacecraft and represents a non-photon source in the observed spectrum.

After the background subtraction, instrumentally-scattered light is removed from the spectrum. To do this, the spectrum is multiplied by the inverse of a 126 x 126 matrix determined from lab measurements of the scattering characteristics of the UVS. This matrix describes the relative intensity on anode X due to a signal on anode Y for each of the 126 anodes of the detector. The process of removing the instrumentally-scattered light is referred to as "descattering" the spectrum. It is important to note that the descattering matrix can only be applied to a spectrum of photoevents.

Finally, the spectrum is multiplied by a calibration spectrum which accounts for the various efficiencies of the detector and grating. This yields the final, processed spectrum in absolute flux units.
C.2 Solar Spectra

Solar spectra (pulse height mode spectra) require a different procedure than stellar or extended source (count mode) spectra. An equivalent to the flat-fielding of the FPN-correction is performed, but the process is more complicated because of nonlinear effects introduced by the high counting rates of the solar spectrum. This process is known as "linearization" and is described in detail below.

The background removal step is not necessary because the background count rates are insignificant when compared to the count rates of the solar spectrum. After linearization, solar spectra are descattered, but the procedure is again more complicated than for count mode spectra (see Section C.2.2 below). Finally, although an absolute calibration is possible, this step is not performed in the analysis of solar occultation spectra because the calibration divides out in the ratio of $I$ and $I_o$ spectra.

C.2.1 Linearization

At low counting rates, the relationship between the number of photoevents on a given anode and the number of counts that they will generate is linear. This is the reason that a simple factor may be applied in the FPN-correction of stellar and extended source spectra. When the intensity of the incoming radiation is high, however, the Voyager UVS detector behaves in a nonlinear fashion, and the number of photoevents corresponding to a given count level increases dramatically as the counts level increases. This nonlinearity is due to a combination of the A-to-D conversion of near-saturation charges in pulse height mode and the effects of current limiting on the gain.

The nature of the descattering matrix requires that spectra be converted
from detector counts to photoevents prior to its application. Therefore, the nonlinear relationship between counts and photoevents in solar spectra must be understood so that the conversion can be properly performed. This conversion process is referred to as "linearization" because through it, the nonlinear effects are corrected and the resulting photoevents spectrum may be further processed using the standard linear operations (descattering and calibration).

Prior to this work, the linearization process was performed using a simple analytical relationship between counts and photoevents. Figure C.1 is a plot of one such relationship, referred to as a "linearization curve". The nonlinearity of the relationship between counts and photoevents is obvious. To linearize a spectrum, we would divide the counts in each channel of a spectrum by the number of scans to produce counting rates (counts per scan). Then, we would find the corresponding

![Figure C.1: Example of an analytical linearization curve. This curve was generated using a detector gain of \(5 \times 10^5\) electrons, the nominal threshold value of \(2.5 \times 10^5\) electrons, a uniform illumination, and an analytical model based on simple assumptions about charge spreading. The various regimes of detector operation are indicated.](image)
photoevent rates using the linearization curve and multiply by the number of scans
to convert the photoevent rates to photoevents. A single curve was used for the
entire spectrum.

There are several problems inherent in the linearization curve approach. The analytical model upon which it is based requires that the threshold levels
and gains of every anode be the same. The number of photoevents is derived
using Poisson statistics, which the UVS obeys, and the corresponding charges are
derived using the measured exponential pulse height distribution, but the resulting
values are statistical averages which are not applicable in many situations. Ideally,
the illuminating spectrum must be uniform over a range of anodes such that the
photoevent rates and derived charges are the same on each anode, but the solar
spectrum is highly variable across the wavelength range of the UVS. Finally, the
even channel problem is not addressed by the analytical model, and in earlier work
the even channels in the resulting photoevents spectrum were obtained by averaging
the adjacent odd channels. This can severely bias the photoevents spectrum when
a line is centered on an even channel.

With the exception of the statistical averages, all of the above problems may
be overcome through an improved version of the analytical model. Unfortunately,
correcting the even channel problem and accounting for nonuniform illumination
require that a new set of 126 curves be developed for each spectrum to account
for the channel-to-channel variations in intensity and the subsequent blending of
charges on the detector anodes. Although the model is an analytical one, generation
of a complete set of linearization curves takes too long to be of any practical use.

To avoid the problems introduced by using the linearization curves, we
have developed a new method of linearization. We use an iterative procedure in
combination with the Monte Carlo detector model of Appendix B. By using the
Monte Carlo detector model, we avoid the problem of statistical averaging inherent
in the linearization curves. Taken over many spectra, the average signal on a given
channel satisfies the necessary Poisson statistics, but each individual spectrum more
closely approximates the randomness of a statistical distribution that is not fully sampled.

The following is an outline of the procedure:

1. Guess an initial photoevents spectrum.

2. Generate a model counts spectrum from the photoevents spectrum.

3. Compare the model counts spectrum to the data counts spectrum.

4. Adjust the photoevents spectrum in accordance with the mismatch in the model and data counts spectra.

5. Repeat steps 2–4 until convergence is achieved.

The adjustment of step 4 is critical to both obtaining an accurate photoevents spectrum and minimizing the time to linearize a spectrum. Despite its problems when used directly, the linearization curve provides a simple way to perform this step. The method is illustrated in Figure C.2 for a single channel. We have 126 such “curves” for the entire spectrum.

We start with the origin and a second point, \( A \). Point \( A \) is determined by choosing photoevent rates for each channel and modeling a counts spectrum. The line between the origin and point \( A \) is then used to guess the initial photoevents spectrum of step 1 by using the photoevent rate corresponding to the data count rate in the given channel.

After the model counts spectrum has been generated, we have a new point, \( B \), which denotes the count rate corresponding to our initial guess at the photoevent rate for this channel. We establish a new line by choosing the two points whose count rates either bracket or are closest to the actual data count rate, and we then estimate the photoevent rate for the next iteration using this line.
Figure C.2: Illustration of the iterative linearization scheme. The dashed line is representative of the data count rate for the spectrum that is being processed. The procedure is discussed in the text.
The next iteration will result in yet another point, $C$. Continuing in this manner will eventually narrow in on the correct photoevent rate for the given channel. The iterative procedure is stopped when further iterations do not yield substantially different results.

An advantage to this method of linearization is that we are able to estimate the uncertainty in the final photoevents spectrum. By repeating the iterative procedure $X$ times, each time starting at a different point $A$, we will get $X$ different photoevents spectra. This is because the photoevents spectrum is non-unique — any one of a number of slightly different photoevents spectra can yield the same counts spectrum because of variations in charge magnitude and spreading. We can then average these spectra to produce a mean photoevents spectrum with standard deviations for each channel.

Because the Monte Carlo model uses random numbers, we are occasionally thrown off in the iterative procedure (e.g., when a particularly large charge results in a point that sends the photoevent rate well away from the true rate). To eliminate this problem, we do the spectrum averaging twice. The first time, we average all the spectra. Then, we use the mean and standard deviation from this averaging to eliminate the anomalies by reaveraging the spectra but excluding any channel whose value is more than five sigma from the original mean. This yields a new mean and standard deviation for each channel.

This new method of linearization represents a substantial improvement over the previous method. We are now accounting for the anode-to-anode variations in detector gain and counting threshold, the variation in the illumination across the detector, the even channel problem, and the statistical uncertainty in the spectrum.

### C.2.2 Descattering

Before any Voyager UVS spectrum can be analyzed, we must remove the effects of instrumentally-scattered light from the spectrum. Instrumentally-scattered light
represents light at wavelength X which falls onto the anode of the detector intended for light of wavelength Y. This scattered component was long believed to originate in the use of a mechanical collimator; however, a comparison of Voyager UVS spectra to spectra from the Galileo EUV has shown otherwise.

The Galileo EUV is a slightly altered version of the Voyager UVS, the primary differences being a shift in the covered wavelength range and the use of a holographic grating. The comparison of spectra revealed a substantially reduced scattered light component despite the use of a similar mechanical collimator, which demonstrated that grating imperfections are the primary source of the scattered light and not the collimator.

The scattered light component of a Voyager UVS spectrum is removed through the linear application of a $126 \times 126$ matrix to the spectrum. This process is referred to as “descattering” the spectrum. The rows of this matrix represent the scattering profiles for each anode of the detector, essentially yielding the fraction of a photon in channel X that ends up in each of the other channels of the spectrum. The matrix was determined pre-flight in the lab by recording the spectrum of a monochromatic light source at many different wavelengths and compiling the results.

As straightforward as the descattering procedure appears, there are several problems that exist. First, the descattering matrix was determined for an on-axis source. Because the majority of spectra are measured when the source is off-axis, the scattered light characteristics are most likely different than those inherent to the matrix. However, it is impossible to account for every possible source position, and as long as the source is near the center of the slit, we must assume that the descattering matrix is applicable.

Second, the descattering matrix is based upon measurements of spectra. This means that the matrix has the gain of the detector built into it. The scattering “wings” of a line source at H Lyman alpha, for example, are not equal. The wing overlying the long wavelength end of the detector, where the filter is located, is at
a higher level than the wing overlying the short wavelength portion of the detector. This is caused by the higher gain of the filter region. The implication here is that the descattering matrix is based upon gains that no longer apply to the detector owing to the in-flight gain degradation of the microchannel plates. Thus, the descattering matrix is likely to overestimate the amount of scattered light in a UVS spectrum.

Third, the descattering matrix was developed for use with the fixed pattern noise correction applied to stellar spectra (see Section C.1). The FPN correction does not account for the gain variations of the detector. With solar spectra, however, the linearization procedure (see Section C.2.1) removes the effect of gain variations across the detector. Thus, when the descattering matrix is applied, the gain signature inherent to the matrix alters the spectrum's shape. This was not a problem in the past because the former linearization procedure used a single detector gain. By accounting for the gain variations, we have been forced to apply a "shape factor" to the spectra prior to descattering to yield a spectral shape consistent with what it expects. After descattering, this "shape factor" may be removed to restore the correct spectral shape.

Fourth, there is the observation that the scattered light characteristics differ for the occultation and airglow ports, primarily in the level of the scattered component, which is smaller for the occultation port. It is easy to understand this in terms of the mechanical collimator, which has fewer scattering edges in the occultation port, but not so easy in terms of grating imperfections. However, a descattering matrix developed for the occultation port of Voyager 2 shows similar scattered light features spectrally but a lower overall level of scattered light. A similar matrix for the Voyager 1 occultation port was not determined, but we have created one by applying the ratio of the Voyager 2 airglow and occultation port matrices to the Voyager 1 airglow port matrix.

Finally, the filter edge has historically been "over-descattered" such that the resulting spectrum is negative over the three to four channels that bracket the filter edge. We have discovered that this is caused by the removal of scattered light.
from the short wavelength channels and not the channels closer to the filter edge. Because the scattering wings fall off rapidly away from a given channel, we have simply eliminated the scattering wings at the filter edge from the shorter wavelength channels. The resulting descattering matrix yields spectra with a reasonable spectral shape at the filter edge.

In the end, the descattering procedure is an uncertain but necessary one because of the potential for misinterpretation of atmospheric absorption. The uncertainties associated with the descattering matrix are unknown and are difficult to estimate. Instead, we have generated two sets of light curves, one from descattered spectra and the other from non-descattered spectra, and compared them. From this comparison, we estimated the percent uncertainty in each of the channels, which ranged from 10 to 30% across the spectrum. These percentages were applied to the final uncertainties from the processing procedure of Chapter 2 to yield the final light curve uncertainties.
APPENDIX D

PHOTOABSORPTION CROSS SECTIONS

The following sections describe how the photoabsorption cross sections for a number of species relevant to Titan’s atmosphere have been compiled. For each species, we give a general description of the source of the data and the means by which we combined various data sets. If multiple sources exist for a given species, we show a table in which the sources for the cross sections are specified according to the relevant wavelength and temperature ranges. Finally, we show figures that illustrate the cross sections as a function of wavelength. These figures show the room temperature cross sections only because any temperature dependence is not visible on the scale of the figures.

In compiling the data, it soon became evident that more laboratory work is desperately needed in this field. Many of the cross section measurements are decades old and should be redone. At the same time, measurements are needed at the range of temperatures applicable to planetary atmospheres because lower temperatures generally yield larger cross section values, especially for band absorptions where the temperature affects the relative populations of the rovibrational levels. Although the temperature dependences measured to date indicate only minor changes in the relevant range, the wavelength and temperature coverage thus far is minimal and general conclusions should not be made. Unfortunately, it is difficult to work in the vacuum ultraviolet and most of the measurements being carried out today are in the more accessible far ultraviolet range.

We also note that problems may exist in the available cross sections. As an example, Bénilan et al. (1995) demonstrated that the most widely accepted C₂H₂
cross sections are contaminated by absorption due to acetone. C$_2$H$_2$ is unstable in air, so it must be stored in either an inert gas (e.g., He) or dissolved in acetone. The latter has been the method used in most of the recent measurements of the C$_2$H$_2$ cross sections. Bénilan et al. pointed out that two supposed “hot bands” (i.e., band absorptions that disappear at cooler temperatures) observed in cross section data for C$_2$H$_2$ at 195 K but absent at 155 K are actually acetone absorption features. At the cooler temperatures, acetone has condensed and no longer contaminates the absorption spectrum; hence, the “hot bands” go away. It is unknown whether similar contaminations exist at shorter wavelengths (the example of Bénilan et al. was for wavelengths near 1900 and 1950 Å) or in other species, primarily because no one has looked for them in the past. As such, all the cross section data given here should be considered the best we have but not necessarily the best there is.

Our preferred units for the photoabsorption data are cross section in cm$^2$ versus wavelength in Å. Much of the compiled cross section data was originally specified in other units. Where necessary, the data have been converted to our preferred units using the following equations:

$$\lambda(\text{Å}) = \frac{12400.0}{E(\text{eV})} = \frac{10^8}{\nu(\text{cm}^{-1})} \quad (D.1)$$

$$\sigma(\text{cm}^2) = 1.0975 \times 10^{-16} \frac{df}{dE} \text{(eV}^{-1}) = \frac{k(\text{cm}^{-1})}{26.8675484 \times 10^{18}} \quad (D.2)$$

### D.1 Molecular Nitrogen (N$_2$)

The photoabsorption cross sections for N$_2$ were taken from Chan et al. (1993), Fennelly and Torr (1992), Stark et al. (1992), and Dalgarno et al. (1967).

The Chan et al. data were generously provided in digital format as differential oscillator strength in eV$^{-1}$ versus energy in eV by G. Cooper and C. E. Brion. The oscillator strengths were converted to photoabsorption cross sections.
in cm$^2$ using equation D.2, and the energies were converted to wavelengths in Å using equation D.1. This data set covers the wavelength range of 550 to 1030 Å at a temperature of 295 K, with the resolution varying from 0.25 Å at short wavelengths to 0.9 Å at long wavelengths.

Fennelly and Torr also kindly provided their data in digital format as photoabsorption cross section in cm$^2$ versus wavelength in Å. This data set covers the wavelength range of 24 to 986 Å. Because the cross sections were determined for use with a standard solar reference spectrum, the resolution varies across the wavelength range, but it is generally between 0.2 and 0.8 Å. This data set is actually a compilation of several other data sets, so it is likely that the temperature corresponding to the cross sections varies; however, they were all most likely obtained at room temperature, and we assume that 295 K applies to them all.

The Stark et al. data were obtained in digital format as photoabsorption cross section in cm$^2$ versus wavenumber from the Harvard Center for Astrophysics WWW site. The wavenumbers were converted to wavelengths in Å using equation D.1. This data set covers several short wavelength ranges of 2–3 Å each between 958 and 994 Å. The resolution of each range is 4.5 x 10$^{-4}$ Å, and the temperature is 295 K.

The Dalgarno et al. data were taken from their Table 2. These are theoretical Rayleigh scattering cross sections covering the wavelength range of 1200 to 2000 Å. The relatively smooth wavelength dependence allows these points to be specified every 100 Å. The temperature is assumed to be 295 K. These data have been scaled to match a measurement of the N$_2$ Rayleigh scattering cross section at 1216 Å by D. Shemansky (B. Sandel, personal communication, 1996).

To construct the actual data set used in the calculations, we chose the highest resolution data available in any given wavelength range. Table D.1 shows which data set was used in the specified wavelength intervals. Figure D.1 shows the final photoabsorption cross sections used for N$_2$. 
Table D.1: N₂ Cross Section Data

<table>
<thead>
<tr>
<th>λ (Å)</th>
<th>All temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>24–986</td>
<td>Fennelly and Torr (1992)</td>
</tr>
<tr>
<td>986–1030</td>
<td>Stark et al. (1992)</td>
</tr>
<tr>
<td>1030–2000</td>
<td>Chan et al. (1993) where available</td>
</tr>
<tr>
<td></td>
<td>Dalgarno et al. (1967)†</td>
</tr>
</tbody>
</table>

† Scaled as indicated in the text.

Figure D.1: N₂ photoabsorption cross sections. The inset shows a close-up of one of the high-resolution regions measured by Stark et al. (1992). We do not show the full set of high-resolution cross sections because they plot as solid, dark bands owing to the small wavelength spacing.
D.2 Atomic Nitrogen (N)

The photoabsorption cross sections for atomic N were taken from Fennelly and Torr (1992), who kindly provided their data in digital format as photoabsorption cross section in $\text{cm}^2$ versus wavelength in Å. This data set covers the wavelength range of 31 to 860 Å. Because the cross sections were determined for use with a standard solar reference spectrum, the resolution varies across the wavelength range, but it is generally between 0.2 and 0.8 Å. This data set is actually a compilation of several other data sets, so it is likely that the temperature corresponding to the cross sections varies; however, they were all most likely obtained at room temperature, and we assume that 295 K applies to them all. Although these data are actually the photoionization cross sections of atomic N, the ionization efficiency is approximately one at these wavelengths, and we may assume they represent the photoabsorption cross sections. This data set is assumed to be valid for all temperatures. Figure D.2 shows the final photoabsorption cross sections used for atomic N.

![Figure D.2: N photoabsorption cross sections.](image-url)
D.3 Methane (CH₄)

The photoabsorption cross sections for CH₄ were taken from Au et al. (1993), Samson et al. (1989), Mount et al. (1977), and Mount and Moos (1978).

The Au et al. data were generously provided in digital format as differential oscillator strength in eV⁻¹ versus energy in eV by G. Cooper and C. E. Brion. The oscillator strengths were converted to photoabsorption cross sections in cm² using equation D.2, and the energies were converted to wavelengths in Å using equation D.1. This data set covers the wavelength range of 248 to 1550 Å at a temperature of 295 K, with the resolution varying from 0.6 Å at short wavelengths to 3.0 Å at long wavelengths.

The Samson et al. data were taken from their Table II and cover the wavelength range of 100 to 950 Å. The Mount et al. data were taken from their Table 1 and cover the wavelength range of 1370 to 1600 Å. Both data sets have a resolution of 10 Å and were measured at a temperature of 295 K.

Mount and Moos provide a measurement of the temperature dependence of the CH₄ cross section. This is in the form of a ratio as a function of wavelength between the cross section at 200 K and the cross section at 295 K. The dependence is shown in their Figure 2, and it exhibits a slow drop-off in the cross section with increasing wavelength at the lower temperature, starting at roughly 1410 Å.

A comparison of the three data sets at 295 K shows general agreement in the regions of overlap. The agreement between the Au et al. data and the Mount et al. data is puzzling given the mismatch between data for C₂H₆ by the same authors (see Section D.6). With no definitive reason to choose one data set over another, we averaged the data sets in the regions of overlap. The actual data set used in the calculations was constructed as indicated in Table D.2 for the possible temperature ranges. Figure D.3 shows the final photoabsorption cross sections used for CH₄.
Table D.2: CH$_4$ Cross Section Data

<table>
<thead>
<tr>
<th>$\lambda$ (Å)</th>
<th>$T \leq 200$ K</th>
<th>$200$ K $&lt; T &lt; 295$ K</th>
<th>$T \geq 295$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>100–248</td>
<td>Samson et al. (1989)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>248–950</td>
<td>Average of Au et al. (1993) and Samson et al. (1989)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>950–1370</td>
<td>Au et al. (1993)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1370–1410</td>
<td>Average of Au et al. (1993) and Mount et al. (1977)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1410–1550</td>
<td>Average of Au et al. (1993) &amp; Mount et al. (1977)$^{\dagger}$</td>
<td>Interpolated</td>
<td>Average of Au et al. (1993) &amp; Mount et al. (1977)</td>
</tr>
<tr>
<td>1550–1600</td>
<td>Mount et al. (1977)$^{\dagger}$</td>
<td>Interpolated</td>
<td>Mount et al. (1977)</td>
</tr>
<tr>
<td>1600–1800</td>
<td>Extrapolated from 1550–1600 Å data</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$^{\dagger}$ Scaled to 200 K according to the temperature dependence shown in Figure 2 of Mount and Moos (1978).

Figure D.3: CH$_4$ photoabsorption cross sections.
D.4 Acetylene (C2H2)

The photoabsorption cross sections for C2H2 were taken from Cooper et al. (1995), Smith et al. (1991), Xia et al. (1991), and Suto and Lee (1984).

The Cooper et al. data were generously provided in digital format as differential oscillator strength in eV\(^{-1}\) versus energy in eV by G. Cooper and C. E. Brion. The oscillator strengths were converted to photoabsorption cross sections in cm\(^2\) using equation D.2, and the energies were converted to wavelengths in Å using equation D.1. This data set covers the wavelength range of 245 to 2450 Å at a temperature of 295 K, with the resolution varying from 0.5 Å at short wavelengths to 7.0 Å at long wavelengths.

The Smith et al. data were obtained in digital format as photoabsorption cross section in cm\(^2\) versus wavenumber via ftp transfer from the Harvard Center for Astrophysics World Wide Web site. The wavenumbers were converted to wavelengths in Å using equation D.1. This data set covers the wavelength range of 1370 to 1740 Å at a temperature of 295 K and the range 1470 to 2015 Å at a temperature of 195 K at a resolution of roughly 0.035 Å. We interpolated these data onto a 0.5-Å grid because the resolution is much higher than warranted for our purposes, and this makes the calculations more tractable.

The Xia et al. data were digitized from their Figure 8 and cover the wavelength range of 1060 to 1100 Å at a temperature of 295 K. The data were sampled approximately every 0.2 Å during the digitization.

The Suto and Lee data were digitized from their Figures 1 and 3 and cover the wavelength range of 1060 to 1400 Å at a temperature of 295 K. The data were sampled approximately every 1.0 Å during the digitization.

A comparison of the Xia et al. data with that of Cooper et al. and Suto and Lee shows that the absolute level of the Xia et al. data is inconsistent with the other two sets although the relative structure is consistent. Because the Cooper
et al. and the Suto and Lee data are consistent with each other, we conclude that the Xia et al. data suffer from a slight absolute calibration error and scale the overall level of that data set until it matches the other data sets averaged over the wavelength interval.

To construct the actual data set used in the calculations, we chose the highest resolution data available in any given wavelength range. Table D.3 shows which data set was used in the specified wavelength intervals for the possible temperature ranges. Figure D.4 shows the final photoabsorption cross sections used for C$_2$H$_2$.

D.5 Ethylene (C$_2$H$_4$)

The photoabsorption cross sections for C$_2$H$_4$ were taken from Cooper et al. (1995) and Zelikoff and Watanabe (1953).

The Cooper et al. data were generously provided in digital format as differential oscillator strength in eV$^{-1}$ versus energy in eV by G. Cooper and C. E. Brion. The oscillator strengths were converted to photoabsorption cross sections in cm$^2$ using equation D.2, and the energies were converted to wavelengths in Å using equation D.1. This data set covers the wavelength range of 248 to 2480 Å at a temperature of 295 K, with the resolution varying from 0.8 Å at short wavelengths to 6.5 Å at long wavelengths.

The Zelikoff and Watanabe data were digitized from their Figures 1, 2, and 3 and cover the wavelength range of 1065 to 1970 Å at a temperature of 295 K. The data were sampled approximately every 1.0 Å during the digitization.

Cooper et al. compare their photoabsorption cross sections to those of Zelikoff and Watanabe and note that there is an absolute level difference between the two data sets, with the Zelikoff and Watanabe data being lower. Cooper et al. give a detailed explanation of this discrepancy, the main point of which is that the Zelikoff and Watanabe data suffer from a poor calibration.
Table D.3: C$_2$H$_2$ Cross Section Data

<table>
<thead>
<tr>
<th>$\lambda$ (Å)</th>
<th>$T \leq 195$ K</th>
<th>$195$ K $&lt; T &lt; 295$ K</th>
<th>$T \geq 295$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>245–1060</td>
<td></td>
<td>Cooper et al. (1995)</td>
<td></td>
</tr>
<tr>
<td>1060–1100</td>
<td></td>
<td>Xia et al. (1991)$^\dagger$</td>
<td></td>
</tr>
<tr>
<td>1100–1370</td>
<td></td>
<td>Suto and Lee (1984)</td>
<td></td>
</tr>
<tr>
<td>1370–1470</td>
<td></td>
<td>Smith et al. (1991) (295 K)</td>
<td></td>
</tr>
</tbody>
</table>

$^\dagger$ Scaled as indicated in the text.

Figure D.4: C$_2$H$_2$ photoabsorption cross sections.
Because the resolution of the Zelikoff and Watanabe data is higher than that of Cooper et al., we prefer to use them where possible. Luckily, we can scale the Zelikoff and Watanabe data to match the Cooper et al. data. We did this over the wavelength range of 1130—1180 Å, where there is little structure in the cross section spectrum. This scaling gives a reasonable comparison between the two data sets over the wavelength range of overlap, and we use the scaled Zelikoff and Watanabe data as indicated in Table D.4. Figure D.5 shows the final photoabsorption cross sections used for C₂H₄.

D.6 Ethane (C₂H₆)

The photoabsorption cross sections for C₂H₆ were taken from Au et al. (1993) and Mount and Moos (1978).

The Au et al. data were generously provided in digital format as differential oscillator strength in eV⁻¹ versus energy in eV by G. Cooper and C. E. Brion. The oscillator strengths were converted to photoabsorption cross sections in cm² using equation D.2, and the energies were converted to wavelengths in Å using equation D.1. This data set covers the wavelength range of 248 to 1648 Å at a temperature of 295 K, with the resolution varying from 0.6 Å at short wavelengths to 3.8 Å at long wavelengths. This data set exhibits band structure between 1200 and 1400 Å that has only been hinted at in previous measurements.

The Mount and Moos data were taken from their Table 2. They cover the wavelength range of 1380 to 1600 Å with a resolution of roughly 10 Å. The corresponding temperature is 295 K.

Mount and Moos also provide a measurement of the temperature dependence of the C₂H₆ cross section. This is in the form of a ratio as a function of wavelength between the cross section at 200 K and the cross section at 295 K. The dependence is shown in their Figure 2, and it exhibits a slow drop-off in the cross
Table D.4: $\text{C}_2\text{H}_4$ Cross Section Data

<table>
<thead>
<tr>
<th>$\lambda$ (Å)</th>
<th>All temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>248–1240†</td>
<td>Cooper et al. (1995)</td>
</tr>
<tr>
<td>1240–1970</td>
<td>Zelikoff and Watanabe (1953)‡</td>
</tr>
</tbody>
</table>

† Although the Zelikoff and Watanabe data extend down to 1065 Å, there is little structure in the cross section spectrum from 1065 to 1240 Å. As such, we consider the Cooper et al. data to be more reliable and use them over this range.
‡ Scaled as indicated in the text.

Figure D.5: $\text{C}_2\text{H}_4$ photoabsorption cross sections.
section with increasing wavelength at the lower temperature, starting at roughly 1520 Å.

A comparison of the two data sets shows that the Mount and Moos data are lower than the Au et al. data. Because the Au et al. data agree well with other measurements of the C₂H₆ cross section at shorter wavelengths and their set-up was the same as used to measure the CH₄ cross sections that agree well with measurements by Mount et al. (1977) (see Section D.3), we assume that the difference lies in a problem with the Mount and Moos data. Because of this, we scale the cross sections of Mount and Moos to be consistent with those of Au et al. in the wavelength region where we use the Mount and Moos data. This should not affect the C₂H₆ temperature dependence of Mount and Moos because this is expressed in the form of a ratio, which should cancel out any absolute calibration error.

The actual data set used in the calculations was constructed as indicated in Table D.5 for the possible temperature ranges. Figure D.6 shows the final photoabsorption cross sections used for C₂H₆.

D.7 Molecular Hydrogen (H₂)

The photoabsorption cross sections for H₂ were treated differently than those for the other species. Instead of compiling a single set of cross sections, the H₂ cross sections were divided into two categories, continuum and band, and a set of cross sections was created for each category. The reason for this is that the H₂ band region, which covers the range of 750 to 1150 Å, can be effectively modeled at much higher resolution than can actually be measured. The temperature corresponding to the cross sections can also be varied during the modeling, so we can generate a set of H₂ band photoabsorption cross sections that correspond to the actual temperatures in the atmosphere. The continuum photoabsorption cross sections are generally smooth, making high resolution less important, and they are usually less dependent
Table D.5: C$_2$H$_6$ Cross Section Data

<table>
<thead>
<tr>
<th>$\lambda$ (Å)</th>
<th>$T \leq 200$ K</th>
<th>$200$ K $&lt; T &lt; 295$ K</th>
<th>$T \geq 295$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>248–1520</td>
<td></td>
<td>Au et al. (1993)</td>
<td></td>
</tr>
<tr>
<td>1520–1570</td>
<td>Au et al. (1993)$^\dagger$</td>
<td>Interpolated</td>
<td>Au et al. (1993)</td>
</tr>
<tr>
<td>1570–1600$^\ddagger$</td>
<td>MM$^*$$^\ddagger$</td>
<td>Interpolated</td>
<td>MM$^*$</td>
</tr>
<tr>
<td>1600–1800</td>
<td>Extrapolated from 1570–1600 Å data</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

† The Au et al. data exhibit strange behavior beyond 1570 Å, so we have chosen to use the Mount and Moos data from 1570 Å on, scaled to match the Au et al. data at shorter wavelengths as indicated in the text.
‡ Scaled to 200 K according to the temperature dependence shown in Figure 2 of Mount and Moos (1978).

![Figure D.6: C$_2$H$_6$ photoabsorption cross sections.](image-url)
upon the temperature. As such, we obtained the H$_2$ continuum cross sections from the literature in a manner similar to that for the other species.

The continuum photoabsorption cross sections for H$_2$ were taken from Samson and Haddad (1994), Chan et al. (1992), Ford and Browne (1973), and Dalgarno and Allison (1969).

The Samson and Haddad data were taken from their Table 1 and cover the wavelength range of 41 to 689 Å at an assumed temperature of 295 K, with a resolution that varies from 1.5 Å at short wavelengths to 35 Å at long wavelengths. The data were specified as cross sections versus energy in eV, so we used equation D.1 to convert the energies to wavelength in Å.

The Chan et al. data were generously provided in digital format as differential oscillator strength in eV$^{-1}$ versus energy in eV by G. Cooper and C. E. Brion. The oscillator strengths were converted to photoabsorption cross sections in cm$^2$ using equation D.2, and the energies were converted to wavelengths in Å using equation D.1. This data set covers the wavelength range of 207 to 1127 Å at a temperature of 295 K, with the resolution varying from 0.45 Å at short wavelengths to 0.6 Å at long wavelengths.

The Ford and Browne data were taken from their Tables V and VI and cover the wavelength range of 1150 to 2000 Å at temperatures of 100 K and 300 K, respectively. The resolution varies from 25 Å at short wavelengths to 50 Å at long wavelengths. These are theoretical calculations of the Rayleigh and Raman scattering cross sections for H$_2$. We summed the Rayleigh and Raman scattering cross sections to provide a single cross section at each wavelength.

The Dalgarno and Allison data were digitized from their Figure 1. This data set covers the range from 710 to 845 Å at an assumed temperature of 295 K. These are theoretical calculations of the continuum cross sections that underlie a portion of the band region. There are three curves in the figure, representing the cross sections related to the B$^1$Σ$^+_u$, C$^1$Π$^+_u$, and B$^1$Σ$^+_u$ excited states. The three
curves were summed together to produce a single set of cross sections representing the $H_2$ continuum over this wavelength range.

The band photoabsorption cross sections for $H_2$ were provided by R. Yelle and were calculated as described in Yelle et al. (1993). They cover the wavelength range of 750 to 1150 Å with a resolution of 3 mÅ. They were modeled at eleven different temperatures from 100 K to 1000 K.

Table D.6 shows which data set was used in the specified wavelength intervals. Figure D.7 shows the final photoabsorption cross sections used for $H_2$.

D.8 Atomic Hydrogen (H)

The photoabsorption cross sections for atomic H were taken from Samson (1966) and Sadeghpour and Dalgarno (1992).

The Samson data were taken from his Table XXXII and cover the wavelength range from 1.0 to 911 Å at an assumed temperature of 295 K. The resolution varies from 1 Å at short wavelengths to 50 Å at long wavelengths. These data are theoretical calculations of the $H$ photoionization cross sections. We assume that the ionization efficiency of atomic H is roughly unity and use these values for the photoabsorption cross sections.

The Sadeghpour and Dalgarno data were taken from their Table 1 and cover the wavelength range of 913 to 1136 Å at an assumed temperature of 295 K with varying resolution. These are theoretical calculations of the Rayleigh and Raman scattering cross sections of atomic H, which we have summed together to generate a set of combined scattering cross sections.

Table D.7 shows which data set was used in the specified wavelength intervals. Figure D.8 shows the final photoabsorption cross sections used for atomic H.
Table D.6: $\text{H}_2$ Cross Section Data

<table>
<thead>
<tr>
<th>$\lambda$ (Å)</th>
<th>$T \leq 100$ K</th>
<th>$100$ K $&lt; T &lt; 295$ K</th>
<th>$T \geq 295$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>41–689</td>
<td>Samson and Haddad (1994)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>689–750</td>
<td>Chan et al. (1992)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>750–800</td>
<td>Interpolated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>800–846</td>
<td>Dalgarno and Allison (1969)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>846–1150</td>
<td>Interpolated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1150–2000</td>
<td>$\text{FB}^*$ (100 K)</td>
<td>Interpolated</td>
<td>$\text{FB}^*$ (300 K)‡</td>
</tr>
</tbody>
</table>

* Ford and Browne (1973).
‡ Although the Ford and Browne are at a temperature of 300 K rather than 295 K, these are close enough to neglect the difference.

Figure D.7: $\text{H}_2$ photoabsorption cross sections. The main plot shows the continuum cross sections, and the inset shows a close-up of one of the high-resolution band cross section regions modeled by Yelle et al. (1993). We do not show the full set of band cross sections because they plot as a solid, dark band owing to the small wavelength spacing.
Table D.7: H Cross Section Data

<table>
<thead>
<tr>
<th>λ (Å)</th>
<th>All temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>1–911</td>
<td>Samson (1966)</td>
</tr>
<tr>
<td>911–913</td>
<td>Interpolated</td>
</tr>
<tr>
<td>913–1136</td>
<td>Sadeghpour and Dalgarno (1992)</td>
</tr>
<tr>
<td>1136–1800</td>
<td>Extrapolated from 913–1136 Å data</td>
</tr>
</tbody>
</table>

Figure D.8: H photoabsorption cross sections.
D.9 Diacetylene (C₄H₂)

The photoabsorption cross sections for C₄H₂ were taken from Okabe (1983). These data were digitized from his Figure 2 and cover the wavelength range of 1194 to 1796 Å at a temperature of 295 K. The data were sampled at varying resolution during the digitization, roughly every 0.1–1.0 Å.

Because the range of wavelengths available to infer the hydrocarbon abundances from the Voyager UVS data extends down to roughly 1050 Å, we substituted the C₂H₂ cross sections determined in Section D.4 for this wavelength range. The cross sections are somewhat similar in the wavelength region of overlap, and the region from 1050–1200 Å is relatively devoid of structure in most of the hydrocarbon species with similar chemical composition to C₄H₂. Thus, while not perfect, this substitution is considered valid enough for our purposes.

Figure D.9 shows the final photoabsorption cross sections used for C₄H₂.
D.10 Cyanogen \((C_2N_2)\)

The photoabsorption cross sections for \(C_2N_2\) were taken from Connors et al. (1974) and Nuth and Glicker (1982).

The Connors et al. data were digitized from their Figure 1, which shows absorption coefficient in \(\text{cm}^{-1}\) versus frequency in wavenumber. The digitized data were converted to photoabsorption cross sections in \(\text{cm}^2\) versus wavelength in \(\text{Å}\) using equations D.2 and D.1, respectively. The converted data cover the wavelength range of 1048 to 1705 \(\text{Å}\) at a temperature of 295 K. The data were sampled approximately every 1.0–2.0 \(\text{Å}\) during the digitization.

The Nuth and Glicker data were digitized from their Figure 3, which shows absorption coefficient in \(\text{cm}^{-1}\) versus wavelength in \(\text{Å}\). The digitized data were converted to photoabsorption cross sections in \(\text{cm}^2\) using equation D.2. The converted data cover the wavelength range of 605 to 1675 \(\text{Å}\) at a temperature of 295 K. The data were sampled at varying resolution during the digitization, roughly every 1.0–5.0 \(\text{Å}\).

Comparison of the two data sets in the region of overlap shows that they are comparable until the longer wavelengths, at which point the Nuth and Glicker data show more structure. With no definitive reason to choose one data set over another, we averaged the data sets in the region of overlap except at the longer wavelengths where we use the Nuth and Glicker data. The actual data set used in the calculations was constructed as indicated in Table D.8. Figure D.10 shows the final photoabsorption cross sections used for \(C_2N_2\).
Table D.8: $\text{C}_2\text{N}_2$ Cross Section Data

<table>
<thead>
<tr>
<th>$\lambda$ (Å)</th>
<th>All temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>605–1050</td>
<td>Nuth and Glicker (1982)</td>
</tr>
<tr>
<td>1050–1620</td>
<td>Average of Nuth and Glicker (1982) and Connors et al. (1974)</td>
</tr>
<tr>
<td>1675–1705</td>
<td>Connors et al. (1974)</td>
</tr>
<tr>
<td>1705–1800</td>
<td>Extrapolated from 1675–1705 Å data</td>
</tr>
</tbody>
</table>

Figure D.10: $\text{C}_2\text{N}_2$ photoabsorption cross sections.
D.11 Dicyanogen (C₄N₂)

The photoabsorption cross sections for C₄N₂ were taken from Connors et al. (1974). These data were digitized from their Figure 5, which shows absorption coefficient in cm⁻¹ versus frequency in wavenumber. The digitized data were converted to photoabsorption cross sections in cm² versus wavelength in Å using equations D.2 and D.1, respectively. The converted data cover the wavelength range of 1050 to 1765 Å at a temperature of 295 K. The data were sampled approximately every 1.0–2.0 Å during the digitization.

The actual data set used in the calculations is simply the Connors et al. data with a linear extrapolation to 1800 Å. Figure D.11 shows the final photoabsorption cross sections used for C₄N₂.

![Figure D.11: C₄N₂ photoabsorption cross sections.](image)
D.12 Hydrogen Cyanide (HCN)

The photoabsorption cross sections for HCN were taken from Lee (1980) and Nuth and Glicker (1982).

The Lee data were digitized from his Figures 2 and 3 and cover the wavelength range of 1050 to 1570 Å at a temperature of 295 K. The data were sampled approximately every 1.0–2.0 Å during the digitization.

The Nuth and Glicker data were digitized from their Figure 2, which shows absorption coefficient in cm$^{-1}$ versus wavelength in Å. The digitized data were converted to photoabsorption cross sections in cm$^2$ using equation D.2. The converted data cover the wavelength range of 628 to 1470 Å at a temperature of 295 K. The data were sampled at varying resolution during the digitization, roughly every 1.0–3.0 Å.

Comparison of the two data sets in the region of overlap shows that they are comparable with the exception of the region near 1075 Å. At this point, the two show mildly differing structure. However, with no definitive reason to choose one data set over another, we averaged the data sets in the region of overlap. The actual data set used in the calculations was constructed as indicated in Table D.9. Figure D.12 shows the final photoabsorption cross sections used for HCN.
### Table D.9: HCN Cross Section Data

<table>
<thead>
<tr>
<th>$\lambda$ (Å)</th>
<th>All temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>1050–1470</td>
<td>Average of Nuth and Glicker (1982) and Lee (1980)</td>
</tr>
<tr>
<td>1470–1570</td>
<td>Lee (1980)</td>
</tr>
<tr>
<td>1570–1800</td>
<td>Extrapolated from 1470–1570 Å data</td>
</tr>
</tbody>
</table>

**Figure D.12: HCN photoabsorption cross sections.**

![HCN Photoabsorption Cross Sections](image-url)
D.13 Cyanoacetylene (HC₃N)

The photoabsorption cross sections for HC₃N were taken from Connors et al. (1974). These data were digitized from their Figure 2, which shows absorption coefficient in cm⁻¹ versus frequency in wavenumber. The digitized data were converted to photoabsorption cross sections in cm² versus wavelength in Å using equations D.2 and D.1, respectively. The converted data cover the wavelength range of 1060 to 1635 Å at a temperature of 295 K. The data were sampled approximately every 1.0–2.0 Å during the digitization.

The actual data set used in the calculations is simply the Connors et al. data with a linear extrapolation to 1800 Å. Figure D.13 shows the final photoabsorption cross sections used for HC₃N.

Figure D.13: HC₃N photoabsorption cross sections.
REFERENCES


Hidayat, T., A. Marten, B. Bézard, D. Gautier, T. Owen, H. E. Matthews,


Lellouch, E., A. Coustenis, D. Gautier, F. Raulin, N. Dubouloz, and C. Frère


Sromovsky, L. A., V. E. Suomi, J. B. Pollack, R. J. Krauss, S. S. Limaye, T. Owen,


Zelikoff, M. and K. Watanabe (1953). Absorption coefficients of ethylene in the