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**Mixing characterization of transient puffs in a rotary kiln
incinerator**

Schenck, Hubert Willem, Ph.D.

The University of Arizona, 1994

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Ann Arbor, MI 48106**

**MIXING CHARACTERIZATION OF TRANSIENT PUFFS
IN A ROTARY KILN INCINERATOR**

by

Hubert Willem Schenck

A Dissertation Submitted to the Faculty of the
DEPARTMENT OF CHEMICAL ENGINEERING

in Partial Fulfillment of the Requirements
for the Degree of

Doctor of Philosophy

in the Graduate College

THE UNIVERSITY OF ARIZONA

1994

THE UNIVERSITY OF ARIZONA
GRADUATE COLLEGE

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Rotary Kiln Incinerator

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Signed: _____

A handwritten signature in black ink, appearing to read "H. J. Schuch", is written over a horizontal line.

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"I will stuff your head with brains. I cannot tell you how to use them, however; you must find that out for yourself."

L. Frank Baum,
The Wonderful Wizard of Oz

TABLE OF CONTENTS

LIST OF FIGURES	10
LIST OF TABLES	17
ABSTRACT	19
CHAPTER 1 INTRODUCTION	21
1.1 Hazardous Waste Incineration and Rotary Kilns	21
1.2 Previous Work on Rotary Kiln Incineration	22
1.3 Scalar Mixing Studies	26
1.4 Scope of this Project	28
CHAPTER 2 THEORY: TURBULENT MIXING OF PASSIVE SCALARS	32
2.1 Momentum, Heat and Mass Transfer - Passive Scalars	32
2.2 The Nature of Turbulence	34
2.3 The Closure Problem and Closure Modeling	36
2.4 Remarks on Turbulent Diffusivity	39
2.5 Length Scales in Turbulent Mixing	43
2.6 Spatial Correlation Functions and Spectra	47
2.7 Mixing and Reaction - Intensity and Scale of Segregation	51
2.8 Probability Density Functions	56
CHAPTER 3 MODELS OF TURBULENT MIXING	61
3.1 Introduction	61
3.2 Mechanistic Models	62
3.3 Closure Models	64
3.4 Linear Eddy Model	66
3.5 Conclusions	74
3.6 Alternatives	77

TABLE OF CONTENTS (continued)

CHAPTER 4	A LINEAR EDDY MODEL FOR MIXING IN TURBULENT PIPE FLOW	78
4.1	Introduction	78
4.2	Radial Diffusivity in Turbulent Pipe Flow	81
4.3	Linear Eddy Modeling Considerations	85
4.4	Simulations and Results	90
4.5	Discussion	91
4.6	Conclusions	96
CHAPTER 5	COLD FLOW MODEL EXPERIMENTS	97
5.1	Design Considerations	97
5.2	Experimental Facility	103
5.3	Optical System	106
5.4	Particle Seeding	109
5.5	Experimental procedure	112
CHAPTER 6	DATA ANALYSIS	114
6.1	Nomenclature	114
6.2	Digitizing and Image Analysis	116
6.3	Spatial Correlation	119
6.4	Calibration	121
6.5	Accuracy	123
CHAPTER 7	EXPERIMENTAL RESULTS	126
7.1	Introduction	126
7.2	Laser Sheet Experiments	126
7.3	Laser Line Experiments	130
7.4	Calibration	138
7.5	Spatial and Temporal Resolution	143
7.6	Probability Density Functions	144
7.7	Spatial Correlation Functions and Spectra	147
7.8	Conclusions	150

TABLE OF CONTENTS (continued)

CHAPTER 8	DISCUSSION OF RESULTS	151
8.1	Cross-stream Variations	151
8.2	Macro-mixing	154
8.3	Local Mixing Characterization I. Spatial Correlation	162
8.4	Local Mixing Characterization II. Micro-mixing	170
8.5	Summary and Significance	177
CHAPTER 9	UNSTEADY STATE LINEAR EDDY MODEL	180
9.1	Objectives	180
9.2	Modeling Considerations	181
9.3	Input Signal	185
9.4	Implementation	189
9.5	Simulation of Experiments	193
9.6	The Effects of Resolution and Schmidt Number	201
9.7	Spatial Correlation	207
9.8	Simulation of Mixing in a Rotary Kiln	210
9.9	Conclusions	215
CHAPTER 10	CONCLUSIONS AND RECOMMENDATIONS - GENERAL	217
10.1	Summary of Experimental Results	217
10.2	Mixing Studies by Digital Image Analysis	219
10.3	Reynolds Number Similarity	222
10.4	Linear Eddy Modeling	225
CHAPTER 11	CONCLUSIONS AND RECOMMENDATIONS - EPA KILN MIXING	230
11.1	Mixing Mechanisms in the Cold Flow Model	230
11.2	Prediction of Puffs	231
11.3	Shortcomings of the Present Work	234
11.4	Comparison between EPA Kiln and Full Scale Kilns	236
11.5	Mixing Enhancement	238
11.6	Project Evaluation	239
11.7	Future Work I. Cold Flow Experiments	242
11.8	Future Work II. Linear Eddy Modeling	243
11.9	Future Work III. Scale Up	245

TABLE OF CONTENTS (continued)

APPENDIX A	OPTICAL PROPERTIES OF PARTICLES	248
A.1	Introduction	248
A.2	Light Scattering	248
A.3	Light Extinction by a Particle Cloud	249
A.4	Conclusions	250
APPENDIX B	STATISTICAL METHODS	252
B.1	Statistical Inference	252
B.2	Analysis of Variance	254
APPENDIX C	COMPUTER PROGRAMS	255
C.1	Linear Eddy Model for Turbulent Pipe Flow	255
C.2	Streamwise Linear Eddy Model	263
C.3	Image Analysis	278
APPENDIX D	EXPERIMENTAL DATA	287
D.1	Cross-stream Average Pixel Value and Standard Deviation	287
D.2	Ensemble Average Pixel Value and Standard Deviation	291
D.3	Probability Density Functions	300
D.4	Spatial Correlation Functions and Scale of Segregation	309
D.5	Characteristics of Mixing	318
APPENDIX E	CALIBRATION ROTAMETER	322
APPENDIX F	LIST OF SYMBOLS AND ABBREVIATIONS	324
REFERENCES		327

LIST OF FIGURES

Figure 2-1: Counter-gradient diffusion, due to non-localness of the turbulent diffusion process.	42
Figure 2-2: Length scales and regimes in turbulent mixing; dependence on Schmidt (or Prandtl) number.	46
Figure 2-3: Theoretical one-dimensional energy spectrum and scalar spectra at low and high Schmidt number.	50
Figure 2-4: Fraction unburnt vs. stoichiometric ratio for partially mixed toluene. Curves are for different intensities of segregation, assuming a Gaussian concentration PDF.	59
Figure 3-1: Time-lines, illustrating the development of a single realization in linear eddy modeling.	68
Figure 3-2: Two possible re-arrangements for implementation of the linear eddy model, and their effects on scalar fields with constant gradient or with peak.	68
Figure 3-3: Flowsheet for simulation subroutine in linear eddy program. Every call to this subroutine constitutes a single realization.	73
Figure 4-1: Dependence of turbulent diffusivity on Reynolds number. Comparison between present model and experimental data.	84
Figure 4-2: Radial profiles of turbulent diffusivity. Comparison between law of the wall, experimental data and linear eddy model. Top: block inversions; bottom: triplet maps after empirical correction.	88
Figure 4-3: Radial profiles of average scalar (a) and scalar fluctuations (b), downstream of wall source. $Re_* = 1125$; $Pr = 0.71$	92
Figure 4-4: Radial profiles of average scalar (a) and scalar fluctuations (b), downstream of wall source. $Re_* = 1125$; various Pr	93
Figure 5-1: EPA rotary kiln incinerator simulator	102

LIST OF FIGURES (continued)

Figure 5-2: Measured and predicted toluene puff shapes. (a) Measured puff shape, $MASS = 100g$, $T_M = 1124\text{ K}$, $RPM = 0.5$. (b) Predicted puff shape for case (a). (c) Predicted "base case" puff shape, $MASS = 125\text{ g}$, $T_K = 1325\text{ K}$, $RPM = 1.25$. From Wendt and Linak (1988).	102
Figure 5-3: Experimental facility.	104
Figure 5-4: Dimensions of cold flow model (in inches). Side view (top) and cross sections of transition section and cavity (bottom).	105
Figure 5-5: Three different optical arrangements. From top to bottom: laser sheet; laser line, horizontal transition section; laser line, vertical transition section.	107
Figure 6-1: Schematic of video images, showing laser line, indicator light and time stamp. One output file is created by combining the laser lines from all digitized images (raw data files) for a given setup and time.	117
Figure 7-1: Typical mixing patterns in cavity (top) and transition section (bottom) of cold flow model.	127
Figure 7-2: Schematic representation of mixing in different regions of the cold flow model cavity.	129
Figure 7-3: Location of laser lines in cold flow model. The numbers indicate pixel locations along the laser lines in the raw data files.	131
Figure 7-4: Digitized images of a laser line at different times in a single run (top) and at the same time ($t = 20\text{ sec.}$) in multiple runs (bottom). Horizontal transition section; $Re = 3.4 \times 10^3$	133
Figure 7-5: Cross-stream average pixelvalue (top); cross-stream standard deviation (bottom). Bars indicate 95% confidence intervals. Horizontal transition section, various Re	136
Figure 7-6: Cross-stream average pixelvalue (top); cross-stream standard deviation (bottom). Bars indicate 95% confidence intervals. Vertical transition section, various Re	137

LIST OF FIGURES (continued)

Figure 7-7: Ensemble average pixel values in horizontal transition section (top) and vertical transition section (bottom). $Re = 3.4 \cdot 10^3$. For graphs at other Re and ensemble standard deviation, see Appendix D.2.	139
Figure 7-8: Calibration of image analysis, by calculating the integral average pixel value. The slope is equal to the corrected pixelvalue of undiluted seeded ("puff") flow.	140
Figure 7-9: Pixel value histograms at different times. Horizontal transition section, $Re = 5.5 \cdot 10^3$	145
Figure 7-10: Pixel value histograms at different times. Vertical transition section, $Re = 5.5 \cdot 10^3$	146
Figure 7-11: One-dimensional scalar spectra at different times. Horizontal transition section, $Re = 3.4 \cdot 10^3$	148
Figure 8-1: Average concentration profiles. Horizontal and vertical transition sections. $Re = 2.0 \cdot 10^3$ and $Re = 1.7 \cdot 10^3$, respectively.	156
Figure 8-2: Average concentration profiles. Horizontal and vertical transition sections. $Re = 3.4 \cdot 10^3$	156
Figure 8-3: Average concentration profiles. Horizontal and vertical transition sections. $Re = 5.5 \cdot 10^3$	157
Figure 8-4: Average concentration profiles. Horizontal and vertical transition sections. $Re = 1.7 \cdot 10^4$ and $Re = 1.6 \cdot 10^4$, respectively.	157
Figure 8-5: Average concentration profiles in vertical transition section. Comparison between experimental data and stirred tank model.	161
Figure 8-6: Average one-dimensional scalar spectra. Vertical transition section, various Re	163
Figure 8-7: Average one-dimensional scalar spectra. Horizontal transition section, various Re	166
Figure 8-8: Scale of segregation as function of time in horizontal transition section (top) and vertical transition section (bottom).	169

LIST OF FIGURES (continued)

Figure 8-9: Concentration fluctuation profiles in horizontal transition section. From top to bottom: absolute fluctuations, relative fluctuations, and intensity of segregation.	172
Figure 8-10: Concentration fluctuation profiles in vertical transition section. From top to bottom: absolute fluctuations, relative fluctuations, and intensity of segregation.	173
Figure 8-11: Probability of exceeding concentration limits, at different times. Horizontal and vertical transition section. $Re = 3.4 \cdot 10^3$	176
Figure 9-1: Convection events in linear eddy model, showing algorithm for by-passing the recirculation zone.	183
Figure 9-2: Concentration PDFs in horizontal transition section. Schematic of measured PDF and input signal for linear eddy model.	188
Figure 9-3: Input signal for linear eddy model.	188
Figure 9-4: Flowsheet for subroutine that creates input signal in linear eddy simulation. This subroutine is called once for every realization, prior to the call to the simulation subroutine (Figure 3-3).. . . .	190
Figure 9-5: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 2.0 \cdot 10^3$ ($1.7 \cdot 10^3$ for experiments in vertical transition section).	195
Figure 9-6: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 3.4 \cdot 10^3$	196
Figure 9-7: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 5.5 \cdot 10^3$	197
Figure 9-8: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 1.7 \cdot 10^4$ ($1.6 \cdot 10^4$ for experiments in vertical transition section).	198

LIST OF FIGURES (continued)

Figure 9-9: The effect of Schmidt number and resolution on concentration profiles. Linear eddy simulations, $Re = 3.4 \cdot 10^3$	202
Figure 9-10: Concentration PDFs from linear eddy simulation. $Re = 3.4 \cdot 10^3$; $Sc = 5.0 \cdot 10^5$; probe size = 0.71 mm.	204
Figure 9-11: Concentration PDFs from linear eddy simulation. $Re = 3.4 \cdot 10^3$; $Sc = 1.9$; full spatial resolution.	205
Figure 9-12: Spatial correlation curve from linear eddy simulation, Hanning taper function, and tapered correlation function. $Re = 3.4 \cdot 10^3$, $Sc = 1.9$	208
Figure 9-13: Scalar spectrum from linear eddy simulation. Fourier transform of the correlation function (top) and of the tapered correlation function (bottom). $Re = 3.4 \cdot 10^3$, $Sc = 1.9$	209
Figure 9-14: Measured and predicted toluene puff shapes. (a) Measured puff shape, $MASS = 100g$, $T_M = 1124 K$, $RPM = 0.5$. (b) Predicted puff shape for case (a). (c) Predicted "base case" puff shape, $MASS = 125 g$, $T_K = 1325 K$, $RPM = 1.25$. From Wendt and Linak (1988).	211
Figure 9-15: Linear eddy simulation of unsatisfied oxygen demand in EPA rotary kiln incinerator. Input follows the evaporation model of Wendt and Linak (1988).	214
Figure 10-1: Random sampling of PDFs for eddy location, in the case of uneven eddy distribution (top) or even eddy distribution (bottom). The shaded area is equal r (a random number between 0 and 1) in both cases.	227
Figure 11-1: Fraction unburnt vs. stoichiometric ratio for partially mixed toluene. Development of a puff with same mixing characteristics as cold flow experiments, assuming a Gaussian concentration PDF.	233
Figure 11-2: Input signal (left) and corresponding PDF (right) of linear eddy model with proposed modifications.	244
Figure 11-3: Schematic of linear eddy model for stratified flow.	246

LIST OF FIGURES (continued)

Figure D-1: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 2.0 \cdot 10^3$	292
Figure D-2: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 3.4 \cdot 10^3$	293
Figure D-3: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 5.5 \cdot 10^3$	294
Figure D-4: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 1.7 \cdot 10^4$	295
Figure D-5: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 1.7 \cdot 10^3$	296
Figure D-6: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 3.4 \cdot 10^3$	297
Figure D-7: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 5.5 \cdot 10^3$	298
Figure D-8: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 1.6 \cdot 10^4$	299
Figure D-9: Pixel value histograms. Horizontal transition section, $Re = 2.0 \cdot 10^3$	301
Figure D-10: Pixel value histograms. Horizontal transition section, $Re = 3.4 \cdot 10^3$	302
Figure D-11: Pixel value histograms. Horizontal transition section, $Re = 5.5 \cdot 10^3$	303
Figure D-12: Pixel value histograms. Horizontal transition section, $Re = 1.7 \cdot 10^4$	304
Figure D-13: Pixel value histograms. Vertical transition section, $Re = 1.7 \cdot 10^3$	305
Figure D-14: Pixel value histograms. Vertical transition section, $Re = 3.4 \cdot 10^3$	306

LIST OF FIGURES (continued)

Figure D-15: Pixel value histograms. Vertical transition section, Re = 5.5×10^3	307
Figure D-16: Pixel value histograms. Vertical transition section, Re = 1.6×10^4	308
Figure D-17: Spatial correlation function and scale of segregation. Horizontal transition section, Re = 2.0×10^3	310
Figure D-18: Spatial correlation function and scale of segregation. Horizontal transition section, Re = 3.4×10^3	311
Figure D-19: Spatial correlation function and scale of segregation. Horizontal transition section, Re = 5.5×10^3	312
Figure D-20: Spatial correlation function and scale of segregation. Horizontal transition section, Re = 1.7×10^4	313
Figure D-21: Spatial correlation function and scale of segregation. Vertical transition section, Re = 1.7×10^3	314
Figure D-22: Spatial correlation function and scale of segregation. Vertical transition section, Re = 3.4×10^3	315
Figure D-23: Spatial correlation function and scale of segregation. Vertical transition section, Re = 5.5×10^3	316
Figure D-24: Spatial correlation function and scale of segregation. Vertical transition section, Re = 1.6×10^4	317
Figure E-1: Calibration curve for rotameter puff flow.	323

LIST OF TABLES

Table 2-1: Recommended parameter values in the k- ϵ model (Launder and Spalding, 1974).	39
Table 5-1: Dimensions and mixing parameters in rotary kiln incinerators. Comparison between a typical full-scale kiln, the EPA simulator, and the cold flow model (at low and high main air flow rates).	100
Table 5-2: Flow conditions for cold flow model experiments (see also Tables 7-1 and 7-2).	113
Table 7-1: Experimental conditions: main air flowrate and derived quantities. Horizontal transition section.	130
Table 7-2: Experimental conditions: main air flowrate and derived quantities. Vertical transition section.	132
Table 7-3: Parameters for image analysis.	134
Table 7-4: Proportionality constants for use in eqns. (7-1, 7-2).	143
Table 9-1: Numerics and parameters in linear eddy simulations.	194
Table 9-2: Input signal for linear eddy simulation of UOD mixing in EPA rotary kiln incinerator.	213
Table 11-1: Stoichiometric ratio and fraction unburnt for toluene with same mixing characteristics as cold flow experiments. $Re = 3.4 \times 10^3$	232
Table D-1: Cross-stream average pixel value and standard deviation. Horizontal transition section; $Re = 2.0 \times 10^3$	287
Table D-2: Cross-stream average pixel value and standard deviation. Horizontal transition section; $Re = 3.4 \times 10^3$	287
Table D-3: Cross-stream average pixel value and standard deviation. Horizontal transition section; $Re = 5.5 \times 10^3$	288
Table D-4: Cross-stream average pixel value and standard deviation. Horizontal transition section; $Re = 1.7 \times 10^4$	288

LIST OF TABLES (continued)

Table D-5: Cross-stream average pixel value and standard deviation. Vertical transition section; $Re = 1.7 \times 10^3$	289
Table D-6: Cross-stream average pixel value and standard deviation. Vertical transition section; $Re = 3.4 \times 10^3$	289
Table D-7: Cross-stream average pixel value and standard deviation. Vertical transition section; $Re = 5.5 \times 10^3$	290
Table D-8: Cross-stream average pixel value and standard deviation. Vertical transition section; $Re = 1.6 \times 10^4$	290
Table D-9: Characteristics of mixing, including 95% confidence intervals for average concentration and RMS fluctuations.	318
Table E-1: Calibration data	322

ABSTRACT

Studies on both full size and pilot scale rotary kiln incinerators have suggested that mixing between evaporating waste and ambient air may be an important factor in the destruction of hazardous wastes in such facilities. Research presented here has addressed the issue of gas phase mixing between one intermittent gas stream, representing a transient puff of evaporating waste, and a continuous stream, representing the primary flame flue gas in a rotary kiln incinerator.

Experiments were performed in a plexiglas cold flow model which is a full scale replica of the rotary kiln simulator used by EPA's Combustion Research Branch. The intermittent gas stream was seeded with TiO_2 particles. Quantitative data were obtained through a combination of laser flow visualization and digital image analysis. Experiments were completed for different main air flow rates, representing Reynolds numbers from 1,700 to 17,000.

The experimental results were compared to a computer simulation model, based on the linear eddy modeling technique. Model results agreed very well with experimental data, if a recirculation zone was explicitly accounted for. The model was used to predict mixing at low Schmidt number, with input conditions obtained from the existing evaporation model of Wendt and Linak (1988).

Conclusions from this research include the following: (1) digital image analysis, based on flow visualization, can be used to quantify gas phase mixing processes; (2) deviations from Reynolds number similarity in these experiments can be explained from differences in relative (main air and puff) flowrates, and in Strouhal number; (3) recirculation zones have a significant effect on macro-mixing (average concentration profiles). However, the effect on micro-mixing is limited; (4) interpretation of high Schmidt number, low resolution measurements as if they were fully resolved low Schmidt number measurements is generally adequate. Specifically for the EPA kiln, it was concluded that: (5) three separate mixing mechanisms are present: jet mixing in the cavity, recirculation zones, and shear turbulence; (6) unmixedness is a likely explanation for failure modes in the EPA rotary kiln incinerator; (7) insufficient macro-mixing (controlled by transient evaporation and large scale motion) is more important than local unmixedness (governed by fine scale turbulence and molecular diffusion).

CHAPTER 1

INTRODUCTION

1.1 Hazardous Waste Incineration and Rotary Kilns

Amendments to the Resource Conservation and Recovery Act in 1984 led to a ban on almost all landfilling of hazardous wastes. These wastes had to be treated and rendered non-hazardous before they could be disposed. The U.S. Environmental Protection Agency's new regulations have recommended incineration as the method of choice for treating many hazardous wastes, although alternatives have sometimes been suggested.

More recently, the preferred waste management hierarchy (in order of decreasing desirability) is as follows: first source reduction, followed by recycling, treatment and, lastly, disposal. Still, incineration remains an indispensable waste treatment technique. On the short term, while new technologies for waste reduction and recycling are being developed, there are often no feasible alternatives to incineration. On the long term, even though the total amount of waste that must be destroyed will hopefully decrease, it is wishful thinking to believe that all waste production can be brought to an end. Therefore, there will always be some need for incineration.

Throughout the years, various incineration technologies have been developed for

destroying hazardous organic wastes. The different types of installations include rotary kilns, fluidized beds, liquid injection incinerators, fixed hearth incinerators, and cement kilns. Of the different types of incinerators, rotary kilns are arguably among the most versatile and the most universal.

A rotary kiln is a large, refractory lined cylinder that may be 60 or more feet long. The cylinder rotates slowly (0.25 to 1.5 rpm) and reclines at an angle of about five degrees. Gaseous and pumpable liquid wastes can be charged through standard burners. Solid materials and liquid filled drums can be fed through entrance chutes, typically co-current with the gas flow. The kiln rotation continuously exposes fresh organic material on the surface of the kiln bed and provides for constant ash removal. Inorganic residues are usually water quenched and removed by conveyor for landfill. A secondary combustion chamber (afterburner) is generally provided for further destruction of unburned gaseous and suspended particulate organics. Combustion gases are then quenched and scrubbed of acid and particulates before being discharged to the environment.

1.2 Previous Work on Rotary Kiln Incineration

Potential problems associated with hazardous waste incineration include the fate of metal and other inorganic constituents during the combustion process, and the incomplete destruction of organic constituents and formation of secondary pollutants or products of incomplete combustion. Issues associated with metal

emissions from incinerators have recently been reviewed by Linak and Wendt (1993). Previous work relating to the combustion of organics in rotary kiln incinerators includes the study of an industrial scale rotary kiln at Louisiana State University (Cundy *et al.*, 1989a, b; Lester *et al.*, 1990). Pilot scale studies on waste evaporation and combustion in rotary kilns were performed at EPA's Combustion Research Branch (Linak *et al.*, 1987a, b; Wendt and Linak, 1988; Wendt *et al.*, 1990; Lemieux *et al.*, 1990), and at the University of Utah (Owens *et al.*, 1991; Larsen *et al.*, 1993). A summary of the results of these studies is given below. A more comprehensive review of issues in hazardous waste incineration and pertaining research will be presented by Wendt (1994).

Cundy and co-workers studied the performance of a 24 MW rotary kiln incinerator at the Louisiana Division of Dow Chemical USA. They measured temperature and stable species concentrations at various locations, and recorded the incineration process on video. Their data demonstrated that, under certain operating conditions, non-uniformities existed at the kiln exit in the vertical (cross-stream) direction. Fluctuations from within the kiln could persist into the afterburner and stack. The authors believed that the production of large quantities of soot in the lower half of the kiln might cause the intermittent evaporation of hydrocarbons.

Research at EPA included a parametric study to determine which waste and kiln parameters affected the instantaneous intensity and total magnitude of the pollutant

"puffs" leaving the kiln, upon batch incineration of sample wastes. This study was performed for both solid wastes and liquids on sorbents. One conclusion was, that high kiln temperatures and high kiln rotation rates increased puff magnitude and intensity, due to increased volatile release rates. A fragmentation model to predict the transient evaporation of organic wastes bound on containerized sorbents was developed. The authors suggested that their model might be used to rank wastes with respect to their ability to produce puffs, based on waste boiling point and the more obvious stoichiometric oxygen requirement of the waste. The results might be quite different from the ranking proposed by Taylor *et al.* (1990), which is based on the thermal stability of organic compounds. Ultimately, the physical and chemical processes combined determine the likelihood that unburnt organic matter leaves the kiln. A comprehensive ranking of wastes should therefore include the effects of both evaporation rate (boiling point) and thermal stability.

At the University of Utah, research has focused on the release of organics from soils at relatively low temperatures, rather than under thermal destruction conditions. Heat transfer and waste evaporation processes were evaluated. The relative importance of convection and radiation in the kiln was assessed, by estimating characteristic times for both processes. It was found that, at wall temperatures under 925 K, convection dominated; at higher temperatures, radiation was more important. Modeling suggested that the temporal evolution of the bed temperature differed significantly between a full-scale kiln and a pilot scale

model at the same fill fraction. The temperature history of the solids in a full-scale kiln at 5% fill fraction was matched closely by a pilot-scale kiln with 25% fill fraction. It was found experimentally that moisture had a profound effect on evaporation rates. Volatile compounds were removed from the bed more rapidly in the presence of water due to steam-stripping, while non-volatile compounds' vaporization rates were decreased by the cooling of the bed which accompanied the evaporation of water. Evaporation models had problems predicting these effects of moisture.

To our knowledge, no fundamental studies of the transient gas phase mixing phenomena in rotary kilns have been completed. The group at Louisiana State University (Lester *et al.*, 1990) called for "more understanding of the large mixing phenomena in the kiln", suggesting that "mixing of relatively cooler gases from the bottom half of the kiln may have an inhibiting effect on waste destruction". Wendt *et al.* (1990), in evaluating their model said that "ultimately, mixing in the gas phase in the kiln environment must also be considered". These remarks justify a more in-depth study of the mixing processes in rotary kilns.

1.3 Scalar Mixing Studies

Numerous experimental studies have been completed on the turbulent mixing of passive scalars¹ (concentration or temperature) in turbulent flow. Three techniques can be distinguished. (1) Concentration of a contaminant can be measured by withdrawing small samples for analysis. This technique has been applied to water vapor (Sherwood and Woertz, 1939), nitrous oxide (Quarmby and Anand, 1969; Sheriff and O'Kane, 1971), and other contaminants. (2) Temperature can be used as a scalar (provided the temperature differences are not so large that they interact with the fluid dynamics) and can be measured with thermo-couples (Bremhorst and Bullock, 1973; Hishida and Nagano, 1979; Durbin and Frost, 1981). (3) Optical probes have been developed, for measurements in water, using a dye (Lee and Brodkey, 1964), and in air, using light scattering by particles (Becker *et al.*, 1966; Rathgeber and Becker, 1983). The possibilities for mixing analysis by optical methods have increased tremendously with the development of more powerful lasers (allowing laser sheet visualization) and of digital image analysis. The main benefit that the new techniques offer is that point measurements are no longer necessary: a single photo or video frame represents simultaneous measurements at various locations. Combination of several images makes it possible to determine local statistics or to follow time development. In the following, three scalar mixing studies are presented. These can be viewed as illustrations of the

¹ The term "passive scalar" will be explained in Chapter 2.1.

recent advances in experimental techniques.

Murayama and Takeno (1988) applied laser sheet visualization to a turbulent premixed flame seeded with titanium dioxide. When the particles moved through the flame surface, the effective cross section for scattering was greatly reduced, for reasons not quite understood (Moss, 1980). This enabled the researchers to distinguish the instantaneous flame surface. Still camera images were digitized, and the fractal dimension was calculated from individual images, for different heights above the burner surface, and different turbulence intensities. The authors reported the fractal dimension to be smaller than that measured for non-reacting flow, and to increase with downstream distance. They suggested that the fractal-like character is not directly connected to the turbulence characteristics of the approach flow. It should rather represent certain aspects of the flamelet itself.

At the International Flame Research Foundation, laser sheet flow visualization was employed in a 35 inch ID furnace (Dugué *et al.*, 1990). An argon ion laser produced a continuous sheet, utilized in cold flow experiments. For flow visualization in gas and coal flames, a pulsing Nd-YAG laser was used. This allowed the researchers to block most of the flame radiation, by using short exposure times. In coal flames, the coal particles acted as scattering particles. In gas flames and cold flows, zirconium oxide powder was added. Visualization results were recorded on photographic film and on video. Digitizing video frames

allowed time-averaging of the images. This research did not yield quantitative results. However, it is probably the largest geometric scale on which mixing studies with laser sheets have been performed.

Gullet *et al.* (1993) developed a method for determining the mixedness in a cold flow model of a tubular gas-solid reactor, based on laser sheet visualization and digital image analysis. In their experimental facility, two air streams were mixed, one of which was seeded with titanium dioxide. They took video recordings of the resulting mixtures at different downstream locations. By assuming a linear relation between the light intensity (pixel value) and the local titanium dioxide concentration, they could determine scale and intensity of segregation (see Chapter 2.7), and thus quantify the mixing process. Both scale and intensity of segregation were found to decrease with increasing downstream distance, indicating improved mixing. The authors reported that the intensity of segregation could be reduced drastically by replacing a straight section in the cold flow model with a venturi throat.

1.4 Scope of this Project

The objective of this work is to better understand the transient "puffs" that occur in the EPA rotary kiln incinerator simulator upon the batch introduction of contained liquid wastes. More specifically, we want to gain insight in the gas phase mixing processes that bring puff material in contact with surrounding air. The research is

directed primarily towards an *application* of turbulent mixing to a practical system, rather than towards an understanding of turbulence *fundamentals* in general. The following questions need to be addressed: (1) How should "puff integrity" be defined and quantified ? A quantitative definition for puff integrity is a prerequisite for any investigation of the transient mixing process. (2) What parameters (such as gas flow rates, transient evolution characteristics of the waste, waste gas density) are important in determining the lifetimes and local mixing characteristics of puffs ? (3) What are the predominant mechanisms in the mixing process, and what model best describes the observed transient mixing phenomenon ? Answers to questions (2) and (3) can help to extrapolate observed behavior, and to suggest methods for improved mixing. (4) Which aspects of the gas phase mixing process that occurs in the EPA kiln are unique, and which aspects are more general and occur in all rotary kilns ? When comparing results between the EPA kiln and similar full scale units, it is essential to know whether or not observations are specific to a particular apparatus.

In the present study, the mixing process of the kiln is reproduced in a cold flow model, in which gas phase mixing can be studied both qualitatively and quantitatively, by means of flow visualization and digital image analysis. The results of the cold flow experiments suggest which mixing phenomena are relevant. Also, the experiments help in selecting and validating a theoretical model; subsequently, predictions of this theoretical model can be compared to the phenomena observed

in the EPA kiln.

The significance of the project is three-fold. First and foremost, we will gain insight into gas phase mixing in the EPA rotary kiln incinerator simulator. A better understanding of the mixing process (and suggestions for enhancing the mixing) may help reduce the impact of hazardous waste incineration on the environment. Typically, the gas stream from a rotary kiln incinerator passes through an afterburner. The design of the afterburner system is clearly determined by the extend to which puffs have maintained their structure and their integrity after evaporation from the waste surface. It is desirable to predict this for the EPA kiln/afterburner system in particular, and for other systems in general. Also, an investigation of transient mixing is important, properly to interpret the EPA laboratory kiln results, and to extrapolate the EPA findings to similar, full scale systems.

Secondly, transient mixing is a generic research area that has applications to a wide variety of pollution control techniques. For example, it has been suggested to employ transient fuel rich eddies in flue gasses to enhance reburning for NO_x control (Breen *et al.*, 1988). Therefore, this study may open up additional avenues for future research in pollution control.

Finally, this work contributes to advances in both experimental and theoretical

techniques for studying turbulent mixing. On the experimental side, digital image analysis is only now being developed as a quantitative measuring technique, and so any progress made here in this area is relevant for a wide variety of applications. Similarly, on the theoretical side, linear eddy modeling of turbulent flow is a very recent development; our new applications and verification against experimental results aid in the validation of this simulation technique.

CHAPTER 2

THEORY: TURBULENT MIXING OF PASSIVE SCALARS

2.1 Momentum, Heat and Mass Transfer - Passive Scalars

The equations of change play a key role in all transport phenomena: the continuity equation and the momentum balance for flow phenomena; the energy balance for heat transfer; and molecular balances for mass transfer. For an incompressible, newtonian fluid, the momentum balance reduces to the well known Navier-Stokes equations. In the absence of a body force (such as gravity), and using cartesian coordinates:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial U_i}{\partial x_j} \right) \quad (2-1)$$

The continuity equation is then:

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (2-2)$$

In the absence of radiation and chemical reaction, and neglecting the effects that temperature and concentration have on bulk fluid properties, such as density, viscosity, or (thermal or mass) diffusivity, the equations of change for heat and mass become identical; in cartesian coordinates:

$$\frac{\partial C}{\partial t} + U_j \frac{\partial C}{\partial x_j} = \frac{\partial}{\partial x_j} \left(D \frac{\partial C}{\partial x_j} \right) \quad (2-3)$$

$$\frac{\partial T}{\partial t} + U_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\alpha \frac{\partial T}{\partial x_j} \right) \quad (2-4)$$

One difference between the Navier-Stokes equations and the energy and concentration balances is, that velocity is a vector quantity, whereas the other two equations deal with scalar quantities. More importantly, the Navier-Stokes equations are non-linear, while the energy and concentration balances are linear (provided transport and material properties are constant). Consequently, the heat and mass transfer depend on the flow field, but they do not affect it. Therefore, heat and mass are said to be passive scalars.

Three fundamental dimensionless parameters arise from the above equations: the Reynolds number (which can be interpreted as the ratio of inertial forces ρU^2 and the viscous forces $\rho \nu U/L$), the Schmidt number (signifying the ratio of momentum to mass transfer) and the Prandtl number (the ratio of momentum to heat transfer):

$$Re = \frac{UL}{\nu} \quad Sc = \frac{\nu}{D} \quad Pr = \frac{\rho C_p \nu}{k} = \frac{\nu}{\alpha} \quad (2-5)$$

2.2 The Nature of Turbulence

In high Reynolds number flows, flow instabilities cannot be suppressed by the viscous forces of the fluid, resulting in irregularities in the fluid flow, that are characteristic of turbulence. Other characteristics of turbulent flows are (Tennekes and Lumley, 1972): (1) turbulent diffusivity causes increased rates of momentum, heat and mass transfer; (2) turbulence is rotational and three-dimensional; (3) turbulent flows dissipate kinetic energy, due to viscous shear stresses; (4) turbulence is a continuum phenomenon; all scales are far larger than any molecular length scale; (5) turbulence is a characteristic of the flow, rather than of the fluid.

Because of the irregularity of turbulent flows, a deterministic approach is difficult¹. Instead, one must rely on such tools as statistical methods and dimensional analysis. One wide-spread statistical approach to turbulence modeling is Reynolds decomposition of velocity, temperature and concentration. For example, the instantaneous velocity U at a point can be thought of as the sum of the time-average local velocity $\bar{U}$ and the velocity fluctuation u . By definition, the average of the velocity fluctuations, $\bar{u}$, is zero. It is therefore common practice to define the fluctuations as a root mean square (RMS) deviation. In steady turbulent flow:

¹ Deterministic computer simulation experiments ("direct numerical simulation") have been completed for low Re turbulence (e.g. Kim and Moin, 1989; Rutledge and Sleicher, 1993).

$$u' = \sqrt{u'^2} = \lim_{\tau \rightarrow \infty} \sqrt{\frac{\int_0^\tau (U(t) - \bar{U})^2 dt}{\tau}} \quad (2-6)$$

In unsteady flow, where the time-smoothed velocity is a function of time, the limit of $\tau \rightarrow \infty$ denotes that τ should be large compared to the time scale of velocity fluctuations, but small compared to a characteristic time for changes in the time-smoothed velocity. Turbulence intensity is usually defined as the relative magnitude of RMS velocity fluctuations and average (or time-smoothed) velocity in the main flow direction.

Two widely used definitions in turbulence theory are isotropy and homogeneity. Turbulence is said to be isotropic, if the turbulence intensity at a point is independent of direction. In other words, the fluctuation field is invariant under rotation. Homogeneous turbulence is defined as flow, in which the turbulence intensity is independent of location; the fluctuations are invariant under translation. Turbulence is generally non-isotropic and non-homogeneous, when the geometric lengthscales of the flow are considered. For steady (i.e. non-decaying) turbulence, there needs to be a supply of turbulent kinetic energy from the main motion, to compensate for viscous dissipation. A steady turbulent flow is therefore by definition non-isotropic. However, local isotropy can generally be assumed over the smaller length scales. Any directionality that might be present is annihilated by the motion of the large eddies.

2.3 The Closure Problem and Closure Modeling

Application of Reynolds decomposition to the continuity equation and subsequent time-averaging leads to:

$$\frac{\partial \bar{U}_i}{\partial x_i} = 0 \quad (2-7)$$

This indicates that the mean flow is incompressible. Subtracting eqn. (2-7) from the instantaneous continuity equation yields:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (2-8)$$

showing that the turbulent velocity fluctuations are also incompressible. We can apply the same procedure to the Navier-Stokes equations:

$$\bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j} + \overline{u_j \frac{\partial u_i}{\partial x_j}} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial \bar{U}_i}{\partial x_j} \right) \quad (2-9)$$

Or, using the observation that velocity fluctuations are incompressible:

$$\bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial}{\partial x_j} \overline{u_i u_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial \bar{U}_i}{\partial x_j} \right) \quad (2-10)$$

Comparing eqn. (2-10) to (2-1), we can see that the co-variation between velocity fluctuations, corresponding to an additional shear stress $\overline{\rho u_i u_j}$, has been introduced in the balance equations for the mean flow. It is customary to relate this turbulent shear stress to the average velocity gradient, introducing the turbulent (or

eddy) viscosity:

$$\nu_T \equiv \frac{-\overline{u_i u_j}}{\partial \overline{U_i} / \partial x_j} \quad (2-11)$$

This leads to the following set of equations for the turbulent flow field:

$$\overline{U_j} \frac{\partial \overline{U_i}}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left((\nu + \nu_T) \frac{\partial \overline{U_i}}{\partial x_j} \right) \quad (2-12)$$

Eqn. (2-10) introduced the co-variation of the velocity fluctuations in the average momentum balance. Balance equations for $\overline{u_i u_j}$ can be derived in a similar way, after multiplying the Navier-Stokes equations by u_j (Frost and Molden, 1977, Chapter 2). When this is done, new terms involving $\overline{u_i u_j u_j}$ appear, due to the non-linear inertia terms. The introduction of higher order correlation functions, when trying to solve for lower order correlations, is generally referred to as the closure problem in turbulence. The only solution to the closure problem is to assume some additional relation between higher and lower order terms. First order closure models (such as the Prandtl mixing length theory) only solve eqn. (2-10) for average velocity, and assume a functional form for the Reynolds stresses. In second order closure, balance equations for $\overline{u_i u_j}$ are included. Probably the most widely used second order closure model for momentum is the k - ϵ model (Launder and Spalding, 1974). Two additional balances are introduced in this model: one for

the specific kinetic energy of the velocity fluctuations ($k = \overline{u_i u_i}$, m^2s^{-2}) and the other for the energy dissipation rate (ϵ , m^2s^{-3}):

$$\frac{Dk}{Dt} = \frac{\partial}{\partial x_j} \left(\frac{v_T}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + v_T \left(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i} \right) \frac{\partial \overline{U_i}}{\partial x_j} - \epsilon \quad (2-13)$$

$$\frac{D\epsilon}{Dt} = \frac{\partial}{\partial x_j} \left(\frac{v_T}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right) + C_1 v_T \frac{\epsilon}{k} \left(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i} \right) \frac{\partial \overline{U_i}}{\partial x_j} - C_2 \frac{\epsilon^2}{k} \quad (2-14)$$

The turbulent viscosity is found by dimensional analysis:

$$v_T = C_v \frac{k^2}{\epsilon} \quad (2-15)$$

Eqns. (2-12 to 2-15) form a closed system, that can be used to calculate both the average flow field and the turbulent energy field. Recommended parameter values are presented in Table 2-1. The k - ϵ model has been applied successfully to a large number of flow configurations, including plane jets, mixing layers and stirred tanks. For some geometries, the model is inadequate, because it assumes local isotropy. To correct for this, various empirical functions have been suggested for the "constants" in the model (e.g. Myong *et al.*, 1989). Still, for highly anisotropic flows, such as swirling flow, the Reynolds stress model or a higher order closure models may be preferable. Various second and third order closure models have recently been reviewed by Launder (1989).

Table 2-1: Recommended parameter values in the k- ϵ model (Launder and Spalding, 1974).

σ_k	σ_ϵ	C_1	C_2	C_v
1.0	1.3	1.44	1.92	0.09

2.4 Remarks on Turbulent Diffusivity

Analogous to the turbulent viscosity, for heat and mass transfer, turbulent diffusivities D_T and α_T can be defined¹, based on the enhanced scalar transport in turbulent flow:

$$D_T \equiv \frac{-\overline{cu_i}}{\partial \overline{C} / \partial x_i} = \frac{-m}{\partial \overline{C} / \partial x_i} \quad (2-16)$$

where m is the average molar flux. According to the Reynolds analogy (Bird *et al.*, 1960), turbulent diffusivity and turbulent viscosity are based on analogous mechanisms, and therefore have the same value. Launder (1978) pointed out that a value of 0.7 for the turbulent Schmidt or Prandtl number has a far stronger claim to normality than a value of unity, as implied by the Reynolds analogy.

Eqn. (2-16) suggests that turbulent diffusivity may be a vector quantity. Indeed, in anisotropic turbulence, different values of the turbulent diffusivity have been observed for different directions (Quarmby and Quirk, 1972).

¹ Many authors use ϵ for turbulent viscosity or turbulent diffusivity. In this case, a subscript indicates the property being transferred.

A shortcoming in the definition of turbulent diffusivity (and turbulent viscosity) is that a relation is assumed between the local gradient and the local flux. The limits of that assumption can be illustrated by deriving the flux from a random walk model. The theory is very similar to the derivation of molecular diffusivity from the kinetic theory of gases (Bird *et al.*, 1960). Assume that turbulent motion in one direction (x) can be described with steps of a single size z . At every step, fluid with the local average concentration $\bar{C}(x)$ is transported over a distance z to the right or left. The frequency of steps to the right and to the left is given by N_R and N_L , respectively. Then the net flux through a plane at $x = 0$ is given by:

$$m_0 = \int_{-z}^0 N_R(x) \bar{C}(x) dx - \int_0^z N_L(x) \bar{C}(x) dx \quad (2-17)$$

The local concentration $\bar{C}(x)$ can be related to the concentration at $x = 0$ through a Taylor series expansion:

$$\bar{C}(x) = \bar{C}(0) + x\bar{C}'(0) + \frac{x^2}{2}\bar{C}''(0) + \frac{x^3}{6}\bar{C}'''(0) + \dots \quad (2-18)$$

In homogeneous turbulence, $N_R = N_L = N/2$. Then, by substituting eqn. (2-18) into (2-17):

$$m_0 = -\frac{N}{2} \left(z^2 \bar{C}'(0) + \frac{z^4}{12} \bar{C}'''(0) + \dots \right) \quad (2-19)$$

Thus, the flux depends not only on the first derivative of the average scalar field, but also on the third, fifth, etc. Therefore, eqn (2-16), implying a linear relation

between the molar flux and the first derivative of the concentration field can only be approximately true. In molecular diffusion processes, where the step size z is of the order of the mean free path length, terms that involve higher order derivatives can easily be neglected, and a linear relation between concentration gradient and molar flux is accurate. However, this may not be the case in turbulent transport: z here represents an eddy size, and can be on the order of the geometric length scale. In that case, non-local effects play a role; consequently, the series in eqn. (2-19) does not converge. Georgopoulos and Seinfeld (1989) derived a set of general non-local integrodifferential equations for turbulent transport. They showed that the turbulent mass fluxes are in general determined by convolutions over space and time of the mean concentration gradients, with space and time dependent kernel functions.

An (extreme) example of the possible consequence of non-localness is counter-gradient diffusion, illustrated in Figure 2-1. If the local scalar gradient has the opposite sign of the average gradient over a larger distance, large eddies will cause a mass flux in the opposite direction of what would be expected locally, from eqn. (2-16).

A "random walk" definition of turbulent diffusivity (Reif, 1965) follows from combination of (2-16) and (2-19), neglecting all higher order derivatives:

Figure 2-1: Counter-gradient diffusion, due to non-localness of the turbulent diffusion process.

$$D_T = \frac{Nz^2}{2} \quad (2-20)$$

We will use this expression for deriving eddy frequencies in the linear eddy model.

In inhomogeneous turbulence, N_R and N_L will be different, and both functions of x . In this case, the turbulent flux depends not only on higher order derivatives of the scalar field, but also on local derivatives of the step frequency N^I , N^{II} , etc.

2.5 Length Scales in Turbulent Mixing

Turbulent motion can be thought of conceptually as motion of eddies of different sizes. The largest eddies are generated by mean shear; their length scale (the "integral scale") is proportional to the width of the flow under consideration, such as the diameter of a pipe, the width of a shear layer, etc. Kinetic energy is transferred from these large eddies to smaller eddies. When viscous dissipation is neglected, the energy transfer rate per unit mass (ϵ) is independent of eddy size. From dimensional analysis:

$$\epsilon \propto u^3/l \quad (2-21)$$

Eqn. (2-21) has two important implications. First of all, it implies that an eddy loses its kinetic energy (u^2) within one turnover time (l/u). Secondly, because ϵ is constant across all scales, the eddy velocity has to be proportional to $l^{1/3}$. An estimate for ϵ can be obtained, by substituting the RMS velocity fluctuations (u')

for the eddy velocity (u), and the integral scale (L) for the eddy size (l) (Tennekes and Lumley, 1972). An alternative estimate is given in Chapter 5.1.

The generation of smaller scales cannot continue down to the molecular level: at some point, kinetic energy of small eddies gets dissipated into heat due to viscosity of the fluid. The length, velocity and time scale at which this happens are referred to as the Kolmogorov scales. Since these scales signify an equilibrium between an inertial "supply" of kinetic energy and viscous dissipation, the controlling parameters should be the dissipation rate (ϵ) and the viscosity (ν). Then, by dimensional analysis:

$$l_K \propto \left(\frac{\nu^3}{\epsilon}\right)^{1/4} \quad u_K \propto (\nu \epsilon)^{1/4} \quad t_K \propto \left(\frac{\nu}{\epsilon}\right)^{1/2} \quad (2-22)$$

The smallest length scale for scalar mixing may be larger or smaller than the Kolmogorov scale, depending on the Schmidt or Prandtl number. In low Schmidt or Prandtl number flows (e.g. heat transfer in liquid metals) molecular diffusion or conduction causes eddies, larger than the Kolmogorov size, to reach equilibrium of the scalar quantity. Equilibrium is established when molecular diffusion is of the same order of magnitude as turbulent convection:

$$D \frac{C}{l^2} \propto \frac{uC}{l} \quad (2-23)$$

Substituting eqn. (2-21) into (2-23) yields the length scale for scalar equilibrium, first recognized by Corrsin (1951):

$$l_C \propto \left(\frac{D^3}{\epsilon}\right)^{1/4} \quad (2-24)$$

This formula is recommended for a Schmidt (Prandtl) number of order unity, or smaller, so that inertial scaling of the turbulent velocity fluctuations applies to all length scales for scalar fluctuations. In the case $Sc = 1$, Corrsin and Kolmogorov scales are identical. Eddy sizes between the Corrsin scale and the Kolmogorov scale ($Sc < 1$) are referred to as the inertial-diffusive range (see Figure 2-2). In high Schmidt number turbulent flows (such as mass transfer in liquids, or mixing of aerosols), the diffusivity is so small, that the mixing at the Kolmogorov scale is governed by convection, rather than molecular diffusion. In this case there are fluctuations with length scales, smaller than the Kolmogorov scale: the viscous-convective range (see Figure 2-2). Batchelor (1959) derived that the smallest mixing scale now is:

$$l_B \propto \left(\frac{\nu D^2}{\epsilon}\right)^{1/4} \quad (2-25)$$

The difference between eqn. (2-24) and (2-25) is that the Corrsin scale follows from equilibrium between diffusion and convection at a single length scale ($\geq l_K$), while the Batchelor scale implies that the Kolmogorov eddy size and velocity are the smallest scales for turbulent convection. It should be noted that eqn. (2-25) can also be obtained from eqn. (2-23), if we substitute the Kolmogorov scales (eqn. 2-22) for the characteristic velocity and length scales at the right hand side of the eqn (2-23).

Figure 2-2: Length scales and regimes in turbulent mixing; dependence on Schmidt (or Prandtl) number.

Since ϵ is of order $(u')^3/L$, all length scales can be written in terms of the turbulent Reynolds number¹ $Re_T = u' L/\nu$ and the Schmidt (or Prandtl) number:

$$\frac{l_K}{L} \sim Re_T^{-3/4} \quad \frac{l_C}{L} \sim (Sc Re_T)^{-3/4} \quad \frac{l_B}{L} \sim Sc^{-1/2} Re_T^{-3/4} \quad (2-26)$$

Thus, from the overall flow characteristics and fluid properties, we can obtain estimates for the smallest length scales of turbulent mixing.

2.6 Spatial Correlation Functions and Spectra

Correlation functions and spectra are two different ways of expressing essentially the same information about turbulent flow. Both can be generated for scalar fluctuations, as well as for velocity fluctuations. They can relate either to the fluctuating quantities at one point at different times (auto-correlation functions and frequency spectra), or to fluctuating quantities at different points at the same time (spatial correlation functions and wave number spectra). We will focus here on scalar spectra and correlation functions, based on separation between two points. For more information on spectral dynamics, the reader is referred to Tennekes and Lumley (1972), Chapter 8, or to Chapter 4 in Frost and Moulden (1977).

Consider a fluctuating scalar C in a turbulent flow field. The spatial correlation function $R(r)$ of C is a measure of how much the value of C at location $(x+r)$ is

¹ Re_T should not be confused with another Reynolds number often used in turbulence theory: Re_λ , based on the Taylor micro-scale (e.g. Champagne, 1978).

related to the value of C at x . If the turbulence is homogeneous, and the average scalar concentration is independent of time t and location x , the spatial correlation function is given by:

$$R(r) = \overline{C(x,t)C(x+r,t)} - \overline{C(x,t)}^2 = \overline{c(x,t)c(x+r,t)} \quad (2-27)$$

$R(0)$ is equal to the RMS concentration fluctuations (compare eqn. 2-6) by definition¹. As the separation distance r gets large, the correlation approaches zero. In general, the separation distance is a vector quantity. In isotropic turbulence, however, the direction of r is immaterial. A negative correlation between two points indicates that when the concentration at one point is above the average concentration, the concentration at the other point is usually below average at the same time. In homogeneous turbulence, the averages in eqn. (2-27) can be determined experimentally either by fixing x and averaging over t , or by moving the pair of points $(x, x+r)$ over the domain at a fixed time t .

The one-dimensional spectrum is the Fourier transform of the spatial correlation function. Formally, a Fourier transform pair is defined as:

$$F(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikr} R(r) dr \quad R(r) = \int_{-\infty}^{\infty} e^{ikr} F(k) dk \quad (2-28)$$

For homogeneous turbulence, $R(r)$ is a symmetrical function (i.e. $R(-r) = R(r)$).

¹ In some texts, the correlation function is normalized, through division by the RMS fluctuations. In that case, $R(0) = 1$.

Consequently, the spectrum is real, and eqn. (2-28) simplifies to:

$$F(k) = \frac{1}{\pi} \int_0^{\infty} \cos(kr) R(r) dr \quad R(r) = 2 \int_0^{\infty} \cos(kr) F(k) dk \quad (2-29)$$

The independent variable of the spectrum, k , is called the wave number; its dimension is reciprocal length. Eddies with an eddy size l have a wave number $k = 2\pi/l$. A spectrum therefore represents a decomposition of the scalar fluctuations into waves of different wave lengths. In the analysis of velocity measurements, the value of the spectrum at a certain wave number represents the mean kinetic energy of eddies of the corresponding size. Similarly, the spectrum of a scalar shows how the scalar variance is divided over different length scales.

Corrsin (1951) showed that the scalar spectrum (like the energy spectrum) is proportional to the wave number to the $-5/3$ rd power (see Figure 2-3) in the inertial-convective range. This follows from an analysis of the dissipation of scalar fluctuations, similar to the dissipation of turbulent kinetic energy (eqn. 2-21). Both the Reynolds number and the Péclet number ($Pe = Re \cdot Sc$) need to be sufficiently large, since molecular effects are neglected in inertial-convective scaling. In the case of high Schmidt number turbulent mixing, the spectrum is inversely proportional to the wave number in the viscous-convective range. Batchelor (1959) derived this, by assuming that (below the Kolmogorov length scale) velocity is a linear function of position.

Figure 2-3: Theoretical one-dimensional energy spectrum and scalar spectra at low and high Schmidt number.

Proportionality constants of order unity are usually omitted in the turbulent length scales (eqn. 2-26) and corresponding wave numbers. However, Hill (1978), from observation of experimental spectra of several authors, remarked that the transition wave number in high Schmidt number mixing is actually $0.05 \cdot k_K$. This suggests that the smallest eddy size is 20 times the Kolmogorov size.

2.7 Mixing and Reaction - Intensity and Scale of Segregation

It has long been recognized that turbulent mixing plays an essential role in many reacting systems. Mixing is particularly important in combustion processes, where the chemical kinetics are very fast, and in many instances mixing becomes the limiting step in the overall reaction process. The relative time scales of mixing and chemical reaction are expressed as the Damköhler number. Mungal and Frierler (1988) defined chemical reaction times, based on multi-reaction calculations (using Chemkin¹ software), while one of their choices for the mixing time was the turnover time of a large eddy. This leads to the following definition of the Damköhler number:

$$Da = \frac{L}{\tau u'} \quad (2-30)$$

At very low Damköhler number, a system is reaction controlled, and the effect of mixing may be neglected. In the high Damköhler number limit, reaction is infinitely

¹ Chemkin is a Fortran chemical kinetics package for the analysis of gas phase reactions, developed at Sandia National Laboratories.

fast, and the system is mixing controlled. This limit has led to the formulation of flame-sheet models, like the coherent flame model of Marble and Broadwell (1977). In this model, the reactions are restricted to a surface, much thinner than the smallest turbulent scale, which is deformed by the straining motion of the flow.

At intermediate Damköhler number, it is necessary to evaluate the combined effect of mixing and chemical reaction. To this end, Danckwerts (1953) proposed two parameters that quantify the "mixedness" of a system: the intensity of segregation ($\mathfrak{S}$) and the scale of segregation (S). He assumed that the mixture is uniform in texture (i.e. it cannot be divided into two parts of equal size in which the mean concentration or scale or intensity of segregation differ significantly). For this to be true, a necessary (but not sufficient) condition is that the turbulence is homogeneous.

The intensity of segregation is a normalized form of the concentration fluctuations:

$$\mathfrak{S} = \frac{\overline{(C - \bar{C})^2}}{\bar{C}(1 - \bar{C})} = \frac{(c')^2}{\bar{C}(1 - \bar{C})} \quad (2-31)$$

C should have values between 0 and 1 (e.g. C is volume fraction), leading to an intensity of segregation from 0 (homogeneous mixture) to 1 (no micro-mixing), independent of the value of $\bar{C}$.

The scale of segregation is the integral over all r of the correlation function $R(r)$,

normalized with the concentration fluctuations:

$$S = \int_0^{\infty} \frac{\overline{c(x,t)c(x+r,t)}}{(c')^2} dr \quad (2-32)$$

Comparing eqns. (2-31, 2-32) to (2-27, 2-29), the intensity and scale of segregation can be written in terms of the spatial correlation function and the spectrum:

$$\mathfrak{S} = \frac{R(0)}{\overline{C}(1 - \overline{C})} = \frac{2 \int_0^{\infty} F(k) dk}{\overline{C}(1 - \overline{C})} \quad (2-33)$$

$$S = \frac{\int_0^{\infty} R(r) dr}{R(0)} = \frac{\pi F(0)}{R(0)} \quad (2-34)$$

As mentioned earlier (Chapter 2.2), steady turbulence and isotropy are mutually exclusive concepts. Nevertheless, it is useful to analyze an imaginary "isotropic mixer", i.e. an apparatus in which the turbulence is steady, as well as homogeneous and isotropic. Not only does this enhance our comprehension of mixing, it is also a reasonable approximation to the smaller scales in high Re steady turbulence. In an isotropic mixer, the intensity of segregation decays exponentially with time (Corrsin, 1964):

$$\mathfrak{S} = \exp\left(-\frac{t}{\tau}\right) \quad (2-35)$$

where, for $Sc \leq 1$:

$$\tau \propto S^{2/3} \quad (2-36)$$

Combining the two equations yields:

$$\frac{d \ln \mathfrak{S}}{dt} \propto S^{-2/3} \quad (2-37)$$

showing that the decay in intensity of segregation is faster for smaller scales.

The way in which the intensity of segregation is defined, its value is always between 0 and 1. While this is convenient for many applications, the normalization has one disadvantage. Consider a system in which a small amount of scalar is being mixed (i.e. $\bar{C} \ll 1$). If the scalar fluctuations are of the same order of magnitude as the average scalar then the intensity of segregation, due to the normalization, is proportional to the scalar concentration. This leads to the somewhat illogical situation that two systems with different average concentration and the same relative fluctuations ($c'/\bar{C}$) have different intensities of segregation.

The effect of mixing on reaction is best illustrated with a second order reaction $A + B \rightarrow P$ in a turbulent flow field. Through Reynolds decomposition, the reaction rate can be expressed as:

$$-\bar{r}_A = k \overline{C_A C_B} = k (\overline{C_A} \overline{C_B} + \overline{C_A' C_B'}) \quad (2-38)$$

In order to find the reaction rate, it is therefore necessary to determine the covariance of the concentration of both species.

Mixing without chemical reaction may be viewed as a limiting case of chemical reacting flow, as the reaction rate constant approaches zero. In this case, the mean of the product of fluctuations of two species is plus or minus 1 times the product of the RMS concentration fluctuations of the individual species when the molecular diffusivities of the two species are equal. For un-premixed feeds:

$$\frac{\overline{C_A' C_B'}}{\overline{C_A} \overline{C_B}} = \frac{-(C_A')^2}{\overline{C_A}(1-\overline{C_A})} = \frac{-(C_B')^2}{\overline{C_B}(1-\overline{C_B})} = -\mathfrak{S} \quad (3-39)$$

Toor (1969) derived an almost identical relationship¹ for very rapid irreversible second-order reaction. The fact that both limits behave the same led Toor to the hypothesis that the mean of the products of the fluctuations is independent of the speed of the reaction. Thus, according to "Toor's hypothesis" (Dutta and Tarbell, 1989) the covariance $\overline{C_A' C_B'}$ depends only on the hydrodynamics of a system, and not on the reaction rate. The overall rate of a reaction with intermediate kinetic rate constant ($Da = O(1)$) and un-premixed feed of reactants in stoichiometric ratio is

¹ To be exact, Toor used the "decay law" of eqn. (2-35) instead of intensity of segregation.

then given by:

$$-\overline{r_A} = k \overline{C_{A,0}} \overline{C_{B,0}} \left(\frac{\overline{C_A C_B}}{\overline{C_{A,0}} \overline{C_{B,0}}} - \mathfrak{S} \right) \quad (2-40)$$

where $\mathfrak{S}$ is the intensity of segregation, determined from a non-reacting mixing experiment in the same apparatus. Dutta and Tarbell (1989) derived several alternative expressions for the co-variance, based on the intensity of segregation, that can be used for parallel-consecutive reactions, as well as single reactions.

As pointed out by Patterson (1981), chemical reaction changes the driving force for molecular diffusion, suggesting that Toor's hypothesis may not be generally valid.

2.8 Probability Density Functions

Consider an ensemble of realizations of a scalar concentration field, each of which is a measured value $C(x,t)$. As the concentration field appears to fluctuate randomly with space and time, the value of $C(x,t)$ is a random variable. Let $Q(C)dC$ be the fraction of the total number of realizations (measurements) in which the measured concentration at particular (x,t) lies between C and $C+dC$. For a sufficiently large number of realizations, $Q(C)$ converges to the probability density function (PDF) $P(C)$, such that $P(C)dC$ is the probability that the concentration at location x and time t lies in the interval $[C, C+dC]$. If C is mixture fraction, then by

definition:

$$\int_0^1 P(C) dC = 1 \quad (2-41)$$

From the concentration PDF, we find the expected value, or average concentration, and the RMS concentration fluctuations:

$$\bar{C} = \int_0^1 C P(C) dC \quad (2-42)$$

$$c' = \sqrt{\int_0^1 (C^2 - \bar{C}^2) P(C) dC} \quad (2-43)$$

The intensity of segregation can be calculated from the concentration PDF. Inversely, we can use the intensity of segregation to find the PDF, only if a shape for the PDF is assumed. This is frequently done, generally by assuming the concentration distribution to be Gaussian. In Chapter 9.3, an alternative PDF shape will be assumed. Thus, while intensity of segregation is a very convenient measure for many applications, it does not contain all the pertinent information that PDFs do.

As an example of the use of PDFs and intensity of segregation, we will now consider the maximum possible extent of reaction of a mixture of organic waste and air, under conditions of incomplete mixing. The overall incineration reaction for

a waste is given by:

Thus, for complete incineration, one mole of waste needs to mix with ν_o moles of oxygen, or ($\nu_a = \nu_o/21\%$) moles of air. For toluene, a typical sample waste, the stoichiometric coefficient ν_o is 9. At a given toluene concentration, C (with $\text{SR} < 1$), the fraction of toluene unburnt, $\phi_{\text{unburnt}}(C)$, is given by:

$$\phi_{\text{unburnt}}(C) = \frac{C - (1-C)/\nu_a}{C} = 1 + \frac{1}{\nu_a} - \frac{1}{\nu_a C} \quad (2-45)$$

Inspection of eqn. (2-45) shows that at $\text{SR} = 1$ ($C = 1/(1+\nu_a)$) the fraction unburnt equals zero, as expected. Assuming a Gaussian concentration distribution, we can generate a concentration PDF from the stoichiometric ratio and the intensity of segregation:

$$P(C) = \frac{1}{\sqrt{2\pi} c'} \exp\left(-\frac{(C - \bar{C})^2}{2c'^2}\right) \quad (2-46)$$

where:

$$\bar{C} = \frac{1}{1+\nu_a \text{SR}} \quad c' = \sqrt{\frac{\bar{C}(1-\bar{C})}{3}} \quad (2-47)$$

By combining eqns. (2-45) and (2-46), the fraction unburned waste in partially mixed waste can be calculated, according to:

$$\phi_{\text{unburnt}}(\text{overall}) = \int_{\text{SR}=0}^1 \phi_{\text{unburnt}}(C) P(C) dC \quad (2-48)$$

Figure 2-4: Fraction unburnt vs. stoichiometric ratio for partially mixed toluene. Curves are for different intensities of segregation, assuming a Gaussian concentration PDF.

The upper limit of integration follows from the fact that low local concentrations (corresponding to $SR > 1$) will burn out completely. Curves of the fraction unburnt toluene vs. stoichiometric ratio, at different intensities of segregation, are presented in Figure 2-4. From this figure, an intensity segregation as low as 0.002 is sufficient to cause incomplete combustion, for stoichiometric ratios up to 2. The reason is, that a very large excess of air is needed, to completely destroy a large molecule like toluene. The fraction unburnt presented here is related to the unsatisfied oxygen demand (UOD), as defined by Wendt and Linak (1988), by:

$$UOD(C) = v_o C \phi_{unburnt}(C) \quad (2-49)$$

CHAPTER 3

MODELS OF TURBULENT MIXING

3.1 Introduction

The balance equations presented in Chapter 2.1 give a complete description of mixing processes. In principle, chemical reaction can be incorporated in the mass balances (provided rate equations are available). It may seem, therefore, that the best approach to predicting turbulent mixing would be to numerically solve the time-dependent Navier-Stokes equations, and the mass balances of all species, involved in chemical reactions. Indeed, direct numerical simulation has been applied to turbulent scalar mixing at low Reynolds number (Kim and Moin, 1989; Rutledge and Sleicher, 1993). The main reason why modeling techniques are of importance is the computational cost of numerical simulations. Because of the three-dimensional nature and the large variation in length scales, an inhibitive number of gridpoints is required for high Reynolds number flows, in order to resolve the smallest scales. Small variations in initial conditions or boundary conditions may have a profound effect on the flow field, due to the non-linearity and chaotic nature of the Navier-Stokes equations.

Computational fluid dynamics software (such as Fluent¹) is deemed inadequate for

¹ Fluent is software from create.x Inc.

many scalar mixing applications, because it predicts merely the distribution of time-averaged (time-smoothed for unsteady flow) scalar field. In this chapter, three different modeling approaches are presented that allow the prediction of "unmixedness". The linear eddy model is explained in more detail than the other models, since this technique will be used later in this work. The chapter is concluded with a comparison between models and a brief mention of alternatives.

3.2 Mechanistic Models

In mechanistic or indirect models of turbulent reacting flow, the dominant mechanisms in the overall transport process are described empirically. This allows the formulation of model, involving the inter-diffusion of inhomogeneous slabs, or the mixing of segregated environments at a prescribed rate.

One example of a mechanistic model is the three-environment model, developed by Ritchie and Tobgy (1979). Two entering environments, one for each reactant feed stream in a two-reactant system, are assumed to supply a single leaving environment. The different environments can be viewed as lumped representations of eddies with corresponding compositions. Micro-mixing is modeled by transfer of material from the entering environments to the leaving environment. The volume fraction of each of the environments is given by:

$$\phi_{EE1} = m\mathfrak{S} \quad \phi_{EE2} = (1-m)\mathfrak{S} \quad \phi_{LE} = 1 - \mathfrak{S} \quad (3-1)$$

where m is the flow rate ratio of the feed streams, and $\mathfrak{S}$ the intensity of segregation, from eqn. (2-35); τ is a fitting parameter.

Other models in this same class include: the coalescence-redispersion model¹ (Curl, 1963); the interaction-by-exchange-with-the-mean (IEM) model (Villermaux and Devillon, 1972); and the four-environment model (Mehta and Tarbell, 1983). All these models are relatively simple. This facet has both advantages and disadvantages, as will be discussed in Chapter 3.5.

Most mechanistic models are deterministic. Only in the coalescence-redispersion model is the meeting between two drops a random process. Curl, in his initial formulation, derived mean rates of creation of drops with different concentrations. As a result, his model results are deterministic also. Spielman and Levenspiel (1965) proposed a Monte Carlo² approach for the coalescence-redispersion model, in which both drop residence times and coalescence events are random functions, thus retaining the non-deterministic nature of the model.

¹ As its name implies, this model was initially developed for dispersed-phase mixing. However, it has been widely applied to single-phase mixing as well. In that case, "drops" denote fluid elements.

² In this context, a Monte Carlo process is defined as a process in which a function of one or more variables is determined by randomly choosing input variable values, and calculating the corresponding function value. From multiple independent realizations, the average function value (and other statistical quantities, including a function value PDF) can be determined.

3.3 Hydrodynamic Mixing Models

The key to the development of hydrodynamic mixing models is, to achieve closure of the different balance equations in a turbulent flow field. In addition to the momentum and turbulent energy balances, as presented in Chapter 2.2, balances for average scalar and scalar fluctuations can be obtained, using the same method of Reynolds decomposition and averaging. For average scalar transport, in the absence of chemical reaction:

$$\overline{U_j} \frac{\partial \overline{C}}{\partial x_j} + \frac{\partial}{\partial x_j} \overline{c u_j} = \frac{\partial}{\partial x_j} \left(D \frac{\partial \overline{C}}{\partial x_j} \right) \quad (3-2)$$

The co-variation term $\overline{c u_j}$ can be replaced by the turbulent diffusivity and the average scalar gradient, using eqn. (2-16)¹. The equivalent of eqn. (2-13) for scalar fluctuations can be found by subtracting eqn. (3-2) from the balance equation for the instantaneous value of the scalar ($\overline{C} + c$), multiplying by c , and averaging or time smoothing (Corrsin, 1953). After re-arrangement, this yields:

$$\overline{U_j} \frac{\partial \overline{c^2}}{\partial x_j} = D \frac{\partial^2 \overline{c^2}}{\partial x_j^2} - \frac{\partial \overline{c^2 u_j}}{\partial x_j} - 2 \overline{c u_j} \frac{\partial \overline{C}}{\partial x_j} - 2D \left(\frac{\partial \overline{c}}{\partial x_j} \right)^2 \quad (3-3)$$

where the terms on the right side represent molecular diffusion, turbulent diffusion, production and dissipation of scalar fluctuations, respectively. The turbulent

¹ Launder (1978) presents alternative closures, for both homogeneous and inhomogeneous flows.

diffusion term can be closed by assuming the same turbulent diffusion for turbulent transport of average scalar and scalar fluctuations (Spalding, 1971):

$$\overline{c^2 u_j} = -D_T \frac{\partial \overline{c^2}}{\partial x_j} \quad (3-4)$$

For production of scalar fluctuations, the definition of turbulent diffusivity can be used, yielding:

$$-2\overline{c u_j} \frac{\partial \overline{c}}{\partial x_j} = 2D_T \left(\frac{\partial \overline{c}}{\partial x_j} \right)^2 \quad (3-5)$$

Proportionality to the gradient squared makes this term particularly sensitive to the local gradient; for a discontinuity in the scalar field, eqn. (3-5) predicts an infinite production of fluctuations. More realistic production terms can be obtained, by considering an average gradient over a characteristic length scale¹. Finally, for closure of the dissipation of scalar fluctuations, a length scale needs to be assumed. Spalding used the local average length scale of turbulence, in combination with an empirical constant:

$$-2D \left(\overline{\frac{\partial c}{\partial x_j}} \right)^2 = -C_3 D_T \frac{\overline{c^2}}{l^2} \quad (3-6)$$

This expression obscures the dependence of scalar fluctuations on Schmidt number. Zipp (1989) maintained the molecular diffusivity in the dissipation term,

¹ Compare the remarks on non-localness of turbulent diffusion in Chapter 2.4.

and used a representative length scale for scalar mixing:

$$-2D \overline{\left(\frac{\partial c}{\partial x_j} \right)^2} = -12D \frac{\overline{c^2}}{l^2} \quad (3-7)$$

where l is a "Taylor type micro-scale for concentration", defined by Corrsin (1964). With this closed set of equations, the average scalar field and the scalar fluctuation field can be calculated, in very much the same way the flow field is calculated with the k - ϵ model. Higher order closure models for turbulent mass balances can also be derived. However, Launder (1989) pointed out that the resources consumed by such models are likely to outweigh the anticipated gain in accuracy.

If chemical reaction is included in a hydrodynamic mixing model, this affects not only the average scalar balance, but also that for scalar fluctuations (Patterson, 1981).

3.4 Linear Eddy Model

Kerstein (1988, 1989, 1990, 1991a&b, 1992a&b) developed a one-dimensional Monte Carlo modeling technique for turbulent mixing of passive scalars. The "linear eddy" modeling approach simulates the random movement of fluid under the action of turbulent eddies. Equations for the flow field are not solved explicitly. Rather, information about the average velocity field and about the turbulent diffusivity are required as input to any particular linear eddy model.

A single realization of a linear eddy simulation represents the time development of a scalar profile under the action of different processes, including (but not necessarily restricted to) turbulent motion and molecular diffusion. This is illustrated in Figure 3.1. Each process (stirring, diffusion, output) has its own time-line, with discrete events at regular time-intervals. A pointer ("clock") proceeds along all the time-lines simultaneously. Whenever an event is encountered along any of the lines, the corresponding process tasks are performed.

Diffusion, expressed as Fick's law:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (3-8)$$

continuously reduces fluctuations in the profile. In the actual simulation code, molecular diffusion is implemented in finite difference form, so that we can speak of discrete "diffusion events". The time between diffusion events is:

$$\Delta t_{\text{diffuse}} = \frac{\alpha (\Delta x)^2}{D} \quad (3-9)$$

where Δx is the grid spacing in the model. For an explicit finite difference scheme (forward Euler method), the maximum value for α that gives a stable solution for the diffusion equation is 0.5 (Ferziger, 1981). A diffusion event consists of updating the entire profile, according to:

Figure 3-1: Time-lines, illustrating the development of a single realization in linear eddy modeling.

Figure 3-2: Two possible re-arrangements for implementation of the linear eddy model, and their effects on scalar fields with constant gradient or with peak.

$$\Delta C_i = \alpha(C_{i-1} - 2C_i + C_{i+1}) \quad (3-10)$$

with index i referring to the location (gridpoint).

Turbulent motion is modeled by instantaneous spatial re-arrangements of the scalar field ("stirring events" or "eddies"). Two possible re-arrangements, the block inversion and the triplet map, are depicted graphically in Figure 3-2. In the block inversion, the scalar profile of a randomly selected interval $[x - l/2, x + l/2]$ of the spatial domain is inverted, replacing the value at $(x + z)$ with the value at $(x - z)$ for $-l/2 < z < l/2$. A block inversion thus corresponds to a rigid body rotation over 180 degrees. The triplet map compresses the scalar profile on the size- l interval to one-third its original length, and then replaces the original profile with three compressed copies, with the central copy spatially inverted. The triplet map is more realistic than the block inversion, since it incorporates both compressive strain (steepening of gradients) and extension (material surface stretching, reflected in tripling of the number of points at which $C = C_0$, for any given C_0).

The main consideration in implementing the linear eddy model for any configuration is to determine the frequency of stirring events, and probability density functions (PDFs) for eddy location and eddy size. The quantity $\lambda(x)dx$, which is the rate of occurrence of linear eddies with centers in the interval $[x, x+dx]$, can be determined from the turbulent diffusivity. The simplest expression for λ is obtained

when eddies are modeled as block inversions, with a single block size (L), and no dependence on location x (i.e. homogeneous turbulence). In this case, we can derive the eddy frequency from the random walk diffusivity (eqn. 2-20) in the following way. The number of steps per unit time is given by:

$$N = \lambda L \quad (3-11)$$

and the mean square displacement is:

$$\overline{z^2} = \int_{-L/2}^{L/2} \frac{(2\xi)^2 d\xi}{L} = \frac{L^2}{3} \quad (3-12)$$

Combination of eqns. (2-20, 3-11, 3-12) yields:

$$\lambda = \frac{6D_T}{L^3} \quad (3-13)$$

Alternative expressions for eddy frequency can be obtained for triplet mappings instead of block inversions (Kerstein, 1991b), for inhomogeneous turbulence (Chapter 4.3), and for Kolmogorov scaling of eddy sizes (Kerstein, 1989; Chapter 9.2). The time between stirring events is found by integration of the eddy frequency over the simulation domain:

$$\Delta t_{\text{stir}} = \left(\int_0^Z \lambda(x) dx \right)^{-1} \quad (3-14)$$

It may seem counter-intuitive that the eddy frequency is a deterministic, rather than

a random function. Randomness is introduced through the placement of an eddy (and the choice of eddy size in the case of Kolmogorov scaling). This ensures that the eddy frequency in any sub-section of the simulation domain is a random function, even though the over-all eddy frequency is deterministic.

For homogeneous turbulence on a simulation domain Z , a stirring event consists of the following steps:

- 1 Draw random number r_1 ($0 < r_1 < 1$). Determine location of eddy center:

$$x = r_1 Z \quad (3-15)$$

- 2 Draw random number r_2 ($0 < r_2 < 1$). Determine eddy size (l) from:

$$r_2 = \int_{l_{\min}}^l P(l) dl \quad (3-16)$$

where $P(l)$ is the PDF for eddy size. For Kolmogorov scaling, this is given by eqn. (9-1).

- 3 Apply re-arrangement to the selected interval $[x-l/2, x+l/2]$.

Typically, the time between stirring events is much shorter than the time between diffusion events. However, diffusion affects the entire simulation domain, whereas a stirring event only covers the size of a single eddy (the location of which varies in a random way). The concentration of an individual cell at a specific location is therefore changed much more frequently by diffusion than by stirring, making the

diffusion a gradual process. As a further consequence, diffusion is generally the most time-consuming procedure in a simulation program.

Figure 3-3 shows a flow diagram for a basic linear eddy simulation subroutine. The main program in a linear eddy model calls this subroutine once for every realization. Output concentration profiles (at a given time) will differ between realizations, because of the random placement of stirring events. Simulation with a linear eddy model can therefore be viewed as the computational equivalent of a physical experiment: each realization is analogous to a measured time history of the scalar profile. Average scalar profiles, scalar fluctuation profiles, spatial correlation curves and spectra can all be determined from multiple realizations. Additional processes (e.g. chemical reaction) can be incorporated by adding more time-lines to the model. Brouwer *et al.* (1994) demonstrated the use of linear eddy modeling in flame analysis, by including detailed chemistry.

Depending on the nature of the model implementation, the line along which diffusion and stirring occur can be perpendicular to the main flow direction, or parallel. In the first case, the line moves downstream with the average fluid velocity, creating a Lagrangian framework, where time is equivalent with downstream distance. Examples of this geometry are the shear layer model (Kerstein, 1989), the round jet model (Kerstein, 1990) and the pipe flow model (Chapter 4). Simulation of a streamwise line can be viewed as interaction between cells along

Figure 3-3: Flowsheet for simulation subroutine in linear eddy program. Every call to this subroutine constitutes a single realization.

a streamline. Neighboring cells interact by diffusion, and stirring events may move the contents of a cell forward or backward along the streamline. Convection by the average fluid velocity needs to be implemented as an additional process, moving the whole profile downstream, adding new fluid at the upstream end of the profile, and removing fluid downstream. Kerstein (1992a) implemented the streamwise model for a turbulent diffusion flame; the linear eddy modeling of the cold flow experiments in this work (Chapter 9) belongs in this same category.

3.5 Conclusions

All three modeling techniques described in the previous chapters have been used for modeling turbulent reacting flows. Comparison between mechanistic models and experimental data is quite good, not only for a single very fast reaction, but also for intermediate rates (Rao and Dunn, 1970; Metha and Tarbell, 1983) and for multiple reactions (Dutta and Tarbell, 1989). Zipp (1989) successfully used a hydrodynamic model to simulate the effect of mixing on an acid-base reaction in a stirred tank. However, closure approximations are greatly complicated if more than one reaction occurs (Patterson, 1981). The most rigorous evaluation of linear eddy modeling predictions for reacting flows is by Kerstein (1992b), who compared simulation of reaction between NO and O₃ in a shear layer to experimental data, at different Damköhler number. Menon *et al.* (1992) compared plots of temperature as a function of mixture fraction in hydrogen-air combustion, from linear eddy simulations and experimental data, and predicted the NO emission index in

hydrogen-air combustion.

Mechanistic models are appealing because of their simplicity. This makes them relatively easy to understand conceptually, and their implementation requires less computational power than that of other modeling approaches. However, they have certain disadvantages, due to their empirical nature. They do not allow modeling of spatial structure of mixing intensity, and therefore cannot yield a distribution of conversion, segregation and temperature. Also, mechanistic models involve parameters which are difficult to relate to the operating variables in real mixers.

Of the different model types presented, only the hydrodynamic mixing model explicitly solves the Navier-Stokes equations; in the linear eddy model, it is necessary to make assumptions or use experimental data for the flow field and the turbulence intensity. Therefore, in complicated geometries, the hydrodynamic mixing model is favorable, with direct numerical simulation or large-eddy simulation (see Chapter 3.6) as alternatives.

Most mechanistic models and the hydrodynamic mixing model are deterministic models, predicting average behavior¹. Even when intensities of segregation are predicted (solution of eqn. 2-35 or 3-3), these do not give complete information;

¹ The Monte Carlo treatment of the coalescence-redispersion model, mentioned earlier, is an exception.

while the "spread" of a concentration PDF can be derived from the intensity of segregation, the shape needs to be assumed separately. The linear eddy model, on the other hand, predicts both the shape and the spread of the concentration PDFs. It can therefore be used in risk assessment studies, to predict the chance of occurrence of a certain event. For example, in hazardous waste incineration modeling, this allows us to estimate the likelihood that a given concentration is exceeded in the outlet of an incinerator, under given inlet conditions. Also, the nature of the model makes it possible to evaluate the effects of spatial resolution on measurements (Chapter 9.6).

The ability of the linear eddy model, to predict excursions from average behavior, made it the model of choice for application to the present study. It is most easily applied to the transition section of the kiln, since the flow pattern in this region is relatively simple; in the kiln cavity, the interaction between two feed streams and the presence of multiple recirculation zones complicate the fluid dynamics considerably. Before the linear eddy model is used to model experimental results (Chapter 9), a model is formulated for radial mixing in fully developed turbulent pipe flow (Chapter 4). The development of this model served two purposes: on the one hand, it was used as an introduction to the technique of linear eddy modeling, in a well-defined system. On the other hand, the model has its own merit: turbulent pipe flow is a very elementary configuration in chemical engineering, and this linear eddy model may help to better understand turbulent reacting flows in many

applications.

3.6 Alternatives

Besides the mixing models presented in this chapter, many others exist, two of which we will mention briefly. One alternative approach consists of direct numerical simulation of the largest scales, in combination with a sub-grid model, that allows for all scales that are not resolved. This technique ("large-eddy simulation") has mostly been used in combination with various closure models. As first demonstrated by Menon (1991), the linear eddy model can also serve as a sub-grid model in large eddy simulations.

PDF models (Borghi, 1988) are deterministic models, in which closed balance equations are obtained for the probabilities of different concentrations. They are therefore similar to the hydrodynamic mixing models, but contain more detailed information about the scalar PDFs.

We did not investigate these and other types of models in sufficient detail to comment on their value for the present study. It should be noted, however, that both large eddy simulations and PDF models exceed the models that were presented earlier both in complexity and in computational demand.

CHAPTER 4

A LINEAR EDDY MODEL FOR MIXING IN TURBULENT PIPE FLOW¹

4.1 Introduction

In this chapter, a linear eddy model for radial mixing in turbulent pipe flow is presented. The development of this model was intended primarily as an exercise in the implementation of linear eddy modeling. Insight gained in developing this model helped in the later development of the unsteady state model (Chapter 9). The choice for turbulent pipe flow was motivated by the availability of both experimental data and theoretical expressions for turbulent diffusivity. We think that the model has some merit of its own, given the importance of turbulent pipe flow in engineering applications. However, there is no *direct* connection between the results of the present chapter and the overall thrust of this dissertation.

Fully developed turbulent pipe flow is one of the most elementary turbulent flow configurations, and one that closely resembles flows in many engineering applications. Average heat and mass transfer in fully developed turbulent pipe flow (and channel flow) have been researched extensively, both experimentally and theoretically, e.g. Sherwood and Woertz (1939), Quarmby and Anand (1969),

¹ This chapter has been submitted for publication elsewhere (Schenck *et al.*, 1994).

Hughmark (1971), Sheriff and O'Kane (1971), Sandall *et al.* (1980). The general approach in all these studies is to use a turbulent diffusivity, or an effective heat or mass transfer coefficient, to calculate the average scalar profile.

In reacting turbulent flows, however, it is usually not sufficient to know only the average local concentration. Concentration fluctuations, in the form of correlations, enter the averaged chemical reaction rates (Dutta and Tarbell, 1989). While there is a fair number of experimental studies of the "unmixedness" in turbulent pipe flow (Lee and Brodkey, 1964; Becker *et al.*, 1966; Bremhorst and Bullock, 1973; Hishida and Nagano, 1979; Durbin and Frost, 1981) and while direct numerical simulations are available for low Re turbulence (Kim and Moin, 1989), adequate theoretical models are more difficult to find.

As pointed out by Fackrell and Robins (1982), point (or line) sources in turbulent boundary layers are characterized by a zero scalar flux at the wall, and therefore differ considerably from situations with constant wall flux or constant wall temperature. Most turbulent mixing models are restricted to either one of those configurations: Lagrangian models for line sources in turbulent boundary layers (Hunt and Weber, 1979; Legg, 1983) cannot be used for boundary value problems; the same is true for the simple model of Parenthoen *et al.* (1988). On the other hand, pseudo-steady state models, such as the surface rejuvenation model (Harriot, 1962; Chung and Pang, 1980) cannot be used to predict the spread of

point or line sources.

Closure models can be used to predict fluctuating quantities, by including a balance equation for scalar fluctuations. Spalding (1971) used this approach to model concentration fluctuations in a turbulent jet. A similar model was used by Sykes *et al.* (1984) for dispersion in a turbulent boundary layer. The main difficulty in closure modeling is to find an appropriate expression for the dissipation term in the scalar fluctuation equation. As Sykes *et al.* pointed out, their model is only valid when molecular diffusion can be neglected (high Péclet number). The expression derived by Zipp (1989) (see Chapter 3.3) accounts for Schmidt number effects, but has not been tested extensively, or found widespread acceptance.

In this chapter, a model is proposed that can be used for both initial value and boundary value problems, based on the linear eddy modeling technique of Kerstein (see Chapter 3.4). The model has certain similarities to other Lagrangian models. It is different from the others because it simulates the development of an entire scalar profile (along the diameter of the pipe), under the dual actions of turbulent stirring and molecular diffusion. The model will be used here to interpret existing experimental data on dispersion from a wall source in turbulent pipe flow by Durbin and Frost (1981). To our knowledge, these data have not yet been modeled successfully. If a boundary value problem were to be modeled, the only model adaptation would be a change in boundary conditions.

4.2 Radial Diffusivity in Turbulent Pipe Flow

A simple expression can be obtained for the diffusivity profile in turbulent pipe flow, based on the "law of the wall" and the Reynolds analogy. Even though more accurate models are available (Quarmby and Anand, 1969; Sandall *et al.*, 1980), this model was chosen because of its simplicity, facilitating derivation of the eddy frequency in the linear eddy model.

A fluid element at distance r from the centerline of a pipe experiences three forces in the axial (Z) direction: pressure, shear force due to the radial gradient of mean velocity, and a force, associated with the turbulent momentum exchange.

$$v \frac{dU}{dr} - \overline{uv} - \frac{r}{2} \frac{dp}{dZ} = 0 \quad (4-1)$$

The radial position is non-dimensionalized, by letting:

$$x = 1 - \frac{r}{R} \quad (4-2)$$

The turbulent viscosity and the friction velocity are introduced:

$$v_T \equiv \frac{-\overline{uv}}{dU/dr} \quad (4-3)$$

$$u_* \equiv \sqrt{\frac{\tau_w}{\rho}} = \sqrt{\frac{-R}{2\rho} \frac{dp}{dZ}} \quad (4-4)$$

A logarithmic velocity profile, derived from the "law of the wall" (Tennekes and

Lumley, 1972) is assumed. in differential form, this can be written as:

$$\frac{dU}{dx} = \frac{u_*}{\kappa x} \quad (4-5)$$

Even though the law of the wall is not valid in the laminar sublayer, the fact that we only use the velocity gradient limits the error substantially. Combining eqns. (4-1 to 4-5) and neglecting molecular viscosity (appropriate outside the laminar sublayer and the buffer layer), gives:

$$\frac{v_T}{u_* R} = \kappa(x - x^2) \quad (4-6)$$

The law of the wall is actually derived for a constant stress layer, and therefore eqns. (4-1) and (4-5) are inconsistent. A turbulent diffusivity in the spirit of the law of the wall leads to the same expression of eqn. (4-6), without the x^2 term (i.e. a linear relation between distance from the wall and turbulent diffusivity). As the term x^2 vanishes close to the wall, eqn. (4-6) may be viewed as an extrapolation of the law of the wall towards the center of the pipe.

From eqn. (4-6), assuming a turbulent Schmidt (or Prandtl) number of one:

$$\frac{D_T}{u_* R} = \kappa(x - x^2) \quad (4-7)$$

Thus, we have obtained an expression for the radial turbulent diffusivity in a pipe, as a function of radial position. This equation is shown as a dotted line in Figure 4-2. It has a maximum value of 0.1 at $r/R = 0.5$. It fits the experimental results of

Quarmby and Anand (1969) very well for $1-r/R < 0.25$. Only in the center of the pipe ($1-r/R > 0.8$) is there a substantial deviation. An empirical relation between u_* and U can be obtained from an expression for the friction factor (Sakiadis, 1984). Taking into account that Re_* has the pipe radius as its length scale, and Re the pipe diameter:

$$Re_* = \frac{u_* R}{\nu} = \frac{0.226 Re}{\ln(Re/7)} \quad (4-8)$$

Combination of eqns. (4-7, 4-8) yields the maximum in D_T/ν ($r/R = 0.5$) as a function of Re . This is depicted in Figure 4-1, together with experimental data, as reported in the literature. The maximum turbulent diffusivity calculated here is consistently higher than experimentally obtained values. The dependence on Reynolds number is in agreement with the semi-theoretical equation by Sherwood and Woertz (1939). It fits the experimental data very well over a wide range of Re ; better than a linear relation between D_T/ν and Re , as suggested by Sheriff and O'Kane (1971).

It should be noted that Durbin and Frost (1981) reported a significantly higher turbulent diffusivity than that derived here (see Figure 4-2)¹. We will correct for this and other incongruities with an empirical factor.

¹ Diffusion from a wall source is determined primarily by the diffusivity close to the wall (where it is minimum). Therefore, large variations in turbulent diffusivity near the center of the pipe have a relatively small effect on the average concentration profiles.

Figure 4-1: Dependence of turbulent diffusivity on Reynolds number. Comparison between present model and experimental data.

4.3 Linear Eddy Modeling Considerations

The linear eddy model presented here simulates a radial line of length $2R$ that moves downstream with the average fluid velocity. Thus, in this model, downstream distance and (Lagrangian) time are equivalent.

Application of the linear eddy model requires expressions for eddy size and frequency. Following Prandtl mixing length theory, the eddy size is assumed to scale with the distance from the wall to the eddy center:

$$\frac{L}{R} = qx \quad (4-9)$$

q (an empirical constant of order unity) is one of two fitting parameters in the model. The maximum possible value for q is 2, since larger eddies (in the radial direction) would straddle the wall.

The quantity $\lambda(x)dx$, which is the rate of occurrence of linear eddies with centers in the interval $(x, x+dx)$, is determined by matching the diffusivity associated with the stirring process to the turbulent diffusivity (eqn. 4-7). Mappings due to block inversions can be viewed as a random walk process (see Chapter 2.4). Allowing displacements of different sizes, eqn. (2-20) for turbulent diffusivity becomes:

$$D = \int \frac{z^2}{2} N(z) dz \quad (4-10)$$

The diffusivity at any point x along the radius of the pipe is due to block inversions that include x , but have their center elsewhere. Necessarily, a block inversion that

moves material at x over a distance z has its block center at $\xi = x \pm z/2$. Its size $L = q\xi$ must be larger than $z = 2|x - \xi|$. Thus, from eqn. (4-10):

$$\frac{D_b}{u_* R} = \int_{ax}^{bx} 2(x - \xi)^2 \Lambda(\xi) d\xi \quad (4-11)$$

where:

$$a = \frac{1}{1 + q/2} \quad b = \frac{1}{1 - q/2} \quad (4-12)$$

are the limits of integration, determined by the local eddy size, and:

$$\Lambda = \frac{\lambda R^2}{u_*} \quad (4-13)$$

is the dimensionless block inversion frequency that needs to be calculated. Eqn. (4-11) is not valid for large values of x , when bx exceeds unity. These points are affected by eddies that have their center on the opposite side of the centerline of the pipe. Therefore, the diffusivity due to block inversions in the center region of the pipe is fixed, because of matching the turbulent diffusivity closer to the wall. A general solution to (4-11) for $x < 1/b$ is:

$$\Lambda(\xi) = \frac{\alpha_1}{\xi^2} + \frac{\alpha_2}{\xi}$$

$$\alpha_1 = \kappa \left(4 \ln \frac{a}{b} + 2 \left(\frac{1}{a} - \frac{1}{b} \right) - 2(a-b) \right)^{-1} \quad (4-14)$$

$$\alpha_2 = \kappa \left(2 \ln \frac{a}{b} - 4(a-b) + (a^2 - b^2) \right)^{-1}$$

For $q = 1.2$ (obtained from a best fit of the temperature fluctuation profiles of Durbin and Frost), $\alpha_1 = 0.6614$ and $\alpha_2 = -0.3534$. As x approaches zero (close to the wall), the eddy frequency gets very high. Therefore, in the wall region, the eddy size was assumed to be constant, and the eddy frequency to be proportional to the distance from the wall. This minimum eddy size was introduced strictly for computational savings. It is sufficiently small (1% of the pipe diameter) that it does not affect the average scalar or scalar fluctuation profiles.

The top graph in Figure 4-2 compares the diffusivity from a linear eddy simulation (using block inversions) to the theoretical curve (eqn. 4-7) and experimental data. The diffusivity, calculated from displacements (eqn. 4-10), matches the theoretical curve up to $1-r/R = 0.4$. Further away from the wall, the theoretical profile is not matched, due to the effect of eddies from the opposite side of the center line. The local gradient diffusivity (eqn. 2-16) was determined by simulating scalar transport across turbulent flow, with fixed scalar concentration at the boundaries. From the molecular diffusivity and the gradient at the wall, the molar flux was calculated. The flux and the scalar gradient at any point were then substituted in eqn. (2-13), to

Figure 4-2: Radial profiles of turbulent diffusivity. Comparison between law of the wall, experimental data and linear eddy model. Top: block inversions; bottom: triplet maps after empirical correction.

calculate the local turbulent diffusivity. As can be seen from Figure 4-2, there is a substantial difference between the random walk diffusivity and the local gradient diffusivity of the simulation. This is most likely due to the facts that the turbulence is inhomogeneous (N is a function of position) and that higher order derivatives of the scalar field can not be ignored.

In order to match the average temperature profiles of Durbin and Frost, it is necessary to account for three incongruities. (1) The local gradient diffusivity and the mean square displacement have different values in inhomogeneous turbulence, as shown above. (2) The diffusivity, associated with triplet maps is lower than that of block inversions. Kerstein (1992a, 1989) derived that in homogeneous turbulence the diffusivity due to block inversions is higher by a factor of $(27/12)$; in inhomogeneous turbulence, there may not be a constant factor. (3) In the wall region, the experiments of Durbin and Frost (1981) suggest a higher turbulent diffusivity than those of Quarmby and Anand (1969). The reason for this is unclear.

One empirical constant was introduced in the expression for eddy frequency (eqn. 4-14), to account for all of these effects. From a best fit to the average temperature profiles, this constant was found to be 4.5, resulting in a triplet map frequency:

$$\frac{\lambda(x) R^2}{u_*} = \frac{-1.59}{x} + \frac{2.98}{x^2} \quad (4-15)$$

Linear eddy simulation of scalar transport across wall-bounded flow with this triplet

map frequency lead to the diffusivity profiles in the bottom graph of Figure 4-2. The diffusivity matches the values, suggested by Durbin and Frost in the wall region; towards the center of the pipe, the diffusivity of the model is lower than suggested by Durbin and Frost, but higher than Quarmby and Anand's data. It is interesting to note that in the wall region, the diffusivities calculated from mean square displacement and local gradient are approximately equal, whereas a large difference was found in the case of block inversions.

4.4 Simulations and Results

Wall source experiments of Durbin and Frost (1981) were simulated with the linear eddy model formulated in the previous section, and a friction velocity Reynolds number $Re_* = 1125$ (corresponding to $Re = 5.0 \cdot 10^4$ in the experimental study. For the Prandtl number a value of 0.71 was assumed. All profiles are normalized with the flow mean scalar, as defined by Durbin and Frost.

The linear eddy simulations were performed with 3000 gridpoints on a domain, representing the pipe diameter of 20 cm. Examination of individual realizations indicated that this number of gridpoints gives resolution of all scales; a typical scale of fluctuations covering 15 or more gridpoints. The number of realizations was 1000. Because each realization gives a profile over the pipe diameter, and the averages are over the pipe radius, both halves of the instantaneous profiles were used independently, effectively doubling the number of realizations. To simulate the

finite probe size in the experimental data (400 μm), temperature profiles were averaged over 6 adjacent gridpoints. The scalar fluctuations were up to 10% higher when this averaging procedure was omitted, the largest discrepancies occurring close to the wall at short downstream distances. Simulation results are compared to experimental data in Figure 4-3. Downstream distance (Z) is expressed in dimensionless form as a Lagrangian time:

$$\tau = \frac{Z u_*}{R U} \quad (4-16)$$

With $U = 4.0 \text{ m/s}$ and $u_* = 0.18 \text{ m/s}$ (Durbin and Frost), one unit of dimensionless time corresponds to 22 pipe radii .

The simulation was repeated for high and low Prandtl number: 6.99 (representing water at 20°C) and 0.021 (mercury at 50°C). Local eddy size and eddy frequency remained unchanged from the previous simulation. Again, 3000 gridpoints were used for the pipe diameter, giving full resolution. Statistics were calculated from 3000 realizations (high Pr) and 100 realizations (low Pr), using a "probe size" of a single grid point (67 μm). Simulation results are presented in Figure 4-4.

4.5 Discussion

The development of the average concentration profile of the model shows good agreement with the experimental data (Figure 4-3a), which reflects the fit of eqn. (4-15). The fluctuation profile (Figure 4-3b) displays a maximum, detached from the

Figure 4-3: Radial profiles of average scalar (a) and scalar fluctuations (b), downstream of wall source. $Re_* = 1125$; $Pr = 0.71$.

Figure 4-4: Radial profiles of average scalar (a) and scalar fluctuations (b), downstream of wall source. $Re_* = 1125$; various Pr .

wall. At longer downstream distances, the peak moves slightly further away from the wall. Quantitatively, the experimental profiles are predicted very well towards the center of the pipe, but strongly under predicted immediately adjacent to the wall, especially at short times. There are two possible explanations for this. The is that the assumed eddy size distribution may not be adequate. The model would predict higher fluctuations in the wall region if a constant eddy size were assumed throughout the laminar sublayer and the buffer layer. Fluctuations in the wall region would also be higher if there were a single eddy size, independent of radial position. This modeling approach is appealing because of its simplicity. However, simulation with a single eddy size model predicted the maximum in the fluctuation profile to be at the wall for all downstream distances, which is contradicted by experimental observations. A second possible explanation for the discrepancy may be due to some conduction along the pipe wall in the experiments (reportedly observed by Durbin and Frost). As a consequence, there would have been a finite gradient at the wall, causing production of scalar fluctuations. By contrast, in the present model, the wall gradient is zero.

Comparison between Figures 4-3b and 4-4b shows a slight difference in the fluctuation profiles at $Pr = 0.71$, at the earliest time. This difference is due to the larger probe size in the simulation of Figure 4-3. Variation of the Prandtl number has effects on both the average temperature profile and the fluctuation profile. At higher Prandtl number, diffusion is slower, due to the increased resistance in the

laminar sublayer (Mizushima, 1974), leading to a profile that is less developed. At any downstream distance, the maximum of the fluctuation profile is closer to the wall, and the peak is both higher and broader, for higher Prandtl number. All these observations agree at least qualitatively with results from direct numerical simulation (Kim and Moin, 1989).

Because the turbulent core of fully developed pipe flow is known to be homogeneous, the present model may seem physically unrealistic near the center of the pipe. Two possible modifications to the model would be (1) to assume a constant eddy size, beyond a certain distance from the wall, or (2) to incorporate Kolmogorov scaling, basing the local Kolmogorov eddy size on the local large eddy size and the large eddy Reynolds number. This means that at any radial position x , there is a range of eddy sizes, compared to a single eddy size for given x in the present model. The Kolmogorov size is then proportional to $x^{1/4}$, leading to homogeneity of the small scales. This second possibility was explored. While it complicated the model considerably, and led to an additional parameter, it did not significantly improve the results. However, including Kolmogorov scaling of some sort would be essential if the model were to be used for Reynolds number extrapolations.

The present model is not recommended for simulating center sources in turbulent pipe flow for three reasons: (1) Axisymmetry has not been accounted for. This is

relatively unimportant for line sources at or near the wall. However, when turbulent dispersion occurs in more than one direction, such as from a center source, or from a point source at the wall, a one-dimensional model will not be adequate. (2) Linear eddy modeling is only valid in the far field, beyond the Lagrangian integral time scale (Kerstein, 1988; 1992b). Since eddy size scales with distance from the wall, so does the Lagrangian integral time scale (assuming no variation in eddy velocity). Therefore, longer times (or downstream distances) are needed for center sources, and most of the interesting developments will take place in a time, shorter than the Lagrangian integral time scale. (3) As mentioned earlier, the model formulation is not realistic in the center region, where homogeneous turbulence has been observed experimentally.

4.6 Conclusions

A linear eddy model was developed for turbulent pipe flow, that can be used both for initial value problems with a source at or near the wall, and for boundary value problems. Average scalar profiles and scalar fluctuation profiles from simulation of a line source agree well with experimental observations, except for the fluctuation profile in the near wall region. Prandtl (or Schmidt) number dependence agrees with direct numerical simulations.

CHAPTER 5

COLD FLOW MODEL EXPERIMENTS

5.1 Design Considerations

The purpose of our cold flow model experiments is to obtain both qualitative and quantitative information on the mixing process in the EPA rotary kiln incinerator, by studying mixing in a comparable environment, in the absence of chemical reaction. The first requirement, therefore, is that the cold flow model has the same geometry as the EPA kiln. For ease of fabrication and undistorted visual access, some compromises were made with respect to the axisymmetry. Although not strictly necessary, it was decided to make the cold flow model the same size as the original.

From the theories that were formulated in Chapter 2, it can be concluded that two mechanisms control the mixing: turbulent motion and molecular diffusion¹. To obtain similarity in turbulent motion between kiln and cold flow model, ideally, the non-dimensional turbulent velocity field at any location in the model should correspond to that in the kiln at the same location. This can be accomplished to some degree by matching the Reynolds number of the kiln, giving the same

¹ It should be noted here that other mechanisms may play a role in gas phase mixing, that have been ignored in the theory. The most likely additional mechanism in rotary kilns is stratification, due to variations of temperature and gas composition. This will be discussed briefly in Chapters 11.4 and 11.9.

balance between viscous and inertial forces, and by matching the turbulence structure at the kiln inlet. Complete dynamical similarity between the kiln and the cold flow model may be impossible to achieve. The main reason is that the temperature varies widely in the kiln (from ambient for the incoming gases at the burner inlet to circa 1400 K at the afterburner), causing a large spatial dependence of viscous and inertial forces, due to variations in density and viscosity. This cannot be accounted for in the model, and the only practical approach is to match the Reynolds number of the kiln at the most prevalent temperature.

The decrease in temperature, compared to the kiln, causes the kinematic viscosity in the cold flow model to be much lower than in the kiln (see Table 5-1). Therefore, in order to match the Reynolds number at a constant geometric length scale, it is necessary to reduce the mean fluid velocity, thus increasing the residence time. According to eqn. (4-8) the friction velocity is roughly proportional to the mean velocity. If we assume that this is true for all turbulent velocities, then turnover times of eddies will increase proportionally to the residence time. Consequently, the whole turbulent mixing process in the cold flow model is a "slow motion" equivalent of the kiln mixing. This slow motion should also be accounted for in the transient phenomena of the kiln. Therefore, the duration of a puff (i.e. the time during which material is released from the bottom of the cold flow model) scales with the kiln residence time. This is expressed in dimensionless form as the Strouhal number, here defined as the ratio of puff duration to residence time

(based on the total volume of the cold flow model).

The relative effect of molecular diffusion is expressed as the Schmidt number. As mentioned in Chapter 2.5, the Schmidt number determines the smallest length scales for scalar mixing at a given Reynolds number (eqn. 2-26). However, the macro-mixing (at length scales much larger than the Corrsin or Batchelor scale, and up to the integral length scale) is not affected by molecular diffusion. Therefore, in studying *large scale* mixing phenomena, the Schmidt number is not an important parameter. The apparent micro-mixing depends not only on the Schmidt number, but also on the spatial resolution of the measurements. The smallest scale that can be observed is the larger of the smallest scale present and the probe size. Therefore, it has been suggested that measurements of high Sc scalar mixing with a finite size probe can be interpreted as higher resolution measurements of low Sc mixing (Becker *et al.*, 1966). The validity of this assertion will be tested with the linear eddy model (Chapter 9.6). While it is impossible to determine the optimum probe size a priori, modeling suggests that the RMS fluctuations are fairly insensitive to the exact dimensions (see Figure 9-9).

In Table 5-1 dimensions and mixing parameters of a typical full-scale kiln, the EPA simulator and the cold flow model are compared. Data for the full-scale kiln are derived from Cundy *et al.* (1989a), and for the EPA kiln from Linak *et al.* (1987a). Figure 5-1 shows a schematic of the EPA kiln.

	full scale kiln	EPA simulator	cold flow model; low	cold flow model; high
diameter (m)	3.2	0.76 ⁽¹⁾ 0.46 ⁽²⁾	0.76 ⁽¹⁾ 0.46 ⁽²⁾	0.76 ⁽¹⁾ 0.46 ⁽²⁾
length (m)	10.7	0.61 ⁽¹⁾ 2.90 ⁽³⁾	0.61 ⁽¹⁾ 2.90 ⁽³⁾	0.61 ⁽¹⁾ 2.90 ⁽³⁾
flow rate (m ³ /s)	29.2	0.185	0.011	0.115
viscosity (m ² /s)	82.56*10 ⁻⁶	15.9*10 ⁻⁵	15.75*10 ⁻⁶	15.75*10 ⁻⁶
waste flow rate (m ³ /s)		8.7*10 ⁻³	8.6*10 ⁻⁴	8.6*10 ⁻⁴
puff time (s)		5	20	20
total volume (m ³)	86	0.74 ⁽³⁾	0.91 ⁽³⁾	0.91 ⁽³⁾
residence time (s)	3	3.8 ⁽³⁾	77 ⁽³⁾	8.1 ⁽³⁾
Re	1.4*10 ⁵	2.0*10 ³ ⁽¹⁾ 3.2*10 ³ ⁽²⁾	1.7*10 ³ ⁽²⁾	1.7*10 ⁴ ⁽²⁾
Sc	O(1)	1.9 ⁽⁴⁾	5.0*10 ⁵	5.0*10 ⁵
St		1.2	0.27	2.5
C ₀		4.7*10 ⁻²	7.1*10 ⁻²	7.5*10 ⁻³
Re _T	3.2*10 ³	118 ⁽²⁾	70 ⁽²⁾	493 ⁽²⁾
Kolmogorov scale (mm)	3.8	6.4	9.5	2.2
Batchelor scale (mm)	~ 4	5.9	1.3*10 ⁻²	3.1*10 ⁻³

Table 5-1: Dimensions and mixing parameters in rotary kiln incinerators. Comparison between a typical full-scale kiln, the EPA simulator, and the cold flow model (at low and high main air flow rates). Notes: ⁽¹⁾ cavity; ⁽²⁾ transition section; ⁽³⁾ to backfire burner/end of cold flow model; ⁽⁴⁾ toluene.

Main gas/air flowrates in the EPA kiln were calculated, based on 5.22 kg/h of natural gas, air at a stoichiometric ratio of 2.0 (giving a total flowrate of 6.7 kg-mole/h), and a temperature of 1200 K. The same temperature was used for fluid property calculations. For the full scale kiln, density and viscosity are based on the design temperature of 800 K. An estimate for the characteristic time of waste release in the EPA kiln was derived from the predicted puff shape of Wendt and Linak (1988), shown in Figure 5-2. At half the maximum height, the time duration of a peak is circa five seconds. The volumetric flowrate of waste was estimated by assuming a charge mass of 100 grams of toluene ($M = 92.14$) to evaporate in five equal puffs, i.e. in a total time of 25 seconds. Both charge mass and composition are representative for experiments at EPA. Data on waste flow were not available for the full scale kiln. The Schmidt number in the cold flow model is based on Brownian diffusion of particles, calculated from the Einstein formula (Levich, 1962):

$$D_B = \frac{kT}{3\pi\mu d_p} = \frac{2.36 \cdot 10^{-17}}{d_p} \quad (\text{m}^2/\text{s}) \quad (5-1)$$

Kolmogorov and Batchelor scales in the transition section are calculated from eqn. (2-26), assuming the velocity fluctuations to be equal to the friction velocity (eqns. 4-4, 4-8), and the large eddy size to the duct radius. The calculated Kolmogorov size is much larger than what is typically observed in laboratory flows. A better value could be obtained from eqn. (2-22), estimating the dissipation rate from (measured) spatial variations in concentration fluctuations (Champagne, 1978):

Figure 5-1: EPA rotary kiln incinerator simulator. From Wendt and Linak (1988).

Figure 5-2: Measured and predicted toluene puff shapes. (a) Measured puff shape, $MASS = 100g$, $T_M = 1124 K$, $RPM = 0.5$. (b) Predicted puff shape for case (a). (c) Predicted "base case" puff shape, $MASS = 125 g$, $T_K = 1325 K$, $RPM = 1.25$. From Wendt and Linak (1988).

$$\epsilon = 15\nu \left(\overline{\frac{\partial u_1}{\partial x_1}} \right)^2 \quad (5-2)$$

One possible explanation for the high value of l_k in Table 5-1 is that the turbulent Reynolds number is too low for Kolmogorov equilibrium theory to apply.

5.2 Experimental Facility

Figure 5-3 shows a schematic of the experimental facility. The heart of the facility is a full scale cold flow model of sections 1 and 2 of the EPA rotary kiln. Dimensions (in inches) are given in Figure 5-4. The model is made of plexiglas, with rounded edges out of 8" diameter PVC pipe. Panels in the sides of the model can be removed for cleaning and for easy access. Inlet and outlet ducting are made of sheet metal. An exhaust blower generates the main air flow through the model; the flowrate can be regulated with a damper on the vent of the model. The main air enters the model through a 6 ft. section of 12" diameter circular ducting, with a flow straightener made out of plastic drinking straws. The velocity across the inlet of the cavity was measured with an Anlor 8500D II thermo-anemometer. It was determined that the variation in average velocity with cross-stream position is less than 10% ($Re = 2.5 \cdot 10^3$ to $2.5 \cdot 10^4$). So, for all practical purposes, plug flow can be assumed at the model inlet. During experiments, the main air flowrate is determined by measuring the velocity upstream of the flow straightener, using the thermo-anemometer. The secondary air stream is supplied by a compressed air

Figure 5-3: Experimental facility.

Figure 5-4: Dimensions of cold flow model (in inches). Side view (top) and cross sections of transition section and cavity (bottom).

cylinder. Parts of this stream pass through TiCl_4 and through water. Both the total flowrate and the flowrate seeded with TiCl_4 are monitored with rotameters. The rotameter for the total secondary air flowrate was calibrated with a Rockwell 1000 gas meter; calibration results are presented in Appendix E. A solenoid valve, operated with a time relay, controls the secondary air stream. The same time relay operates an indicator light, which burns whenever the solenoid valve is open. The seeded flow enters the cold flow model through an 8" circular hole in the bottom of the cold flow model, covered with a flow straightener of 1.5" thickness, made out of plastic straws.

5.3 Optical System

A 5 W argon ion laser (Spectra Physics model 165), placed under the cold flow model, is operated at 514.5 nm. The laser beam is expanded with a series of lenses, and positioned in the cold flow model through the use of mirrors. Three different optical configurations are used (see Figure 5-5): (1) For qualitative analysis, the laser beam is positioned along the center line of the horizontal transition section, and diffracted into a vertical sheet, using a 5/8" glass rod. This rod is placed inside the cold flow model, in the recirculation zone. (2) Quantitative measurements in the horizontal transition section are performed with the laser beam positioned vertically, 10 cm downstream of the contraction. This the closest to the cavity that measurements can conveniently be performed. (3) For quantitative measurements in the vertical transition section, the laser beam is

Figure 5-5: Three different optical arrangements. From top to bottom: laser sheet; laser line, horizontal transition section; laser line, vertical transition section.

positioned horizontally, 1.0 m above the center line of the horizontal transition section. Measurements further downstream might be affected by flow interference from the vent. At the points where the laser line enters the model (for laser line experiments) 2 mm holes were drilled, in order to minimize loss of light intensity by reflections off the plexiglass.

A laser line (as opposed to a sheet) was used in quantitative analysis for two reasons. First of all, the light intensity of a laser line is much higher than that of a sheet. Therefore, lower particle densities are required, reducing the likelihood of multiple scattering (see Appendix A). Secondly, in a diverging laser sheet, the light intensity is a function of location, so that it is necessary to calibrate each position independently. The light intensity along a laser line is constant, and therefore a single calibration for the entire line suffices. It should be noted that the use of a stronger laser (or operation of the current laser in multi-line mode) would not resolve the second issue. One alternative approach would be the use of a scanned sheet (Balint *et al.*, 1985), produced by a rotating mirror. In a scanned sheet, the light intensity is a function of the distance from the mirror, but independent of the angle, relative to the incoming beam.

5.4 Particle Seeding

In a windbox under the cold flow model, seeding particles are formed by the (very fast) reaction between water and TiCl_4 :

In order to estimate the dynamics of the particles, first of all, we need to know the particle size and the particle number density.

From impactor experiments, using a Delron cascade impactor (model DCI-5), we determined the particle size to be between 0.5 and 1.0 μm , which agrees fairly well with the primary particle size of 1.1 μm , reported by Freymuth *et al.* (1985) and the sub-micron size, reported by Murayama and Takeno (1988). The particle number density can be estimated as follows: In all our experiments, the total puff flowrate is 0.86 liter/sec, of which 0.008 l/s (0.97%) is seeded with TiCl_4 . If the TiCl_4 -containing flow is saturated ($p = 10$ mm Hg; Weast, 1986), the total Ti seeding is $(10/760) \cdot 0.97\% \cdot (40 \text{ mol/m}^3) = 5.1 \text{ mmol/m}^3$. Assuming all TiCl_4 reacts¹ to form TiO_2 ($M = 189.7$), the particle mass density (m) is 967 mg/m^3 . The number density (n) can be found from the particle mass density and the weight of a single particle:

$$n = \frac{6m}{\rho_p \pi d_p^3} \quad (5-4)$$

The density of TiO_2 is $4.17 \cdot 10^3 \text{ kg/m}^3$ (Weast, 1986). With a particle diameter

¹ Note: the flowrates are such that water is available in excess (see Table 5-2).

between 0.5 and 1.0 μm , the number density is found to be between $4.4 \cdot 10^{11}$ and $3.5 \cdot 10^{12}$ particles/ m^3 .

A key assumption in the cold flow model mixing experiments is that the seeding particles act as markers of the puff. This requires that particles follow the flow of the surrounding gas. Two mechanisms that may cause a deviation between local gas velocity and particle velocity are gravitational settling and particle inertia. The terminal settling velocity can be calculated from Stokes' law (Bird *et al.*, 1960):

$$u_s = g \frac{d_p^2 (\rho_p - \rho)}{18\mu} \quad (5-5)$$

With the particle size determined earlier, the terminal settling velocity is between 0.04 and 0.15 mm/s. For residence times up to 77 s (Table 5-1), the total settling distance may be as much as 1 cm, which is small, compared to the geometric length scale of the model. It should further be noted that the gravitational force results in a steady settling, and has no effect on the local instantaneous fluctuations in particle velocity. Levich (1962) estimated the velocity of a particle, relative to the surrounding fluid, due to particle inertia (effectively a slip velocity). His result, based on a balance between drag, inertia and local fluid acceleration, obtained from scaling arguments:

$$u_i \approx \frac{1}{6\sqrt{3}} \frac{\rho_p - \rho}{\rho} d_p^2 \frac{\epsilon^{3/4}}{\nu^{5/4}} \quad (5-6)$$

The direction of u_i varies randomly, with the frequency of the smallest eddies.

Combining with eqns. (2-21, 2-22) yields:

$$\frac{u_i}{u_K} \approx \frac{1}{6\sqrt{3}} \frac{\rho_p - \rho}{\rho} \left(\frac{d_p}{L} \right)^2 Re_T^{3/2} \quad (5-7)$$

Consequently, the slip velocity due to inertia is less than 1/5000th of the velocity of Kolmogorov eddies. We therefore conclude that particle inertia does not play a role, and particles do indeed follow the flow.

In quantitative experiments, we determine puff concentrations by calculating the particle density from the pixel value. It is implied that the puff concentration and particle concentration are proportional. This is not necessarily true: the particle number density in the flow may decrease, due to a loss of particles (e.g. gravitational settling or electrostatic diffusion to the walls), or due to coagulation. The gravitational settling, estimated in the previous paragraph, is unlikely to have a substantial effect. Electrostatic diffusion (or some other, unknown mechanism) may be relevant; over long periods of time, we noticed some deposition of particles on the walls of the cold flow model. Unfortunately, we do not have a good way to quantify this. Coagulation can be estimated from the diffusivity of particles (eqn. 5-1) using Smoluchowski's theory (Levich, 1962):

$$n = \frac{n_0}{1 + 4\pi D_B d_p n_0 t} \quad (5-8)$$

For residence times up to 77 seconds (Table 5-1), the particle concentration might drop from an initial 3.5×10^{12} particles/m³ down to 3.2×10^{12} particles/m³, and is therefore negligible. Most likely, coagulation is even slower than calculated here, because of dilution of the puff.

5.5 Experimental Procedure

Experiments consist of the temporal release of seeded secondary air into the main air stream, under known flow conditions (see Table 5-2). In quantitative experiments, the only parameter that is varied is the main air flowrate. We keep the puff flowrate constant, because this gives us the most confidence that the puff is seeded in a reproducible manner. The laser beam is positioned perpendicular to the main flow direction. Because of the random nature of the mixing process, multiple releases under identical circumstances are necessary, to obtain statistically significant data. Therefore, one set of experiments consist of multiple (between 9 and 18) runs.

The seeding particles in the secondary air stream scatter (and absorb) the laser light, as described in Appendix A. The scattered light is recorded on video, using an RCA camcorder, operated with the iris fully open and a shutter speed of 1/120th second. All recordings are made on Scotch EG+ VHS tape. Video frames

also include a time stamp (obtained from the monitor of a Gateway personal computer with 486DX/33 processor, displaying the clock of Microsoft Windows 3.1), and the solenoid valve indicator light. This allows us to determine the time of any video frame, relative to the time at which the puff was first released. Data analysis, based on video recordings, is performed independently (i.e. not in "real time"). This will be described in the next chapter.

Table 5-2: Flow conditions for cold flow model experiments (see also Tables 7-1 and 7-2).

Main air flowrate	0.011 to 0.115 m ³ /s
Puff flowrate	0.86 l/s
puff - TiCl ₄ seeded	0.0083 l/s
puff - H ₂ O seeded; estimate	~ 0.4 l/s
puff duration	20 s

CHAPTER 6

DATA ANALYSIS

6.1 Nomenclature

Before describing the image analysis techniques and presenting the experimental results, it is useful to define some terms and naming conventions that will be used throughout this and the following chapters:

A run is defined as the release of a single puff of seeded material. The term setup is used to signify a combination of experimental settings (main air and puff flowrates, puff duration, and location of the laser line). Thus, one setup consists of multiple (between 9 and 18) runs. Time is measured relative to the time at which a puff was first released; $t = 0$, therefore, at the beginning of each run.

The coordinate system used in digitized images has its X-axis aligned with the laser line, perpendicular to the main flow direction; the Y-axis is aligned with the main flow direction. Indices i and n both relate to the X-axis: i is the absolute index, and n a relative index, given by $n = i - i_{\min}$; j is the absolute index along the Y-axis. Index m refers to the run number in a particular setup. The value of m ranges from 1 to M , the number of runs per setup; n has values between 1 and N , the number of pixels that are determined along the laser line in an individual image.

Three different types of average pixelvalue are calculated. The ensemble average

is an average over all runs (M), for a given setup, time and cross-stream location (n). The cross-stream average is a spatial average of the ensemble average, and is determined over multiple runs and locations (M,N), for given setup and time. Finally, the integral average is the time-integral of the cross-stream average, and is only dependent on the setup. Two types of standard deviation are calculated, analogous to average pixel values: the ensemble standard deviation and the cross-stream standard deviation. It should be noted that the second is not simply an average over the ensemble standard deviations. This follows from analysis of the variance, as presented in Appendix B.2.

Average concentration, concentration standard deviation, intensity of segregation and scale of segregation are calculated as functions of time only, with no cross-stream dependence. Similarly, PDFs and spectra are based on a combination of cross-stream data. All spectra to be presented are one-dimensional scalar spectra. Average spectra are geometric means of multiple spectra, determined at different times in a single setup. Profiles of average concentration, RMS fluctuations, etc. denote the development of these quantities over time, at a fixed (downstream) position.

Some additional terms are introduced throughout the rest of this chapter, in the context in which they appear. All terms are printed italic/underlined when they are defined. Naming conventions for data files are given in Appendix C.3.

6.2 Digitizing and Image Analysis

The first step in the data analysis process is to decide, what video frames will be digitized. To this end, we first of all register the clock times of all puff releases (indicated by a light on the video tape), and the approximate clock times at which the puffs appear and disappear in the field of view. Then, for every setup, we choose ca. ten different times, the first one equal to the average arrival time of the puff, and the last one equal to the time when the puff has died out. For each run in a setup, we then digitize video images at all these times. A 320x200 pixel, 256 gray level digitizer is used; however, only 320x50 pixels of each image, containing the laser line, are actually digitized. These digital images constitute the raw data files.

The position of the laser line in the raw data files: $i_{\min}$ and $i_{\max}$, $j_{\min}$ and $j_{\max}$ (see Figure 6-1) is determined, using Improces¹ image processing software². This position is the same for all files from a particular setup.

Images from multiple runs, for given setup and time, need to be combined. Also, we want a single pixel value for each combination of run number and cross-stream location. Finally, statistics need to be calculated. All processing tasks are

¹ Improces is "shareware" from John Wagner Software.

² To view images in Improces, it was necessary to transform raw data files to GIF format.

Figure 6-1: Schematic of video images, showing laser line, indicator light and time stamp. One compressed data file is created by combining the laser lines from all digitized images (raw data files) for a given setup and time.

performed by three separate programs, written in Microsoft Fortran (see Appendix C.3), and run on a 486DX/33 PC. The input for the first program (PROPERTIES) consists of the raw data files of a given setup and time, plus the values of $i_{\min}$ and $i_{\max}$, $j_{\min}$ and $j_{\max}$. It creates two files. One output file (the compressed data file) contains a two-dimensional array of $M \times N$ processed pixel values, with M the number of runs and N the number of cross-stream locations. The second output file gives the ensemble average and standard deviation of the processed pixel values at each location n , plus the cross-stream average and standard deviation. Figure 6-1 shows schematically how the video images are translated into a data file. Generating a processed pixel value for a given run number and cross-stream location $PPV(m,n)$ consists of three steps. First, pixel values $RPV(i,j)$ are read from the raw data files, for fixed position $i = i_{\min} + n$, and different positions j ($i_{\min} < j < j_{\max}$). Pixel values are translated from hexadecimal to integer numbers. Then, each pixel value is filtered, according to:

$$FPV_{i,j} = \sum f_k RPV_{i,j+k} \quad (6-1)$$

where: $f_{-3} = f_{-2} = -1$; $f_{-1} = 0$; $f_0 = f_1 = f_2 = f_3 = 1$; $f_4 = 0$; $f_5 = f_6 = -1$.

The filter is chosen such that the background pixel value is subtracted from the image, while it accommodates for the fact that the width of the laser line may be more than a single pixel (up to four pixels). The third step in the image analysis is determining the maximum of the filtered pixel values $FPV(i,j)$. This maximum is saved as the local processed pixelvalue $PPV(m,n)$, and used in the statistical calculations.

The compressed data files are used by the other two analysis programs. Of these, the program CORRELATION calculates the spatial correlation function, the scale of segregation, and the spectrum; this is described in more detail in Chapter 6.3. The program PDF creates a pixel value PDF, simply by performing a bin count on the array of processed pixel values.

6.3 Spatial Correlation

Spatial correlation functions, the scale of segregation, and scalar spectra serve to quantify spatial correlation of the scalar field. While the theoretical expressions of eqns. (2-27, 2-29 and 2-32) define all three quantities, they are impractical for actual computations. The main difficulty is that the maximum separation distance ($r_{\max}$) over which the correlation function can be determined is not infinity. Rather, it is limited by the maximum distance between measurement points, or at best by the physical dimensions of the mixing device. This would not be a problem if all mixing scales were much smaller than this dimension, so that $R(r_{\max})$ would essentially be zero. However, problems arise in situations where the largest mixing length scales are of the same order of magnitude as $r_{\max}$, or in mixtures with spatial inhomogeneity. One of two situations can arise, depending on how the correlation curves are determined: (1) If the correlation is determined by following the concentration fluctuations at two points as functions of time, $R(r_{\max})$ may be positive for large r . (2) If a correlation curve is determined from a single instantaneous concentration profile, by moving pairs of points along the profile, the

resulting $R(r)$ will be negative for $r > (r_{\max}/2)$ because the average concentration of one half of the domain is lower than the global average, and that of the other half higher. Both situations pose a problem. If $R(r_{\max})$ is positive, we cannot accurately calculate the spectrum, because the high end of the integral over the correlation curve is missing. The occurrence of negative correlations raises the question, whether they are imaginary (i.e. an artifact of the bounds of the measurement domain) or real.

In our experimental analysis, each correlation curve is determined for a single setup and time, by combining processed data files from multiple runs, and moving pairs of points along the laser line in each file. Therefore, both situations (1) and (2), outlined above, might occur.

Gullet *et al.* (1993) determined the scale of segregation from analysis of a single image at a time, and then calculated the average and standard deviation of ten scales, determined under identical conditions. They circumvented the question of whether or not to include negative values $R(r)$ in their integration, by defining an alternative (related) scale. However, the exact physical significance of their scale is unclear. It seems unlikely that it is quantitatively identical to Danckwerts's scale of segregation. Also, the same method cannot be applied to determination of the scalar spectrum. Therefore, we do not follow their approach. Instead, for all measurements, we determine the scale of segregation in two ways, namely by

integrating over positive values $R(r)$ only, and by integrating over all values of $R(r)$, up to $r_{\max}$. A large discrepancy between the two indicates a strong negative tendency in the spatial correlation function, suggesting large scale unmixedness (spatial inhomogeneity) within individual data files.

In the image analysis program, negative values $R(r)$ are excluded from the calculations of the scalar spectrum, for two reasons. Mostly, spectra show less scatter when negative values are excluded, because there is no discontinuity in the correlation function. When negative values are included, this causes a discontinuity at $r_{\max}$, producing high wave number components in the spectrum. Also, inclusion of negative values results in a positive derivative $dF(k)/dk$ for large wave numbers¹. All spectra are multiplied by $(\pi/R(0))$, so that the value of the spectrum has the units of length. Therefore, the calculated value of $F(0)$ corresponds to the scale of segregation (compare eqn. 2-34).

6.4 Calibration

A key assumption in the data analysis is that the pixelvalue at any point is proportional to the local particle density, and thus to the relative amounts of secondary and main air. Unfortunately, we are not able to verify this directly, due to unsteady state phenomena and inhomogeneities in the mixture. Instead, for

¹ Under assumption of isotropy, this leads to negative values for the three-dimensional spectrum, which is physically impossible.

calibration, we rely on the integral average signal. At any time, the cross-stream average particle density is proportional to the relative flowrate of seeded (compared to total) air, under the assumption that the observed laser line is representative of the entire cross-stream area. The integral average particle density is therefore proportional to the product of relative flowrate and duration of puff. Thus, when the total air flowrate is increased a factor Q , under further identical conditions, the integral average pixelvalue should be $1/Q$ times its original value, if pixel value and particle density are indeed proportional. The calibration procedure implies that the cross-stream averages are mixing cup averages; in other words, transverse variation of average velocity can be neglected. Detailed measurements of the velocity profile, that might serve to correct the mixing cup averages, are not available. Therefore, in cases where the average pixelvalue is highly dependent on transverse position, mixing cup averages cannot be determined accurately.

Proportionality between particle density and pixel value was confirmed by Gullet *et al.* (1993) in a very similar setup. There are several reasons why we cannot do the same calibration as they did. First of all, their system is for continuous, rather than transient mixing, eliminating time dependence of the mixing process. Secondly, their data analysis is based on laser sheet images (giving more measurement points per video frame than a laser line), and they achieve almost complete mixing at the downstream end of their system. Thus, one can have confidence that in the measurements of Gullet *et al.* a single image gives the average particle density.

From calibration, a theoretical pixel value can be calculated for undiluted puff:

$$PV_{\text{puff}} = \frac{\int PV dt}{t_{\text{puff}} C_0} \quad (6-2)$$

where C_0 is the relative puff flow rate, at the time a puff is being released. It should not be surprising that PV_{puff} is higher than 256 (the maximum pixel value in the raw data files, for two reasons: (1) Due to the filtering, processed pixel values are generally higher than raw pixel values. (2) Given the high dilution rate, it is very unlikely that undiluted puff would be found anywhere in the cold flow model.

6.5 Accuracy

Several factors determine the accuracy of the measurements. The two that we will consider here are statistical inference and temporal resolution. Of the other factors, cross-stream inhomogeneity (Chapter 8.1) probably has the largest effect. However, this is difficult to quantify.

Statistical inference theory gives the confidence intervals for average and standard deviation of a quantity, based on the number of independent observations and the average and standard deviation of the observations. The relevant formulas are presented without proof in Appendix B.1. The main problem in applying statistical inference to our measurements lies in the fact that neighboring pixels are correlated. Therefore, the number of independent observations is lower than the

total number of observations. According to Tennekes and Lumley (1972), the integral time scale is a rough measure of the interval over which the velocity $u(t)$ is correlated with itself. We will assume that the same is true for the scale of segregation, being a measure of the distance over which a scalar quantity is correlated with itself. Thus, the number of independent observations per digitized image equals the length of the laser line that has been analyzed, divided by the scale of segregation. It is necessary, therefore, to calculate the scale of segregation, before the confidence intervals for PV and pv' can be determined.

From the 95% confidence interval for PV , the 95% confidence interval for $\bar{C}/C_0$ can be calculated directly. Likewise, the confidence interval for c'/C_0 follows from that for pv' . Calculating a confidence interval for $c'/\bar{C}$ or for $\mathfrak{S}$ is more complicated, because these are functions of both PV and pv' . Therefore, both confidence intervals contribute to a confidence interval for $c'/\bar{C}$ or $\mathfrak{S}$.

The standard deviations in pixel value (both ensemble and cross-stream) are determined from independent measurements at a certain time. However, measurements that are said to be taken at the same time t are really taken somewhere in the interval $(t-\Delta t/2, t+\Delta t/2)$. If the average pixel value changes significantly during this time interval, the calculated standard deviation will have two contributions: one is from the fluctuations at any time t' ($t-\Delta t/2 < t' < t+\Delta t/2$). The other contribution is due to the variation of the average pixel values at different

times t' . This partitioning of the standard deviation can be related to the analysis of variance (Appendix B.2), when the different groups are taken to be different times t' . The true standard deviation at any time will therefore be lower than the value we calculated. If each time t' is sampled with equal likelihood, and the time-derivative of the average pixel value is constant, then the contribution of the time dependence of the average pixel value to the total variance (variance of group means) is:

$$\frac{\sigma_B^2}{N} = \int_{-\Delta t/2}^{\Delta t/2} \left(t \frac{dPV}{dt} \right)^2 dt = \frac{1}{12} \left(\frac{dPV}{dt} \right)^2 (\Delta t)^3 \quad (6-3)$$

Using eqns. (6-3, B-5, B-6, B-8), a time interval of one second, and experimentally determined dPV/dt , the corrected variance at time t (pooled sample variance) is:

$$(pv')^2 \approx (pv')^2_{\text{observed}} - \frac{1}{12} \left(\frac{dPV}{dt} \right)^2 \quad (6-4)$$

Eqn. (6-4) was used to correct all cross-stream pixel value fluctuations. However, the effect turned out to be very small (smaller than the round-off error) in most cases.

CHAPTER 7

EXPERIMENTAL RESULTS

7.1 Introduction

In this chapter, experimental results are presented. Two types of experimental data were obtained: qualitative data from laser sheet experiments, and quantitative data, using a laser line. Laser sheet experiments were performed mainly to distinguish regions with different mixing patterns in the cavity of the cold flow model. Line experiments were completed at two different downstream locations. From digitized video images, we determined the time-development of average pixel value, standard deviation, and pixel value PDFs, as well as spatial correlation curves and spectra. Pixel values are related to puff concentrations through a calibration procedure. Of the quantitative data, we will use primarily the cross-stream average pixel value and standard deviation in subsequent chapters, to characterize and model the mixing of puffs in our cold flow model and in the EPA rotary kiln. The scale of segregation is used for estimating the accuracy of the measurements.

7.2 Laser Sheet Experiments

Laser sheet flow visualization was used for qualitative analysis of the mixing in the cold flow model. The laser sheet was positioned vertically, along the center line of the model (Figure 5-5, top). Figure 7-1 shows photographs, representative of the mixing patterns in the cavity and in the transition section. Additional laser sheet

Figure 7-1: Typical mixing patterns in cavity (top) and transition section (bottom) of cold flow model.

experiments were recorded on video.

Figure 7-2 schematically shows our observation of the mixing in different regions of the cavity. It can be described as follows. As the seeded puff stream enters the cavity (1), some fairly small scale mixing occurs at the edges, reminiscent of shear layer mixing. In this region, the effects of the main air inlet flow are negligible in most cases: the unseeded air is quiescent. Only at very high main air flowrates can a slight motion towards the main air inlet be observed, and seeded flow is entrained by the main air jet. In the center of the cavity (2), large scale mixing between the two streams occurs. There is a clear interface between seeded and unseeded air; the fluid shows strong circulation in this region. Near the top of the contraction (3), most fluid moves into the transition section. However, some fluid (from both feed streams) turns upward, and enters a recirculation zone in the top of the cavity (4). More seeded flow enters this recirculation zone at higher puff flow rate or lower main air flow rate. According to the jet/cross-flow model of Rathgeber and Becker (1983) presented in Chapter 8.1, the puff trajectory is determined by the relative velocities of the two streams. The recirculation zone is very well mixed (and therefore difficult to record on video). Coherent structures can be observed at the interface of the recirculation zone and the top of the main air jet, where fluid from the recirculation zone is entrained by the jet. The region near the bottom of the contraction (5) was hard to observe. There seems to be a recirculation zone here also. From the cavity, the fluid enters the transition section (6). Depending on

the relative flow rates of puff and main air, the seeded flow may distribute over all or only part of the cross section of the transition section: at low relative puff flow rates, the puff stays near the bottom of the duct, while at higher puff flow rates (or lower main air flow rates), the seeded material is distributed over the entire cross section, with the highest concentration near the top. Large scale turbulent motion was observed throughout the transition section.

7.3 Laser Line Experiments

Quantitative experiments, using laser line flow visualization, were performed with fixed puff duration (20 sec) and puff flowrate (0.86 liter/sec). The air flowrate through the TiCl_4 was 0.5 liter/min in all experiments. Four different main air flowrates were chosen. The length of the laser line recorded on the video images is circa 25 cm, in the middle of the cross-sectional area (see Figure 7-3). Experimental conditions are summarized in Tables 7-1 and 7-2.

Table 7-1: Experimental conditions: main air flowrate and derived quantities. Horizontal transition section.

setup #	main air flowrate (l/s)	C_0 (v/v)	τ (sec)	Re transition section	St
2	13	0.062	66	$2.0 \cdot 10^3$	0.30
4	22	0.037	39	$3.4 \cdot 10^3$	0.51
3	37	0.023	24	$5.5 \cdot 10^3$	0.84
1	115	0.007	8	$1.7 \cdot 10^4$	2.54

Figure 7-2: Schematic representation of mixing in different regions of the cold flow model cavity.

Figure 7-3: Location of laser lines in cold flow model. The numbers indicate pixel locations along the laser lines in the raw data files.

Table 7-2: Experimental conditions: main air flowrate and derived quantities. Vertical transition section.

setup #	main air flowrate (l/s)	C_0 (v/v)	τ (sec)	Re transition section	St
4	11	0.071	77	$1.7 \cdot 10^3$	0.26
1	22	0.037	39	$3.4 \cdot 10^3$	0.51
2	37	0.023	24	$5.5 \cdot 10^3$	0.84
3	112	0.008	8	$1.6 \cdot 10^4$	2.47

Video frames were digitized, as described in the previous chapter. Numbers in Figure 7-3 indicate the relation between the pixel location in the raw data files (index i in Figure 6-1) and the location along the laser line in the cold flow model. Figure 7-4 shows some of the resulting images (raw data files) for a single setup.

Raw data files were processed, by running the image analysis program PROPERTIES (Appendix C.3), using the i and j values specified in Table 7-3. This provided us compressed data files, as well as cross-stream average and standard deviation of pixel values, and ensemble average and standard deviation¹. The compressed data files have been discarded (after using them to calculate PDFs, spatial correlation functions and spectra). Cross-stream average pixel values and standard deviations are tabulated in Appendix D.1. Also included are the time derivative of the average pixel value and the corrected standard deviation, as

¹ Nomenclature follows the definitions of Chapter 6.1.

Figure 7-4: Digitized images of laser line at different times in a single run (top) and at the same time ($t = 20$ sec.) in multiple runs (bottom). Horizontal transition section; $Re = 3.4 \cdot 10^3$.

defined in eqn. (6-4). As can be seen from the tables, this correction is negligible in most cases.

Table 7-3: Parameters for image analysis.

setup #	# runs	$i_{\min}$	$i_{\max}$	$j_{\min}$	$j_{\max}$
Horizontal transition section					
1	16	2	317	29	38
2	14 ¹	38	317	33	36
3	18	44	319	30	35
4	16	48	319	30	35
Vertical transition section					
1	14	2	317	43	52
2	14	2	317	32	41
3	14	2	317	33	44
4	9	2	317	32	44

Confidence intervals (95%) were determined, as described in Chapter 6.5. For estimating the number of independent observations, we used the scale of segregation (in pixels), obtained from integration over positive values of $R(r)$ (see Appendix D.4). This "positive-only" integral results in a larger scale of segregation than the total integral, and thus in a more conservative estimate for the confidence intervals.

¹ At 180 seconds, only 12 runs were analyzed.

Cross-stream average pixelvalue and standard deviation, with corresponding 95% confidence intervals, are presented graphically in Figures 7-5 and 7-6. As can be seen from the graphs, confidence intervals are rather large. In order to reduce the size of the confidence intervals, a large increase in the number of measurements would be necessary; confidence intervals for average pixel value are proportional to $N^{-1/2}$ (see Appendix B.1). The figures display a peak of circa twenty seconds in both average pixel value and fluctuations, at all Re . When comparing the results from the two figures, it can be seen that the fluctuations are lower in the vertical transition section (further downstream), which is evidence of improved micro-mixing. The time integral of the average pixel value peak increases by roughly a factor of two (see Chapter 7.4). However, the maximum (over time) of the cross-stream average pixel value does not change so dramatically (with the exception of the experiment at $Re = 3.4 \cdot 10^3$), indicating that the puff has distributed over a longer time (improved macro-mixing).

In the absence of a laser line, the cross-stream average and standard deviation are 9 and 4, respectively. This was determined by using the same procedure for the digital images of one setup and time, but choosing j_{min} and j_{max} such that the laser line was outside the area considered in the data compression.

Ensemble average pixel values and standard deviations, presented graphically in Appendix D.2, are three-dimensional versions of the curves for cross-stream

Figure 7-5: Cross-stream average pixelvalue (top); cross-stream standard deviation (bottom). Bars indicate 95% confidence intervals. Horizontal transition section, various Re.

Figure 7-6: Cross-stream average pixelvalue (top); cross-stream standard deviation (bottom). Bars indicate 95% confidence intervals. Vertical transition section, various Re.

average and standard deviation, with location as the third dimension. Two representative graphs for ensemble average pixel value are also shown in Figure 7-7. It is apparent that in the vertical transition section, average and standard deviation are virtually independent of location, and the 3D graphs therefore do not show any additional qualities. In the horizontal transition section, however, there is an important feature. At $Re = 1.7 \times 10^4$, the peaks in both ensemble average and ensemble standard deviation are highest for the highest pixel location, and virtually absent at low pixel locations. At $Re = 2.0 \times 10^3$ and $Re = 3.4 \times 10^3$, the peaks for average pixel value are higher at low than at high pixel locations. The standard deviation peaks show a similar trend but less pronounced. Finally, for $Re = 5.5 \times 10^3$ we can detect a maximum in both average and standard deviation, around the 100th pixel along the line, indicating that the maximum puff concentration occurs close to the center of the duct.

7.4 Calibration

Calibration was performed separately for the two measurement locations. For every setup, the cross-stream average pixel values were corrected, by subtracting 9 (the value found when the laser line was absent). The corrected pixel values were integrated over time, and then divided by the duration of a puff (20 sec). The resulting integral signal has been plotted as a function of C_0 , the fraction seeded

Figure 7-7: Ensemble average pixel values in horizontal transition section (top) and vertical transition section (bottom). $Re = 3.4 \cdot 10^3$. For graphs at other Re and ensemble standard deviation, see Appendix D.2.

Figure 7-8: Calibration of image analysis, by calculating the integral average pixel value. The slope is equal to the corrected pixelvalue of undiluted seeded ("puff") flow.

flow, in Figure 7-8. From linear regression of the data¹, we find a slope K of 7435 for the horizontal transition section and 13441 for the vertical. Therefore, the theoretical pixel value of pure, undiluted puff would be 7435 and 13441 respectively, at these two locations. The dimensionless average concentration and standard deviation are given by:

$$\frac{\bar{C}}{C_0} = \frac{(PV - 9)}{KC_0} \quad (7-1)$$

$$\frac{c'}{C_0} = \frac{(pv' - 4)}{KC_0} \quad (7-2)$$

Where 9 and 4 are the average pixel value and standard deviation in the absence of a laser line.

The following can be observed from Figure 7-8. (1) The signal is roughly a factor two higher in the vertical than in the horizontal transition section. There are three explanations for this. (a) The laser line is reflected by three mirrors to reach the horizontal section, and by two to reach the vertical section (see Figure 5-5). Therefore, the laser light intensity will be less in the first case, due to absorption by the mirror surfaces. This effect is thought to be small. (b) The distance between the laser line and the camcorder was larger in the measurements of the horizontal section. Therefore, less of the scattered light was received by the camcorder

¹ For regression in the vertical transition section, the measurement at the highest fraction seeded flow was discarded.

optics, inversely proportional to the distance $(r)^1$. While r was not measured directly, it can be inferred from the pixel size (Chapter 7.5). Based on this, the proportionality constant is expected to be 15% lower in the horizontal than in the vertical transition section. (c) Additional discrepancies are probably due to (flow and mixture) inhomogeneities in the horizontal transition section. (2) In the vertical section, all but one of the integral signals show proportionality to the fraction seeded flow. The signal at the highest fraction seeded flow (lowest Re) is lower than expected. A likely (partial) explanation for this is as follows: In this setup, the pixel value is significantly higher than the "zero value" (i.e. 9) at the latest measurement time. Therefore, the integral is not complete. A higher value for the integral would have been found, had measurements at later times been available. Other possible reasons why the integral pixel value is lower than expected may be settling or electrostatic diffusion of particles (largest at the longest residence time) and multiple scattering (most likely at the highest puff concentration). (3) In the horizontal transition section, the correlation between the data is fairly poor. This is probably due to the inhomogeneity of the flow. Because the observed line is only slightly more than half of the diameter of the duct, the calculated cross-stream average may not be representative of the true cross-stream average.

¹ The irradiance due to scattering from a single particle at distance r is $\propto r^{-2}$. The total number of particles observed along a line element is $\propto r$, making the total irradiance $\propto r^{-1}$. Note that for a laser sheet, the number of particles observed is $\propto r^2$, and therefore the total irradiance is constant (independent of r).

As a result of the poor correlation in the horizontal transition section, the average concentration profiles are inconsistent, i.e. the integral average concentration is not equal to the product $C_0 \cdot t_{\text{puff}}$, when the average slope (obtained from regression: $K=7435$) is used. To correct for this, in addition to calculating the average concentration by using the average slope in eqn. (7-1), we also used the slope of each setup separately. Corresponding values for K are presented in Table 7-4. The same renormalization procedure was applied to the average concentration profile at $Re = 1.7 \cdot 10^3$ in the vertical transition section.

Table 7-4: Proportionality constants for use in eqns. (7-1, 7-2).

location	Re	K
horizontal	all	7435
horizontal	$2.0 \cdot 10^3$	6764
horizontal	$3.4 \cdot 10^3$	10994
horizontal	$5.5 \cdot 10^3$	6449
horizontal	$1.7 \cdot 10^4$	10119
vertical	all	13441
vertical	$1.7 \cdot 10^3$	8736

7.5 Spatial and Temporal Resolution

The smallest length scale that can be resolved experimentally is the size of a pixel.

The pixel size was determined by placing a ruler inside the cold flow model at the location of the measurements, recording the ruler on video, digitizing an image, and counting the number of pixels along the ruler. We found that in the horizontal

transition section the resolution is 30.3 pixels per inch, and in the vertical transition section 36.0 pixels per inch. This means that the pixel size is 0.84 and 0.71 mm respectively, at the two locations.

The temporal resolution of the clock used in our experiments (Microsoft Windows) is one second. We could improve the resolution by interpolation. However, this gain is probably offset by a slight irregularity that was observed: not every second on the clock display had the exact same duration.

7.6 Probability Density Functions

From compressed data files, pixel value histograms were determined, by running the program PDF (see Appendix C.3). These histograms are essentially the same as concentration PDFs, with a linear relation between pixel value and puff concentration (compare eqn. 7-1). They have not been normalized¹. Histograms for $Re = 5.5 \cdot 10^3$ (both horizontal and vertical transition section) are presented in Figures 7-9 and 7-10. Each figure consists of eight histograms, representing different times in a single setup. Appendix D.3 contains histograms for all Reynolds numbers; qualitatively, all histograms correspond to those at $Re = 5.5 \cdot 10^3$.

In the horizontal transition section (Figure 7-9), the histograms are essentially

¹ See Appendix D.3 for a description of the normalization procedure, which allows quantitative interpretation of pixel value histograms.

Figure 7-9: Pixel value histograms at different times. Horizontal transition section, $Re = 5.5 \times 10^3$.

Figure 7-10: Pixel value histograms at different times. Vertical transition section, $Re = 5.5 \cdot 10^3$.

bimodal, indicating the presence of two distinct phases. They consist of a narrow peak at pixel value zero ("unseeded air phase") and a very broad peak ("puff phase", made up of various puff concentrations). During a cycle, the magnitude of the second peak increases and then again decreases. At very short and very long times, there is no local maximum in this peak. The maximum is also less pronounced or virtually absent for experiments at other Reynolds numbers.

In the vertical transition section (Figure 7-10), the histograms are unimodal, so that we can no longer distinguish two separate phases. During a puff cycle, the maximum moves from zero to some finite concentration, and back to zero.

7.7 Spatial Correlation Functions and Spectra

Spatial correlation functions $R(r)$, scales of segregation, and one-dimensional scalar spectra $F(k)$ were determined from compressed data files, by running the program CORRELATION (see Appendix C.3). The maximum separation distance in calculation of the correlation functions was chosen to be 200 pixels¹. Correlation functions for different times in each setup, and corresponding scales of segregation, are presented in Appendix D.4.

¹ Calculations at larger separation distances were deemed of little value, because of insufficient data. For example, to calculate $R(300)$, on a domain of 315 pixels, only 15 combinations are possible. The problem is aggravated by the fact that those 15 combinations would be correlated.

Figure 7-11: One-dimensional scalar spectra at different times. Horizontal transition section, $Re = 3.4 \cdot 10^3$.

Each spectrum that was calculated is for a given setup and time. Figure 7-11 shows spectra at six different times from a single setup. Interruption of the curves at any point indicates a negative value for $F(k)$, which cannot be represented on a logarithmic scale. Because the curves are noisy, and because there is no clear trend in the time-development of the spectra, we decided to combine spectra that were obtained at different times in a given setup. By doing this we imply that the spatial correlation of the mixture does not change over time. This does not mean that the micro-mixing should be independent of time (in fact, we know that it is not). It does mean that the way fluctuations in pixel value are divided over different length scales is the same at all times. The fact that the correlation functions and the scale of segregation are not definite functions of time (Figures D-17 to D-24) supports this supposition. The scale of segregation tends to be somewhat higher at short than at longer times in the vertical transition section. By averaging, we ignore this difference. Spectra at very short and very long times were excluded from the averaging procedure, because we thought that the signal to noise ratio would be lower when pixel values are low. We also excluded the spectrum from a time that corresponds to an outlying value for the scale of segregation ($t = 22$ s in the horizontal transition section, $Re = 5.5 \cdot 10^3$). Average spectra will be presented and interpreted in Chapter 8.3.

7.8 Conclusions

We have successfully completed qualitative and quantitative flow visualization studies. Image analysis of video images (between 9 and 18 per measurement point) gave us time-development of average pixel value and standard deviation, pixel value PDFs and spectra. The accuracy of the measurements was adequate, and can easily be improved further by increasing the number of runs. A more serious problem was the uncertainty, caused by cross-stream variations in the horizontal transition section. As a consequence, regression for calibration of the measurements was poor. Regression was very good in the vertical transition section for all but the lowest Reynolds number, for which the signal was lower than expected. Several possible explanations for the lower signal at low Re have been presented. From the data presented here, we can infer profiles of cross-stream average concentration and RMS fluctuations as functions of time. These will be presented in the next chapter, and form the main data set for model development.

CHAPTER 8

DISCUSSION OF RESULTS

8.1 Cross-stream Variations

The raw experimental data in the horizontal transition section (Figures 7-7, D-1 to D-4) show a strong cross-stream variation in ensemble average pixel value. At low Reynolds number (i.e. high relative puff flowrate), it is maximum near the top of the duct; at high Reynolds number near the bottom. These results are consistent with the qualitative observation, that the seeded flow traverses further through the duct at lower relative main air flowrate (Chapter 7.2). In the vertical transition section, cross-stream variations have largely disappeared (Figures 7-7, D-5 to D-8). Three issues need to be addressed here: (1) What is the reason for the cross-stream variations; can this phenomenon be modeled ? (2) What are the consequences of the cross-stream variation for the mixing characterization (Chapters 8.2 to 8.4) ? (3) Are the observations (qualitatively and quantitatively) representative for the EPA kiln ?

(1) The cross-stream variation in the horizontal transition section can be linked to the initial mixing between the two streams in the cavity. This is a complicated process: two jets meet under a right angle in a bounded domain. While in principle the transient nature of the secondary jet might have an effect as well, this seems unlikely, because most of the turbulent energy for mixing is provided by the

(steady) main air flow. Okamoto and Enokida (1982) reported that deflection of a jet, under the action of a secondary jet at a right angle, can be modeled adequately with an impulse balance. This result applies to unconfined flow. Mixing between a jet and a cross-flow has been investigated by Rathgeber and Becker (1983). They proposed for the trajectory of the jet:

$$\frac{x}{M d_0} = 0.42 \left(\frac{Z}{M d_0} \right)^{0.20} \left(\frac{d_0}{d_c} \right)^{-0.39} \quad (8-1)$$

where x is the cross-stream position, Z the downstream position, d_0 and d_c are the initial jet and the cross-flow (pipe) diameters, respectively, and M is the ratio of jet and cross-flow velocities. Expressions for the jet width were also presented. Interestingly, the jet trajectory is virtually independent of Reynolds number ($68,000 < Re < 160,000$); the authors posed the question, whether the slightly greater jet deflection at higher Reynolds number is a non-ideality or a trend.

Qualitatively, our observations agree with both the jet/jet model and the jet/cross-flow model: both predict the puff to transverse the main stream further at lower Re (keeping the puff flowrate constant). Quantitatively, the deflection of the seeded flow is much less than that predicted by either model. This should not be too surprising. Compared to Rathgeber and Becker, our Reynolds number is a factor 10 lower; M is between 0.016 and 0.16 in our setup, when the ratio between the puff and main air inlet jets is taken (a factor 6.25 higher, if the main air is

considered to be distributed evenly over the cavity). The corresponding (d_o/d_c) is 0.67 (0.27 for cavity) By contrast, eqn. (8-1) was developed for values $2 < M < 13$ and $0.02 < d_o/d_c < 0.06$. The extrapolation to other velocity ratios and diameter ratios may not be valid. The contraction downstream of the incoming puff flow may affect its path as well.

(2) Cross-stream variations in the horizontal transition section make the mixing characterization somewhat inaccurate. The main reason is, that experimental data are available for only half of the cross-section. In stratified flow, this may not be a representative sample. The poor results for calibration (Figure 7-8) are indicative of this problem. The proportionality constant K , that relates concentrations to pixel values (eqns. 7-1, 7-2), cannot be determined accurately. A further consequence of the stratification is a negative correlation for the scalar field at large separation distances. This introduces an undesirable component in the spatial correlation functions, which may also affect the scale of segregation and the spectra. In spite of these complications, we treated the measurements in the horizontal transition section as if there were no cross-stream variation, for lack of an alternative. Mixing characteristics determined in the vertical transition section are thought to be more reliable, since cross-stream variations are very small here.

(3) Entrainment of evaporating waste in the main air stream in the EPA kiln would likely be similar to what has been observed in the cold flow model. A quantitative

prediction cannot be given, however, for two reasons. First, the area over which the waste is being released from the kiln bottom is not known, and most likely time-dependent, as the bed is moved continuously by the motion of the kiln. As can be seen from eqn. (8-1), this is an important parameter¹. Secondly, the model of Rathgeber and Becker does not account for density differences between jet and cross-flow. This is possibly a significant factor in the kiln mixing.

8.2 Macro-mixing

The fact that puffs are transient introduces an important large scale phenomenon: macro-mixing or a distribution of residence times. If macro-mixing were absent (all fluid elements had the same residence time), the average concentration profile $\bar{C}(t)$ at any location Z would be identical to the input profile, shifted over a time $\tau(Z)$. Also, under steady state conditions (inlet concentration constant), a residence time distribution would have no effect on the output concentration². In our experiments, the inlet concentration profile consisted of a 20 second pulse of concentration C_0 . Any deviation from this shape at the two measurement locations indicates a distribution in residence time.

¹ At constant relative volumetric flowrates, M is a function of the area over which the puff is released. Consequently, the cross-stream position at any downstream location will be proportional to $d_0^{-1.19}$.

² This is true for pure mixing only. In reacting flow, mixing or residence time distribution can have an effect on the conversion and the product distribution, also under steady-state conditions. See Levenspiel (1972), Chapter 10.

Average concentrations, for both the horizontal and the vertical transition sections, are presented as functions of time in Figures 8-1 to 8-4. Average concentration was calculated from ensemble average pixel value, using eqn. 7-1. In the vertical transition section, all conversions were made with the same proportionality constant ($K = 13441$). In addition, at $Re = 1.7 \times 10^3$, a renormalized curve was calculated ($K = 8736$). In the horizontal transition section, for each Re , calculations were done with both the average proportionality constant ($K = 7435$) and the renormalized constant for that particular Re (see Table 7-3).

Points that correspond to average K values and to K values of individual setups are represented by filled and hollow symbols, respectively. While the filled symbols form the most accurate representation of the actual measurements, they do not always predict the correct integral puff concentration, i.e. the area under the curves is inconsistent with the theoretical value ($t_{puff} = 20$ sec). By definition, the area under all renormalized curves (hollow symbols) is 20 seconds.

At all Re , we can detect a significant "tail" in the concentration profiles from the vertical transition section, while the maximum average concentration is always much less than C_0 . Both observations indicate a considerable spread in residence time. A further important feature of the curves is, that they are highly asymmetrical.

Figure 8-1: Average concentration profiles. Horizontal and vertical transition sections. $Re = 2.0 \cdot 10^3$ and $Re = 1.7 \cdot 10^3$, respectively.

Figure 8-2: Average concentration profiles. Horizontal and vertical transition sections. $Re = 3.4 \cdot 10^3$.

Figure 8-3: Average concentration profiles. Horizontal and vertical transition sections. $Re = 5.5 \cdot 10^3$.

Figure 8-4: Average concentration profiles. Horizontal and vertical transition sections. $Re = 1.7 \cdot 10^4$ and $Re = 1.6 \cdot 10^4$, respectively.

In the horizontal transition section, the amount of macro-mixing varies, depending on Re . At $Re = 1.7 \cdot 10^4$, the dispersion is significant. Referring back to the remarks on stratification in the previous section, and to the laser sheet experiments (Chapter 7.2), we suspect that at high Re (low relative puff flowrate) the puff material is likely to be held up in the recirculation zone at the bottom of the kiln cavity (region 5 in Figure 7-2). At intermediate Re , when deflection of the puff stream is less, more puff material by-passes the bottom recirculation zone, and the dispersion diminishes. At $Re = 5.5 \cdot 10^3$, the amount of backmixing is negligible, as indicated by a very strong drop in average concentration after 20 seconds. At lower Re , more of the puff reaches the top recirculation zone of the cavity. Consequently, we can again observe more dispersion. Profiles in the horizontal transition section at $Re = 5.5 \cdot 10^3$ and at $Re = 1.7 \cdot 10^4$ include values $\bar{C}/C_0 > 1$, which does not seem realistic. Given the inaccuracy, both from statistical inference (intervals in Figures 7-5 and 7-6) and from cross-stream variations, we suspect that these values are due to experimental error, and have no physical significance.

Several mechanisms may be responsible for the macro-mixing process: (1) axial turbulent motion, (2) radial spread in axial velocity, and (3) holdup of fluid in one or more recirculation zones.

(1) Axial turbulent motion can be accounted for with the dispersion model (Levenspiel, 1972). For large amounts of dispersion, the residence time distribution

becomes asymmetrical. This is best illustrated by considering the response to an impulse (δ) tracer input: the spreading tracer curve will change shape during the time that it passes the observation point. The average concentration measurements in Figures 8-1 to 8-4 therefore agree (qualitatively) with the dispersion model. However, large amounts of backmixing are necessary, for concentration profiles to become noticeably asymmetrical; according to Levenspiel: $D/UZ \approx 0.2$. In our experiments, estimating the turbulent diffusivity to be of order u_*R , and letting $Z = 10R$ in the vertical transition section:

$$\frac{D_T}{UZ} \approx 0.1 \frac{u_*}{U} \approx 0.01 \quad (8-2)$$

which suggests that the contribution of turbulent dispersion to macro-mixing is minimal. Therefore, while turbulent axial dispersion is likely to be present in our experiments, it is probably not the only relevant mixing mechanism.

(2) Turbulent motion suggests plug flow in the transition section: fluid at different radial positions moves with approximately the same average velocity. Radial mixing eliminates any residence time distribution that might otherwise be present due to a spread in average velocity. In laminar flow, fluid along different streamlines would have different velocities, and radial mixing would be minimal, resulting in a spread in residence time. However, laminar flow does not agree with qualitative experimental observations (presence of large scale cross-flow motion), and would not be expected at any but the lowest Reynolds number in our experiments.

(3) Recirculation zones have been observed in the cavity of the model, and we proposed that they are responsible for the residence time distribution at the first measurement location. In the transition section, recirculation zones are likely to be present in the dead end (representing the ram port of the EPA kiln), and downstream of the 90° bend. They would cause a spread in residence time, as observed experimentally. Because we suspect that recirculation zones may play an important role in the macro-mixing in the transition section, they will be incorporated in our linear eddy model (Chapter 9), and the effect will be assessed.

Presently, we will formulate a simple empirical model to describe the macro-mixing, based on classical reaction engineering modeling. The response of a stirred tank to a step change on the inlet is (Levenspiel, 1972):

$$\frac{C(t)}{C_0} = 1 - \exp\left(-\frac{Qt}{V}\right) \quad (8-3)$$

where Q is the volumetric flowrate, and V the tank volume. Regarding a pulse of duration t_d as a positive step, followed by a negative step with time delay t_d , it can be seen that the response of a stirred tank to a pulse is ($t > t_d$):

$$\frac{C(t)}{C_0} = \exp\left(-\frac{Q(t-t_d)}{V}\right) - \exp\left(-\frac{Qt}{V}\right) \quad (8-4)$$

while for $t < t_d$ eqn. (8-3) can be used. This set of equations, with a tank volume of 0.7 m³, fits the average concentration profiles in the vertical transition section quite well, especially at intermediate Reynolds number (see Figure 8-5). In this

Figure 8-5: Average concentration profiles in vertical transition section. Comparison between experimental data and stirred tank model.

graph, time has been non-dimensionalized with the residence time in the cold flow model (Tables 7-1, 7-2). Note that a correction was made for dead time (displacement of curves along the time axis by $\tau/2$). The model under-predicts the dispersion at the highest and lowest Reynolds numbers, probably because of additional mixing in the recirculation zones of the cavity. It should be noted that the volume used in eqns. (8-3) and (8-4) is strictly a fitting parameter, without physical significance, since the model is not an attempt at explaining the mixing process.

8.3 Local Mixing Characterization I. Spatial Correlation

In this and the following sections, we will evaluate local unmixedness. Presently, the different local mixing length scales are determined. Three types of information are available: spatial scalar correlation curves, scales of segregation, and one-dimensional scalar spectra. However, all these quantities are related, as discussed in Chapter 2. Therefore, we restrict our attention mostly to interpretation of the spectra. Scale of segregation is considered also, because it is available as a function of time¹.

Spectra for different Reynolds numbers in the vertical transition section are presented in Figure 8-6, and for the horizontal transition section in Figure 8-7. The wave number (x axis) is given both in units (pix^{-1}), and in (mm^{-1}). The relation

¹ Recall that spectra were obtained by averaging multiple spectra, representing different times in a setup (see Chapter 7.7).

Figure 8-6: Average one-dimensional scalar spectra. Vertical transition section, various Re .

between the two is determined by the resolution of the measurements: 0.84 mm/pix in the horizontal transition section, and 0.71 mm/pix in the vertical transition section (Chapter 7.5). The value of the spectrum (F) is given in units of pixels only; to determine F in mm, multiply by 0.84 or 0.71 in horizontal or vertical transition section, respectively.

Let us consider the spectra from the vertical transition section (Figure 8-6) first. We expect mixing to be fully developed here, so the spectra might look like the theoretical high Sc scalar spectrum of Figure 2-3: a constant value $F(k)$ for low wave number, followed by an inertial-convective range (slope of $-5/3$), and a viscous-convective range (slope of -1). It should be kept in mind, however, that the theoretical spectra are derived for homogeneous, high Re turbulence. In our system, Re is between 1700 and 17,000 and turbulence is definitely non-homogeneous, because of the geometry of the experimental facility. The integral wave number (marking the low wave number cut-off of the inertial-convective range) is independent of Reynolds number. However, Kolmogorov and Batchelor wave number increase at increasing Re . Kolmogorov scales between 2 and 10 mm were calculated¹ (Table 5-1), so $k_K (=2\pi/l_K)$ would be between 0.6 and 3 mm^{-1} . Based on the observation of Hill (1978), referred to in Chapter 2.6, we would expect the transition between the inertial-convective range and the viscous-

¹ The actual Kolmogorov scale is probably smaller than this; compare the discussion on page 101.

convective range to be between 0.03 and 0.15 mm^{-1} . From the theoretical Batchelor scale (between 3 and $13 \text{ }\mu\text{m}$), the viscous-convective range should extend to wave numbers well beyond 100 mm^{-1} .

Spectra in Figure 8-6 are approximately constant for $k < 0.01 \text{ mm}^{-1}$, suggesting an integral length scale of about 0.61 m . This corresponds quite well to the duct diameter of 0.46 m . For all but the highest Re , there is no clear inertial-convective range. Instead, we can detect a direct transition to the viscous-convective range. Most likely, the Reynolds number in these experiments is too low to have a fully developed inertial range of eddies. At $Re = 1.6 \times 10^4$, there seems to be an inertial-convective range ($0.02 \text{ mm}^{-1} < k < 0.09 \text{ mm}^{-1}$), followed by a fairly constant value for the spectrum. We suspect that this constant value may be caused by noise in the optical system: since the particle concentration was lowest in this setup, the signal to noise ratio would also be lowest. Because of this unlikely behavior of the high wave number part of the spectrum, we are not sure whether the observed slope of $-5/3$ at lower wave number is truly an indication of an inertial-convective range, or merely a coincidence. All spectra have a high end cutoff around 1.4 mm^{-1} (1 pix^{-1}). The reason why the high wave number end of the spectra is not observed is simply a matter of resolution of the measurements: any fluctuation on a scale, smaller than the size of a pixel, cannot be detected.

Comparing the spectra from the horizontal transition section (Figure 8-7) to those

Figure 8-7: Average one-dimensional scalar spectra. Horizontal transition section, various Re .

from the vertical transition section (Figure 8-6), we can detect three differences. (1) The integral wave number is slightly larger, and dependent on Re : $k \approx 0.01 \text{ mm}^{-1}$ at $Re = 2.0 \times 10^3$, but between 0.02 and 0.03 mm^{-1} for the higher Re experiments. (2) The high wave number cutoff is below the pixel wave number, and also dependent on Re : values range from 0.25 mm^{-1} ($Re = 1.7 \times 10^4$) to 0.8 mm^{-1} ($Re = 2.0 \times 10^3$). (3) Between the low and high wave number cutoffs, the decay of the spectrum is steeper than the (-1) slope of the viscous-convective range.

Observation (1) implies that the integral length scale is smaller in the horizontal than in the vertical transition section. Because the measurement point is only 10 cm downstream of the contraction, it is unlikely that the effect of the largest eddies of the transition section can be observed here. Probably, the integral scale is determined by the largest eddies of the kiln cavity, which are created by the main air jet.

Observations (2) and (3) both indicate that the scalar spectrum is developing in the horizontal transition section. An equilibrium between length scales has not yet been established, and fluctuations have not yet reached the smallest length scales. The high wave number cut-off is at lower wave number for higher Re . This cannot be explained from the shorter residence time, since (under the assumption of Reynolds similarity) all time scales are proportional. Two possible explanations are as follows: (a) There may be a departure from Reynolds number similarity. We

already observed qualitative differences between high and low Re experiments (Chapter 8.1). Likewise, there may be differences in turbulence structure, causing the ratio of eddy turnover times to main flow residence time to vary, depending on Re . (b) The mixing process may in part be determined by factors that are not related to Re , such as the puff flowrate. If a non-related mechanism controls the initial decrease in scalar mixing micro-scale, the development (as a function of time) is independent of Reynolds number, and higher Re flow will show a larger micro-scale at the same downstream distance, due to a shorter residence time.

By definition, the scale of segregation is equal to the value of the scalar spectrum at zero wave number (eqn. 2-34)¹. Physically, it can be seen as a representative average mixing length scale. In Figure 8-8, scales of segregation are presented as functions of time, for different Reynolds numbers, at both measurement locations. For all conditions, there is a fairly large discrepancy between the scale, calculated by integration over all values of the correlation curve (open symbols), and the scale that was calculated by integration of positive values $R(r)$ only (filled symbols). This indicates that the largest length scales are larger than the maximum separation distance in the measurements, which is in agreement with the observed integral scale from the spectra. The scale of segregation is larger in the horizontal than in the vertical transition section. Figure 8-8 shows one feature that could not

¹ Recall that all spectra presented here have been multiplied by $(\pi/R(0))$ (Chapter 6.3).

Figure 8-8: Scale of segregation as function of time in horizontal transition section (top) and vertical transition section (bottom).

be observed from the spectra: in the vertical transition section, the scale of segregation is larger at short than at longer times. After about 2τ , it reaches a steady-state value. This implies that the mixing scales at the front end of a puff are larger than those at later times. Possibly, if we had more accurate scalar spectra at different times in the vertical transition section (i.e. data from a larger number of runs), we could see a trend in the spectra at subsequent times. The earliest ones might look somewhat like the average spectra in the horizontal transition section. We therefore suspect that the transient nature of the puffs has some effect on the local mixing length scales.

8.4 Local Mixing Characterization II. Micro-mixing

After having determined which length scales play a role in the local mixing process, we will now look at mixing beyond the smallest mixing length scales. In a pure physical sense, micro-mixing is mixing at a molecular level. For our experiments, the Batchelor scale would form the cut-off between macro-mixing and micro-mixing. However, due to the resolution of our images, apparent micro-mixing takes place at a larger scale (i.e. the size of a pixel). This process might be called "optical diffusion"; like molecular diffusion, it creates blurring at interfaces, and causes intermediate local concentrations to form from combination of high and low concentrations.

Micro-mixing is characterized with the concentration fluctuations and the

concentration PDFs. Figures 8-9 and 8-10 show the concentration fluctuations, in three different forms: "absolute" fluctuations (c'/C_0), relative fluctuations ($c'/\bar{C}$), and intensity of segregation ($\mathfrak{S} = (c')^2/\bar{C}(1-\bar{C})$), all as functions of dimensionless time. The profiles of absolute fluctuations were obtained from the cross-stream pixel value fluctuations (Figures 7-5, 7-6), using eqn. 7-2, with average values for K . They are similar in appearance to the average concentration profiles: we can observe low fluctuations at short times, with an increase starting at $t/\tau \approx 0.5$, followed by a more gradual decay. The maximum in the fluctuation profiles generally precedes the maximum in the corresponding average concentration profiles. Since the duration of the increase in fluctuations is roughly equal to the puff duration (20 seconds), in dimensionless units (t/τ) the duration is longer at higher Re . Fluctuations are about five times higher in the horizontal than in the vertical transition section.

Profiles of relative fluctuations were obtained by dividing the concentration fluctuation profiles by the average concentration profiles. In the vertical transition section, profiles for all but the highest Reynolds number collapse at short times. Relative fluctuations are maximum at short times, and drop sharply. There are two reasons for the high initial fluctuations: (1) The first puff material that passes the measurement point has a shorter than average residence time. Therefore, it has had less time to mix than material, exiting later. (2) Axial gradients in average concentration (slope dC/dt in Figures 8-1 to 8-4) form a source of concentration

Figure 8-9: Concentration fluctuation profiles in horizontal transition section. From top to bottom: absolute fluctuations, relative fluctuations, and intensity of segregation.

Figure 8-10: Concentration fluctuation profiles in vertical transition section. From top to bottom: absolute fluctuations, relative fluctuations, and intensity of segregation.

fluctuations, as is apparent from eqns. (3-3, 3-5). Therefore, transients will promote concentration fluctuations. The minimum in the relative fluctuations coincides with the maximum in the average concentration. At longer times, as the average concentration decreases, the relative fluctuations increase gradually. Profiles in the horizontal transition section show the same general trend as in the vertical transition section. There is more scatter of data here, making it more difficult to interpret the profiles. The relative fluctuations differ much less in magnitude between horizontal and vertical transition section than the absolute fluctuations, indicating that the decrease in concentration fluctuations is in part due to a decrease in average concentration, by macro-mixing of the puff (as discussed in Chapter 8.2). This fact, and the fact that the relative concentration fluctuations are minimum when the average concentration is maximum, suggest that the transient nature of the puff has an important effect on the micro-mixing.

Profiles for the intensity of segregation show an overall decrease with time in the horizontal transition section. At all times, the intensity of segregation is significantly below unity, indicating substantial micro-mixing. This seems to contradict the observed scalar spectra in the horizontal transition section, which displayed a transient micro-scale (suggesting that the scale over which diffusion occurs has not yet been reached). A possible explanation for the simultaneous existence of micro-mixed fluid and a transient length scale is staged mixing. Very fast micro-mixing between the puff and a portion of the main air may occur in the cavity, followed by

much slower mixing between this diluted puff and the remaining air.

In the vertical transition section, profiles for intensity of segregation show an initial peak, followed by a slight local minimum, and then a constant value. The intensity of segregation is lower and features are generally less pronounced at higher Re . This can be attributed to the fact that the intensity of segregation is roughly proportional to the average concentration (at low concentrations), as discussed earlier in Chapter 2.8.

The fluctuation profiles leave one question unanswered: what is the maximum instantaneous concentration, and at what time in the puff does it occur ? This is an important question if we want to assess the occurrence of puffs. The best way to approach this issue is by inspection of the PDFs (Appendix D.3). The maximum concentration is simply given by the highest value in the concentration PDF that has a finite probability of occurring at any time. From the PDFs, we can determine the probability that a certain concentration is exceeded, by measuring the area to the right of that concentration. This was done for PDFs at $Re = 3.4 \times 10^3$ in both the horizontal and the vertical transition section. Results are shown in Figure 8-11.

It is informative to view Figure 8-11 in the context of the occurrence of puffs: if the same concentration limits were exceeded in the EPA kiln, would they explain the occurrence of puffs ? Answering this question requires two additional pieces of

Figure 8-11: Probability of exceeding concentration limits, at different times. Horizontal and vertical transition section. $Re = 3.4 \cdot 10^3$.

information: the fraction seeded flow (C_0) and the maximum concentration that can be destroyed in the kiln (C_{SR} , corresponding to $SR = 1$). At $Re = 3.4 \times 10^3$, $C_0 = 0.037$ (Table 7-2), which is actually a conservative estimate for a typical puff ($C_0 = 0.047$, Table 5-1). C_{SR} is determined from the stoichiometric coefficient ($\nu_o = 9$ for toluene, Chapter 2.8), and the oxygen mole fraction in the primary flame flue gas. For the latter, Wendt and Linak (1988) give a value of 0.09775. Thus, for $SR = 1$, $C_{SR} = 0.09775/9 = 0.0109$. Therefore, $C_{SR}/C_0 = 0.29$. In other words, whenever C/C_0 exceeds 0.29, the local oxygen concentration is too low to completely oxidize all the waste. Figure 8-11 shows that this relative concentrations has a considerable probability of occurring. Interestingly, the probability is higher in the vertical than in the horizontal transition section. This is due to the fact that the concentration PDFs are broader in the horizontal transition section. Therefore, both high and low concentrations have a higher probability of occurring here. This is illustrated by the fact that the probability of exceeding $C/C_0 = 0.80$ is negligible ($< 3\%$) in the vertical transition, but substantial (up to 20%) in the horizontal transition section.

The micro-mixing in the cold flow model experiments may not be representative of micro-mixing in the EPA kiln, because of the large difference in Schmidt number. In gas phase mixing, the viscous-diffusive range in the scalar spectrum is very small, because $l_B/l_K \sim Sc^{-1/2}$ (from eqn. 2-26). The high wave number cut-off of the scalar spectrum in the EPA kiln is expected to be at lower wave number than in

the cold flow model experiments (i.e. $k_{B,kiln} < 1/\text{pix}$). Consequently, micro-mixing will be larger, resulting in lower concentration fluctuations, and narrower PDFs than found in our experiments. This issue will be addressed further in the next chapter.

If cold flow model results are representative of EPA kiln mixing, then the above analysis suggests mixing between waste and ambient air in the kiln is insufficient to accomplish complete destruction of organics.

8.5 Summary and Significance

In this chapter, the experimental results were interpreted, and a connection was made between the cold flow model experiments and mixing in the EPA kiln.

Mixing in the cavity is a complicated process. Rapid mixing occurs between the transient stream and part of the main air stream, while the remainder of the main air stream by-passes the puff. Two available models (Okamoto and Enokida, 1982; Rathgeber and Becker, 1983) could explain the puff trajectory qualitatively, but not quantitatively. Prediction of mixing in the EPA kiln cavity is further hampered by the fact that no detailed information is available about the area over which waste is released from the kiln bottom.

For the transition section, we have been successful in characterizing the mixing process quantitatively. This makes it possible to develop and calibrate a model. If

we may assume cold flow model mixing to be representative of mixing in the EPA kiln (differences will be discussed in Chapter 11.3), experimentally determined PDFs yield information about stoichiometric ratios in the kiln. Based on this, we determined the likelihood of incomplete combustion due to unmixedness, in both the horizontal and the vertical transition section. We concluded that unmixedness is a likely explanation for the incomplete destruction of wastes in the EPA rotary kiln incinerator. In Chapter 11.2, an alternative analysis will be presented, based on average concentration and RMS fluctuations.

Results were interpreted as a combination of macro-mixing and local mixing. The extent of macro-mixing was too large to be explained from turbulent dispersion alone; we hypothesized that recirculation zones cause a spread in residence time. Locally, turbulent dispersion was important. Because the Reynolds numbers in the experiments were moderate ($1.7 \cdot 10^3 < Re < 1.7 \cdot 10^4$), we could not distinguish an inertial-convective range in the scalar spectra. However, a viscous-convective range was observed. The smallest scalar mixing length scales were determined by the resolution of the measurements. Micro-mixing was therefore governed by "optical diffusion", rather than molecular diffusion. We have not yet shown whether the resolution of the measurements is representative for low Sc mixing; this issue will be discussed further in Chapter 9.6. The transient nature of the mixing process turned out to be important for the micro-mixing process: concentration fluctuations were largest during the rise in average concentration at the beginning of a puff.

CHAPTER 9

UNSTEADY STATE LINEAR EDDY MODEL

9.1 Objectives

In this chapter, a linear eddy model is presented for interpretation and extrapolation of the experimental data. The model is intended to predict the mixing characteristics in the vertical transition section, based on experimental data from the horizontal transition section. The development had several objectives: (1) Linear eddy simulations with and without recirculation zone serve to indicate, whether the presence of recirculation zones is vital to the mixing process in the transition section. (2) The effect of spatial resolution (probe size) on the measurements is determined, as well as the effect of Schmidt number. This will quantitatively verify the claim of Becker *et al.* (1966), that low resolution measurements of high Schmidt number flow are equivalent to higher resolution measurements of low Schmidt number flow. Also, extrapolations to lower Schmidt number are essential for predicting EPA kiln mixing from cold flow model experiments. (3) Finally, the model is used to predict the occurrence of puffs in the EPA kiln under typical operating conditions, by analyzing the distribution of the unsatisfied oxygen demand as a passive scalar.

9.2 Modeling Considerations

For a general description of linear eddy modeling, the reader is referred to Chapter 3.4, and to the papers by Kerstein 1988, 1989, 1990, 1991a, b, 1992a, b). To allow time dependence, the present model is streamwise, i.e. gridpoints along the simulation line represent cells at subsequent downstream locations. As a consequence, the model does not allow cross-stream variations to be modeled directly. The cross-stream variation in the horizontal transition can be modeled indirectly, however, as will be explained in the next section. The concentration in each cell changes with time, due to three mechanisms: convection, molecular diffusion, and turbulent stirring. Unsteady behavior follows from the fact that the input signal (the concentration at the inlet of the simulation domain) is a function of time. The fluid dynamics of the simulation are assumed to be in steady state, i.e. average velocity and eddy frequency do not change. Our motivation for this is, that the transient stream makes up a very small part of the total flow rate (between 0.8 and 7.2%), and therefore its absence or presence has only a minor effect on the flow phenomena in the transition section.

The initial concentration of all cells in the simulation domain is zero. During convection events, the inlet concentration feeding into the first cell is a periodic signal, with period (d/U) ; the phase at $t=0$ is chosen at random. The way in which the input signal is constructed will be discussed in more detail in Chapter 9.3.

A recirculation zone is modeled explicitly. During convection events, the contents (concentration) of each cell is shifted to a neighboring downstream cell, corresponding to the average fluid motion. Of the convection events, $n\%$ are "normal", i.e. include all cells of the simulation domain, and $(100-n)\%$ by-pass the recirculation zone (Figure 9-1). Consider the recirculation zone consisting of the cells $(n_j + 1)$ through $(n_j + n_r)$. Then, in a by-passing convection event, cell (n_j) feeds directly into cell $(n_j + n_r + 1)$, while the contents of each of the cells $(n_j + 1)$ through $(n_j + n_r)$ remains unchanged. As a consequence, the average fluid velocity is lower in the recirculation zone than in the rest of the simulation domain. A disadvantage of the by-passing procedure is, that it creates discontinuities in the scalar field. Recirculation zone size, and the probability that convection events by-pass the recirculation zone ($P_{\text{by-pass}}$) are fitting parameters. At time intervals (L/U) , a random choice between inclusion or by-passing of the recirculation zone is made: if random number $r < P_{\text{by-pass}}$, convection events for the next period (L/U) by-pass the recirculation zone; if $r > P_{\text{by-pass}}$, they include it.

Molecular diffusion is implemented in finite difference form. The only unusual feature of a diffusion event is that the contents of cells (n_j) and $(n_j + n_r)$ get mixed, prior to updating the profile. The motivation for this is that the two cells occupy the same physical space (see Figure 9-1).

Turbulent stirring is implemented as triplet maps, with randomly selected location

Figure 9-1: Convection events in linear eddy model, showing algorithm for by-passing the recirculation zone.

and size. The relative frequency of eddies of different sizes has been derived from Kolmogorov scaling (Kerstein, 1989):

$$P(l) = \frac{5}{3L} \frac{1}{(L/l_{\min})^{5/3} - 1} \left(\frac{l}{L} \right)^{-8/3} \quad (9-1)$$

The smallest eddy size ($l_{\min}$) is 20 times the Kolmogorov size, based on the observation of Hill (1978), referred to in Chapter 2.6; for the largest eddy size, we chose the duct radius. The total triplet map frequency is constant throughout the model, independent of time or location. As shown by Kerstein (1991b):

$$\lambda = \frac{54}{5} \frac{D_T}{L^3} \frac{(L/l_{\min})^{5/3} - 1}{1 - (l_{\min}/L)^{4/3}} \quad (9-2)$$

Turbulent diffusivity is estimated by:

$$D_T \propto u(L)L = Re_L \nu \quad (9-3)$$

Re_L is assumed to be equal to Re_* (eqn. 4-8). The proportionality factor of order unity is neglected.

In stirring events, there is one shortcoming: eddies around point n_j (Figure 9-1) do not include $n_j + n_r$ and neighboring points, and vice versa. In reality, since the separation distance between these points is small, there would be interaction due to turbulent motion. This might be incorporated by selecting any two branches emanating from the junction for stirring events in the vicinity of the point n_j .

9.3 Input Signal

The input signal for the linear eddy simulations needs to reflect two experimentally observed facts. First of all, in the horizontal transition section, there is considerable cross-stream (vertical) segregation, i.e. the average concentration is dependent on location. Secondly, the concentration PDF of the input signal should match the PDFs of the experiments. Both the model and the available experimental data restrict us to a simplified representation.

Because of its one-dimensional nature, the model does not allow cross-stream variations¹. Thus, the only option for incorporating a mixing scale in the input signal is by streamwise variation: making the input signal periodic, with a length, corresponding to the dominant scale, in this case the kiln diameter. This is acceptable in our particular application, because the cross-stream variation is temporary (in the Lagrangian sense), and cross-stream variation of average concentration has largely disappeared after one large eddy turnover time. The same argument could not have been used if cross-stream variations had been persistent, due to a separating force. For example, stratification in full scale kilns is probably induced by gravity, and therefore requires an alternative modeling approach. Suggestions will be made in Chapter 11.9.

¹ The alternative of modeling a cross-stream line, as described in Chapter 4, does not allow unsteady state mixing, which is deemed a more severe restriction in the present application.

In principle, experimentally determined PDFs from the horizontal transition section could be used for the input signal (see Chapter 11.8). However, because of the inaccuracy of the measurements in the horizontal transition section, this is not deemed the best choice at present. Instead, we use the experimentally determined average concentration profiles and relative fluctuation profiles, and an assumed (simplified) PDF shape. From inspection of the experimental PDFs in the horizontal transition section (Figures 7-9 D-9 to D-12) a Gaussian shape is not an adequate description. A better shape would consist of a sharp peak at zero concentration, and a long tail. To develop such a PDF, however, we would need the skewness (in addition to the average and the standard deviation). Implementation would also require an additional length scale, similar to implementation of the experimental PDFs (Chapter 11.8).

We propose an alternative PDF for the input signal, that maintains the peak at zero concentration, but requires only average and standard deviation, and a single length scale. The PDF essentially consists of two delta functions: one at zero concentration, and one at concentration C_1 (Figure 9-2). Simplifying the PDF to two delta functions may not seem realistic. However, the effect on the simulation results is probably minimal. We make this assertion, based on a connection between the spatial variation and the PDFs: since different levels of puff intensity (other than clean air) are close together spatially, they will be mixed by small eddies, with short turnover times. On the other hand, the average separation distance between puff

and clean air is large (the order of the duct diameter); thus, the large eddies (with long turnover times) are responsible for the initial mixing between puff and clean air. This gives sufficient time for the small eddies to substantially reduce the concentration variation inside the puff, making the concentration PDF approach the assumed shape. The value of C_1 and the relative size of the two peaks (ϕ_0 and ϕ_1) are determined from the average and standard deviation, such that:

$$\phi_1 C_1 = \bar{C} \quad \phi_1 (C_1 - \bar{C})^2 + \phi_0 (\bar{C})^2 = (c')^2 \quad (9-4)$$

For $\bar{C}$ and c' , the renormalized average concentration profiles ($\bar{C}/C_0$; Chapter 8.2) and relative fluctuation profiles ($c'/\bar{C}$ Chapter 8.4) from the horizontal transition section are used. Thus, effectively, c' is renormalized also. Because both quantities are functions of time, C_1 and ϕ_1 are time-dependent as well.

The model input consists of a periodic signal (see Figure 9-3), with period (d/U), and randomly selected phase, different for each realization. The period reflects the dominant length scale, which is the duct diameter, from experimental observation. The random phase ensures that the ensemble average input signal is a smooth (transient) function, and not a periodic function. The signal alternates between 0 and C_1 , with relative durations ϕ_0 and ϕ_1 , matching the PDF of Figure 9-2. As mentioned previously, C_1 and ϕ_1 are time-dependent. Each peak in the input signal therefore has a different height and width.

Figure 9-2: Concentration PDFs in horizontal transition section. Schematic of measured PDF and input signal for linear eddy model.

Figure 9-3: Input signal for linear eddy model.

It is important to note that the peaks in the input signal represent the spatial structure within a single transient, and should not be interpreted as short time fluctuations in the transient stream (i.e. all the peaks of a linear eddy simulation, Figure 9-3, lie within a single peak of the evaporation model of Wendt and Linak (1988), Figure 5-1 or 9-14).

A flow diagram for the subroutine that creates the input signal is presented in Figure 9-4. First of all, for every cycle, the time of the concentration burst is determined. These times correspond to t_a , t_b , and t_c in Figure 9-3. At a given time, C_1 and ϕ_1 (eqn. 9-5) are determined, by interpolation of experimental data. The times at which a burst starts (t_{up}) and ends (t_{down}) are calculated from:

$$t_{up} = t - \frac{\phi_1 d}{2 U} \quad t_{down} = t + \frac{\phi_1 d}{2 U} \quad (9-5)$$

Values for t_{up} (with corresponding C_1) and t_{down} are stored, for use in the simulation subroutine.

9.4 Implementation

The actual simulation subroutine is an extension of the generic linear eddy simulation routine (Figure 3-3). Three additional processes (time-lines) are included in the subroutine: one for convection, and two that create step changes in the inlet concentration, based on the inlet signal subroutine discussed in the previous

Figure 9-4: Flowsheet for subroutine that creates input signal in linear eddy simulation. This subroutine is called once for every realization, prior to the call to the simulation subroutine (Figure 3-3).

section¹. Input for the model consists of values for C_1/C_0 and ϕ_1 at different times, calculated prior from experimental values $\bar{C}/C_0$ and $c'/\bar{C}$, using eqn. (9-4). The main program calculates average concentration, standard deviation, and concentration PDFs as functions of time from the instantaneous concentrations in multiple realizations, at a single location. For spatial correlation calculations, every realization and output time gives one pair of points for each separation distance, centered around the output point. The maximum separation distance between points is 1.5 duct diameters. In order to accommodate the correlation measurements, and to allow turbulent interaction with fluid further downstream, the simulation domain extends one duct diameter beyond the output location. The scale of segregation is calculated for each time separately. Like in the cold flow model experiments, spectra are calculated by Fourier transformation of the spatial correlation curves, and then averaged (compare Chapters 6.3, 7.6). For the purpose of program output, correlation curves are averaged in a similar fashion. Correlation curves and spectra are not included in the average when $t/\tau < 0.7$ or when $c'/C_0 < 0.01$, in order to minimize the effect of the transient. Anticipating the simulation results, we want to remark here that the calculated spectra are unsatisfactory. This will be discussed in more detail in Chapter 9.7.

The model was coded in Fortran. A program listing is given in Appendix C.2. It was

¹ Note that the times for t_{up} and t_{down} are not spaced equally. Therefore, these times are read from an array, rather than incremented by Δt at every step.

compiled/vectorized and run on a Convex mini-super computer. A typical simulation (500 realizations) required circa 10 hours of CPU time.

We validated the model, by determining the dispersion of an impulse (δ -function) input, due to molecular diffusion, in the absence of a recirculation zone. Stirring events were disabled in the program. Then, we enabled the stirring events and disabled molecular diffusion. From multiple realizations, we determined the average dispersion of an impulse (δ) input, due to turbulent stirring. In both cases, the standard deviation in residence time of the output signal agreed with the theoretical value from the axial dispersion model (Levenspiel, 1972). We also verified the occurrence of eddies in the simulation model: a PDF for eddy size distribution followed eqn. (9-1), while eddies were indeed evenly distributed throughout the simulation domain.

The model needs to reflect the fact that we do not have full resolution in our experiments. Therefore, the instantaneous output concentration for a given realization and time is not the concentration of a single grid point. Instead, we determine the average over a number of grid points, whose total length corresponds to the probe size. While the simulation results (like the experimental results) are expected to be dependent on probe size, they should be independent of the grid size. The required grid size was determined by comparing results with different numbers of grid points. We found 200,000 elements for the length of the

domain (5 diameters, plus recirculation zone and area downstream of output point) to be sufficient for all high Sc simulations. In predictions at low Sc , the number of grid points could be decreased, reflecting the larger length scales in the mixing process.

As mentioned earlier, the size of the recirculation zone and the relative flow rate are fitting parameters in the model. However, preliminary simulations indicated that the model results are fairly insensitive to the value of either of these parameters.

9.5 Simulation of Experiments

Parameters and model numerics are summarized in Table 9-1. Also included are the corresponding variable names in the Fortran code. Inlet conditions followed the experimental conditions, as outlined earlier. The input signal for the model, at different Reynolds numbers, is given in Appendix C.2.

Model results consist of predictions for average concentration, fluctuations, PDFs, and scale of segregation, all as functions of time. In addition, time-average spectra and spatial correlation curves are predicted. Average concentration and fluctuation profiles are compared to experimental data in Figures 9-5 to 9-8, for different Re . Profiles at the inlet of the simulation domain have been included also. Experimental points here are renormalized values (for the average concentration: open symbols in Figures 8-1 to 8-4). Concentration PDFs will be presented in connection with the

discussion of resolution and Schmidt number (Chapter 9.6). Model predictions for spatial correlation will be discussed separately in Chapter 9.7. At $Re = 3.4 \cdot 10^3$ and $Re = 1.7 \cdot 10^4$, simulations were repeated in the absence of a recirculation zone. The results are included in Figures 9-6 and 9-8.

Table 9-1: Numerics and parameters in linear eddy simulations.

variable	var. name	value
# grid points	nn	200,000
# realizations	nsim	500
Z/d	zout	5.0
d_{probe}/d	dp	0.0016
L/d	ql	0.5
l_{min}/l_K	qh	20
D_T/ν	qf*rel	Re_*
U_R/U	1-pbp	0.4 (1.0)
Z_R/d	zrc	2.0 (0.0)
Sc	sc	500,000

Figure 9-5: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 2.0 \cdot 10^3$ ($1.7 \cdot 10^3$ for experiments in vertical transition section).

Figure 9-6: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 3.4 \times 10^3$.

Figure 9-7: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 5.5 \cdot 10^3$.

Figure 9-8: Average concentration profiles and concentration fluctuation profiles. Comparison between experiments and linear eddy model. $Re = 1.7 \cdot 10^4$ ($1.6 \cdot 10^4$ for experiments in vertical transition section).

Model input profiles of average concentration and fluctuations match the experimental points in the horizontal transition section very well. This reflects the fit to the experimental data for the constructed input signal. The oscillations in the input signal (most apparent in the relative fluctuation profiles) are probably due to discretizing of time in the model.

In general, the model output fits the shape of the experimental profiles from the vertical transition section both qualitatively and quantitatively. There are three discrepancies between the experiments and the model predictions, however. (1) For all but the highest Re , the model predicts a 50% larger time lag than is observed experimentally. This indicates that the velocity of the bulk of the fluid is considerably larger than what would be expected under plug flow conditions, suggesting the presence in the transition section of several regions with different flow characteristics (in addition to the recirculation zone at the end of the horizontal transition section). These regions might include a recirculation zone downstream of the 90° bend, and boundary layers or recirculation zones along the walls of the transition section. (2) The experimentally determined relative fluctuations ($c'/\bar{C}$) gradually increase at long times, whereas the linear eddy simulations predict constant relative fluctuations. We suspect that the experiments may not be accurate here. It should be noted that the relative fluctuations are obtained from division of fluctuation profiles and average concentration profiles; since both approach zero at long times, a small systematic error may cause the quotient to

deviate substantially from the true value. In light of the overall motivation for our research (the prediction of puffs) the exact structure at long times is of limited interest, because the concentrations are much lower than at shorter times. Therefore, the occurrence of puffs is not associated with this long time behavior.

(3) At $Re = 5.5 \cdot 10^3$ and $Re = 1.7 \cdot 10^4$, the model over-predicts the maximum average concentration. This can be attributed to the inaccuracy of the input signal. The experimentally observed average concentration ($\bar{C}/C_0$) exceeds unity, which we suspect is not the true value (Chapter 8.2). If the maximum inlet concentration were lower, the model predictions for the average concentration in the vertical transition section would also be lower.

Comparison between the simulations with and without recirculation zone show a marked difference in average concentration profile at $Re = 3.4 \cdot 10^3$. Without recirculation zone, the output concentration is very similar to the input profile, displaced over a time $t = \tau/2$. This indicates that turbulent motion does not cause significant macro-mixing, supporting the assertion in Chapter 8.2. With recirculation zone, the model predicts a substantial change in the average concentration profile at low Re (Figure 9-5), and the predicted profile matches the experimental observations very closely (disregarding the lag time, mentioned in the previous paragraph). At $Re = 1.7 \cdot 10^4$ (Figure 9-8), the effect of the recirculation zone is smaller, because of the larger Strouhal number: the transient time is large, compared to the characteristic time of the recirculation zone. The same Strouhal

number effect can be observed in the empirical stirred tank model (Figure 8-5), where profiles at high Re look more like the 20 second pulse input than curves at lower Re.

The recirculation zone has only a minor effect on the concentration fluctuations. This indicates that the presence of a recirculation zone affects the macro-mixing, but not the micro-mixing. The simulation without recirculation zone predicts slightly lower fluctuations at $Re = 3.4 \times 10^3$, but the same or higher fluctuations at $Re = 1.7 \times 10^4$, at short times. We do not know whether this qualitative difference is a non-ideality or a trend.

9.6 The Effects of Schmidt Number and Resolution

The linear eddy simulation at $Re = 3.4 \times 10^3$ was repeated with lower Schmidt number ($Sc = 1.9$, representing molecular diffusivity of toluene in the EPA kiln). The number of realizations remained constant (500); however, full resolution was achieved with 10,000 gridpoints. The results are compared to the earlier high Sc simulation in Figure 9.9. It can be seen that the average concentration profile is not affected by a change in Schmidt number. The reason is that this is controlled by macro-mixing, which is identical in both cases.

The change in Schmidt number does affect the micro-mixing, as is evident from the difference in profiles for concentration fluctuations. The RMS fluctuations from the

Figure 9-9: The effect of Schmidt number and resolution on concentration profiles. Linear eddy simulations, $Re = 3.4 \cdot 10^3$.

low Sc simulation are circa 20% lower at all times. This implies that the molecular diffusion in the low Sc simulations is higher than the optical diffusion of the experiments, simulated in the linear eddy model. The fluctuations in the high Sc simulation can be suppressed by increasing the probe size (i.e. the number of gridpoints over which the instantaneous concentration is averaged). When the probe size is increased from 0.71 mm to 9.2 mm, fluctuations in a high Sc simulation match those for $Sc = 1.9$ closely (Figure 9-9). This suggests that for the low Sc simulation, the Batchelor scale is around 9 mm. We will discuss this further in Chapter 9.7.

The decrease in concentration fluctuations for lower Sc implies that the concentration PDFs should be narrower. This can indeed be observed. In Figures 9-10 and 9-11, the concentration PDFs at different times are presented, for high Sc flow with 0.71 mm probe and for $Sc = 1.9$, respectively. While the maximum in the PDFs is generally the same (identical average concentration), high Sc simulations have a broader range of possible values, most noticeable at $t/\tau = 1.0$. PDFs agree (at least qualitatively) with those determined from cold flow model experiments (Figure D-14).

It is important to note that a more than tenfold increase in probe size is required to accomplish a 20% drop in RMS fluctuations. This reflects the (-1) decay in the viscous-convective range of the scalar spectrum (Figure 2-3): the concentration

Figure 9-10: Concentration PDFs from linear eddy simulation. $Re = 3.4 \cdot 10^3$; $Sc = 5.0 \cdot 10^5$; probe size = 0.71 mm.

Figure 9-11: Concentration PDFs from linear eddy simulation. $Re = 3.4 \cdot 10^3$; $Sc = 1.9$; full spatial resolution.

fluctuations are contained primarily in the low wave numbers (large eddies). Therefore, they are fairly insensitive to the high wave number cut-off of the spectrum. This is fortunate, because it makes the fluctuation profiles fairly insensitive to the exact probe size. While a probe size of 9.2 mm is required to closely match the concentration fluctuations of low Sc flow in a high Sc experiment, a 0.71 mm probe is adequate for many applications, since the error is not larger than the accuracy of the measurements.

Our model predictions at first seem inconsistent with findings of Dowling and Dimotakis (1990), who compared experimental centerline concentration PDFs in high a low Sc turbulent jets. Essentially, no Sc dependence was observed. However, in the same article, the authors point out that this conclusion is valid for the centerline only, and that RMS concentration fluctuations may depend on Re and/or Sc near the edge of the jet. Therefore, Sc dependence in a different configuration does not contradict their results. Miller and Dimotakis (1991) studied turbulent mixing in a water jet ($3000 < Re < 24,000$; $Sc \sim 10^3$). They used scaling arguments to analyze the effect of spatial resolution on scalar spectra, and concluded that their "measurements of $c'/\bar{C}$ are not significantly affected by resolution difficulties". The reason is, that the fluctuations are contained primarily in the largest eddies, which have the longest turnover times (compare the discussion in Chapter 9.3). As our simulations of experiments are at much higher Sc , a slight increase in RMS fluctuations with increasing resolution is to be expected.

9.7 Spatial Correlation

Spectra from simulations (both at low and high Schmidt number) showed considerable scatter. One reason is that the spatial correlation function does not drop off to zero for large separation distances (Figure 9-12). This causes a discontinuity at the maximum separation distance, resulting in spikes in the spectrum. The largest distance considered for correlation functions and spectral calculations in the simulations was 1.5 times the duct diameter. Correlation between points at this and larger separation distances is probably a consequence of the transient nature of the simulated experiments.

One way to eliminate the discontinuity is by "data windowing". Prior to the Fourier transform, the correlation function is multiplied by a Hanning taper, given by (Koopmans, 1974):

$$W(r) = \frac{1 + \cos(\pi r/r_{\max})}{2} \quad (9-6)$$

The tapered function (see Figure 9-12) is then Fourier transformed. In Figure 9-13, spectra, obtained from correlation functions with and without tapering are compared. Like in the spectra from cold flow model experiments, interruption of the curves indicates negative values for the spectrum. It can be seen that the high wave number end of the spectrum is modified substantially by the tapering procedure. There is substantially less scatter, and the highest wave number that has a positive value is lower. Still, the spectrum from the tapered correlation

Figure 9-12: Spatial correlation curve from linear eddy simulation, Hanning taper function, and tapered correlation function. $Re = 3.4 \cdot 10^3$, $Sc = 1.9$.

Figure 9-13: Scalar spectrum from linear eddy simulation. Fourier transform of the auto-correlation function (top) and of the tapered auto-correlation function (bottom). $Re = 3.4 \cdot 10^3$, $Sc = 1.9$.

function does not display a viscous-convective range, as would be expected. The Batchelor wave number is ambiguous: it may be at 0.1 mm^{-1} , or at 0.2 mm^{-1} .

High Sc simulations show similar trends: the spectrum can be improved by tapering of the correlation function, but the outcome is not quite satisfactory. We do not know whether the poor results are due to insufficient data, or if there is some more fundamental problem.

A final comment concerns the scale of segregation. This quantity was determined as a function of time in the linear eddy simulations. However, because the value of the correlation function is larger than zero at the maximum separation distance, the true scale of segregation is larger than what was determined.

9.8 Simulation of Mixing in a Rotary Kiln

In the cold flow model experiments, the transient stream of seeded flow (puff) was a 20 second pulse. The flowrate remained constant for the duration of a puff. This is not the most accurate representation of the transient evaporation process in the EPA kiln. The evaporation model of Wendt and Linak (1988) predicts a virtually instantaneous rise in waste concentration, followed by a sharp decay (see Figure 9-14, which is identical to Figure 5-2). Also, both measurements and evaporation model predictions show multiple peaks. The maximum intensity (highest peak) occurs during the middle of a puff.

Figure 9-14: Measured and predicted toluene puff shapes. (a) Measured puff shape, $MASS = 100g$, $T_M = 1124 K$, $RPM = 0.5$. (b) Predicted puff shape for case (a). (c) Predicted "base case" puff shape, $MASS = 125 g$, $T_K = 1325 K$, $RPM = 1.25$. From Wendt and Linak (1988).

In this section, a linear eddy simulation is used to predict the transient mixing of a single peak in a more realistic puff. The same transient model is employed that was presented for modeling of the cold flow experiments. As passive scalar, we use unsatisfied oxygen demand (UOD), defined in eqn. (2-49), rather than concentration. The Schmidt number is taken to be the same as that for toluene.

The input signal for the linear eddy simulations is based on a combination of results from Wendt and Linak, and results presented earlier in this dissertation. The average UOD is taken from the maximum peak in the base case puff shape of Wendt and Linak (Figure 9-14c). The relative RMS fluctuations are estimated, based on cold flow model experiments in the horizontal transition section (Figure 8-9):

$$\text{UOD}' / \overline{\text{UOD}} = 1.0 \quad (9-7)$$

Note that higher relative fluctuations occur primarily after most of the puff has passed, and have therefore not be included in this estimate. If the waste concentration were to be zero, the UOD would be negative. However, because the peak that we model is preceded by several other peaks, zero waste concentration seems unlikely. We therefore assume a minimum value $\text{UOD} = 0$ (both for the initial condition and for the low value in the inlet signal), corresponding to a finite waste concentration. Then, by combining eqns. (9-4 and 9-7):

$$\text{UOD}_1(t) = 2\text{UOD}_{\text{base case}}(t) \quad \phi_1 = 0.5 \quad (9-8)$$

A simulation was performed with $\tau v/d^2 = 2.855 \times 10^{-3}$ ($\tau = 3.8$ sec.), $\text{Re} = 3.2 \times 10^3$, and $\text{Sc} = 1.9$. The simulation domain included 10,000 gridpoints. The input signal is listed in Table 9-2. All other parameters were the same as for cold flow model experiments (Table 9-1). Resulting average UOD and UOD fluctuations are presented graphically in Figure 9-15.

Table 9-2: Input signal for linear eddy simulation of UOD mixing in EPA rotary kiln incinerator.

t/τ	UOD_1	ϕ_1
0.	0.614	0.5
0.1316	0.614	0.5
1.842	0.142	0.5
3.421	0.070	0.5
6.842	0.	0.5

Results are qualitatively similar to the cold flow model experiments and corresponding linear eddy simulations (Figures 9-5 to 9-8). The present simulation suggests a 25% decrease in maximum average UOD (from 0.32 to 0.24), and a very large decrease in RMS fluctuations (from 0.3 to 0.09, maximum). Like in the cold flow model experiments, the relative fluctuations are maximum at the beginning of the peak, which may be attributed to the very large transient.

Figure 9-15: Linear eddy simulation of unsatisfied oxygen demand in EPA rotary kiln incinerator. Input follows the evaporation model of Wendt and Linak (1988).

From the simulation of mixing in the EPA rotary kiln incinerator, we conclude that turbulent mixing in the transition section is very effective in reducing local unmixedness. Macro-mixing causes a slight reduction in the maximum UOD. Based on comparison of simulations with and without recirculation zone (Figure 9-6), we suspect that this macro-mixing is largely due to recirculation, and therefore unique to the EPA kiln.

9.9 Conclusions

In this chapter, a linear eddy model was formulated for interpretation of the cold flow model experiments. Input of the model consisted of experimental data in the horizontal transition section. Model output was compared to experimental data in the vertical transition section. If a recirculation zone was included in the model, agreement between experiments and model predictions for average concentration, RMS fluctuations and PDFs was very good. Without recirculation zone, the macro-mixing was under-predicted, most noticeably at low Reynolds number.

The model was used to predict Schmidt number dependence of micro-mixing. Simulations indicated that the RMS fluctuations in gas mixing would be circa 20% lower than the high Sc cold flow model experiments, at $Re = 3.4 \times 10^3$. It was suggested that lower resolution measurements ($d_{probe} = 9.2 \text{ mm}$) mimic low Sc mixing more accurately. An attempt at relating this probe size to the Batchelor scale was not quite successful: information on spatial correlation was difficult to

extract from the model, in part because of the transient nature of the simulations.

We then simulated (part of) a typical puff in the EPA rotary kiln incinerator, using unsatisfied oxygen demand as a passive scalar. The model predicted a substantial decrease in RMS fluctuations over the length of the transition section. The average UOD was abated by 25%. This macro-mixing is mostly due to the recirculation zone, and may therefore not be present in other kilns.

CHAPTER 10

CONCLUSIONS AND RECOMMENDATIONS - GENERAL

10.1 Summary of Experimental Results

We have analyzed the mixing in a cold flow model of EPA's rotary kiln incinerator simulator by means of flow visualization and digital image analysis. From multiple runs, we determined pixel value histograms, spatial correlation functions, and (ensemble and cross-stream) average pixel values and standard deviations. We used the time-integral of the cross-stream average pixel value to calibrate the experimental technique. In the vertical transition section, calibration results gave good correlation for all but the lowest flow rate; in the horizontal transition section, correlation was poor, due to the fact that experimental data included only half of the cross-section, and there was substantial cross-stream variation in the local ensemble average concentration. We used cross-stream average pixel value, cross-stream standard deviation and correlation curves to calculate the average concentration, concentration fluctuations, intensity of segregation and scale of segregation, all as functions of time. In addition, we determined time-average scalar spectra from the correlation functions.

Experiments were completed at two downstream locations, for four different main air flow rates, giving values for Re between 1700 and 17,000. The flow rate and duration of the puff flow were kept constant. In the horizontal transition section, we

observed cross-stream variation, with the location of the highest ensemble average pixel value dependent on Re . Cross-stream variations had largely disappeared at the second measurement point, in the vertical transition section.

In the horizontal transition section, we observed a transient micro-scale in the scalar spectra, maximum at the highest Reynolds number (Figure 8-7). This suggests that the mixing process is in a developing stage, and the smallest length scales are too large for molecular mixing to have occurred. This would imply complete unmixedness of the two streams: an intensity of segregation of unity, and a concentration PDF, consisting of two delta-functions. The observed mixture is quite different, however, with intensity of segregation below 0.03 under all conditions (Figure 8-9), and a considerable spread in the PDFs (Figures 7-9; D-17 to D-24). To explain this, we hypothesized a two-step mixing mechanism in the cavity: fast, intense mixing between the puff and part of the main air, followed by much slower mixing between this diluted puff and the remainder of the main air.

In the vertical transition section, we observed a spread in average concentration (macro-mixing). Most scalar spectra displayed a viscous-convective range (Figure 8-6), while the concentration fluctuations were substantially lower than in the horizontal transition section (Figure 8-10), indicating improved micro-mixing.

10.2 Mixing Studies by Digital Image Analysis

The experimental work presented here resembles the work of Gullet *et al.* (1993): both study scalar mixing in a cold flow model, using TiO_2 particles to mark one of the incoming flows. The particles scatter laser light, which is recorded on video. Video images are then digitized and analyzed on computer, assuming the light intensity to be proportional to the instantaneous local concentration of seeded flow. Our measurements differed from the work of Gullet *et al.* in two ways. We used a laser line, whereas the other authors diffracted the laser light into a sheet. Also, in our study, the mixing was not a steady-state process; time was an independent parameter in the analysis.

The use of a laser line has several consequences. The main advantage is, that the light intensity is independent of location. When using a laser sheet, the light intensity may be higher in the center than near the edges. Unless a convergent lens or mirror is used to make the sheet parallel, the light intensity is lower, further away from the source. A second advantage of a laser line, especially in large scale experiments, is that the light intensity is much higher. Therefore, lower seeding concentrations and less light-sensitive optics are needed than for a laser sheet. There are disadvantages to the use of a laser line as well. First of all, two-point measurements (such as the spatial correlation function) can be performed in one direction only. Gullet *et al.* calculated both axial and radial scales of segregation; with our laser line analysis, that would not be possible. Another disadvantage is

that a single video frame, obtained from a laser line, has fewer measurement points than one from a sheet. Therefore, more video frames are needed, in order to obtain a sufficiently large number of measurements to calculate statistical quantities. Finally, the information from a laser line is more difficult to interpret qualitatively; for observing distinct features in a flow field, laser sheet visualization is superior.

The unsteady nature of our mixing process makes the calibration procedure somewhat more involved (Chapters 6.4 and 7.4). It also requires additional "book-keeping" in the data analysis, in order to combine the images from corresponding times for calculating statistics. However, these are not fundamental differences between characterizing a steady or an unsteady mixing process. More importantly, in an unsteady process, macro-mixing is important. In non-reacting, steady-state mixing, it is irrelevant, and cannot be determined.

Becker *et al.* (1966) asserted that low resolution measurements of high Sc mixing can be interpreted as fully resolved low Sc mixing. Their reasoning was, that the high wave number cut-off in the scalar spectrum of high Sc mixing, determined by the probe size, is about the same as the Corrsin or Batchelor wave number in low Sc scalar spectra. Linear eddy simulations suggested that the argument of Becker *et al.* can be quantitative, when the correct probe size is chosen (Chapter 9.6). There are some complications, however. First of all, the scalar spectrum is not

known a priori. It is therefore impossible to choose a probe size for the experiments, before the data have been analyzed and extrapolated to lower Sc . Secondly, the scalar mixing micro-scales depend on Re , as well as Sc (eqn. 2-26). Therefore, in an analysis of the effect of Re on mixing, it would be necessary to choose different probe sizes for experiments at different Re . In practice, the exact choice of probe size is not very critical, because the largest scalar fluctuations are associated with low wave numbers. From linear eddy simulations, we concluded that the scalar fluctuations decreased by only 20% when the probe size was increased more than tenfold. The analogy is therefore adequate for most practical applications.

The probe size analogy would clearly break down if the average concentration profiles were to depend on Sc . Linear eddy simulations indicated that the average concentration is not affected by the resolution or Schmidt number for gas phase mixing (Chapter 9.6). The reason is that macro-mixing is governed by the largest scales of the flow. However, when heat or mass transfer between phases involves molecular transport at the interface, the average concentration profile does depend on Sc or Pr (see Figure 4-4 and discussion in Chapter 4.5). Therefore, simulation of low Sc mixing with a high Sc experiment and finite probe size would be inadequate in such a case.

10.3 Reynolds Number Similarity

In a fully turbulent flow, the Reynolds stresses are much greater than the mean viscous stresses over most of the flow field. The mean motion and the motion of the energy containing components of the turbulence in this region are determined by the boundary conditions of the flow alone; viscosity does not affect the main structure of the flow. This implies that the main flow properties are independent of Reynolds number. Therefore, while geometrically similar flows are expected to be dynamically and structurally similar if their Reynolds numbers are the same, their structures are also very nearly similar for all Reynolds numbers which are large enough to allow turbulent flow. This phenomena is known as Reynolds number similarity.

The question arises, whether Reynolds number similarity applies to our experiments. We have presented all experimental data as functions of Reynolds number. It is important to realize that a change in Re has several consequences, some of which are unique to the way we conducted our experiments. (1) The turbulent diffusivity is proportional to the turbulent Reynolds number (eqn. 9-3), which in turn is roughly proportional to the main flow Reynolds number (eqn. 4-8). (2) The mean residence time is inversely proportional to the volumetric flowrate, and therefore in our experiments inversely proportional to Re . (3) With a constant large eddy size, the Kolmogorov and Batchelor scales decrease at increasing Re (eqn. 2-26). (4) Because the puff flowrate was kept constant in the experiments,

the puff concentration (C_0) is inversely proportional to Re . (5) The puff duration is constant, while the residence time is inversely proportional to Re , leading to a proportionality between Reynolds number and Strouhal number.

The first two effects cancel, resulting in equal large scale motion at different Re (when time is normalized with the residence time). This in effect constitutes the Reynolds number similarity. The micro-mixing is determined by the turbulent length scales. One may be inclined to think that the mixing to smaller scales at higher Re causes a more rapid decrease in concentration fluctuations. However, it is the large scales that have the largest eddy turnover times, and therefore affect the rate of micro-mixing most. Consequently, Reynolds number similarity holds approximately for the level of concentration fluctuations as well. The scalar spectra should differ, however: we expect the transition between the inertial-convective range and the viscous-convective range to be at higher wave number for higher Re . Indeed, the only spectrum in which an inertial-convective range can be observed is at the highest Re (Figure 8-6). The high wave number cut-off of the spectra is determined by the probe size. If we had full resolution in our measurements, this, too, would have been Re dependent.

The difference in puff concentration between high and low Re flows has been eliminated from the results, by normalizing the results with C_0 . Only the intensity of segregation is affected by the average concentration, as pointed out earlier

(Chapter 2.8). However, the difference in relative flowrates of main air and puff has an important effect on the flow structure in the cavity (Chapter 8.1). The flow structure is qualitatively different, leading to a break-down in the Reynolds number similarity. The observed Reynolds number dependence of the cross-stream variations in the horizontal transition section is therefore really a dependence on relative flowrates of the two streams. Even though this assertion has not been proven in our experiments, Rathgeber and Becker (1983) arrived at the same conclusion, in a study that included variation of relative flowrates and Reynolds number separately.

The difference in Strouhal number leads to different macro-mixing at long times only, since at short times (before the end of a puff has effectively reached the measurement point) the puff appears as a step change in inlet concentration, independent of Strouhal number. This can be seen most clearly from the average concentration profiles and concentration fluctuation profiles in the vertical transition section (Figures 8-5, 8-10). Profiles collapse at short times (with the exception of the profiles at $Re = 1.6 \cdot 10^4$), while they vary at longer times, due to the difference in Strouhal number. The fact that the profiles at the highest Re do not collapse, even at short times, is probably due to the strong stratification at the entrance of the horizontal transition section. Because the seeded material is concentrated near the bottom of the transition section, its velocity will be below the average velocity, which results in a longer delay time in both average concentration and fluctuations.

The stratification also reduces the area over which mixing between the two streams occurs, leading to an increase in relative fluctuations.

In conclusion, all the differences between the experimental results at different Reynolds number, with the exception of the scalar spectra in the vertical transition section, can be attributed to differences in inlet conditions: relative flowrates of main air and puff, and puff duration. We suspect that Reynolds number similarity would have been observed in our experiments, if the relative puff flowrate and the Strouhal number had been kept constant.

10.4 Linear Eddy Modeling

Two different linear eddy models have been presented: a model for radial mixing in fully developed turbulent pipe flow (Chapter 4), and a model for axial mixing in the cold flow experiments (Chapter 9). Below, we will compare the two models, and point out the similarities and differences between them.

The most apparent difference between the models is the orientation of the simulation line: radial (cross-stream) for the pipe flow model, and streamwise for the unsteady state model. When the simulation domain of a linear eddy model is perpendicular to the main flow direction, Lagrangian time and downstream distance are equivalent. The model therefore loses its time-dependence (in the Eulerian sense), but includes two spatial dimensions. A streamwise model contains only

one spatial dimension, and time. Each case has advantages for specific applications, as should be clear from the context in which the models were presented. It is important to note that the local small scale structure is not affected by the direction of the simulation domain. Kerstein (1991b) points out that "although the model ostensibly simulates mixing-field evolution along a straight line, it is more accurate for some purposes to regard the computational domain as a time-varying space curve locally aligned with the concentration gradient".

In the pipe flow model, the eddy frequency is a function of radial position: according to eqn. (4-14), λ is maximum near the wall. This implies that of stirring events, the majority should be in the wall region. This is accomplished by randomly sampling the eddy location PDF, which is a normalized eddy frequency:

$$P(x) = \frac{\lambda(x)}{\int_0^1 \lambda(x) dx} \quad (10-1)$$

In the unsteady state model, the stirring events are distributed evenly, so that the location of each eddy is proportional to the random number drawn. While this may seem to be a different procedure, it is essentially the same. This is illustrated in Figure 10-1. In each case, a random number (r) is drawn. The eddy location (x ; shown with an arrow in the figure) is then determined from:

Figure 10-1: Random sampling of PDFs for eddy location, in the case of uneven eddy distribution (top) or even eddy distribution (bottom). The shaded area is equal r (a random number between 0 and 1) in both cases.

$$r = \int_0^x \lambda(\xi) d\xi \quad (10-2)$$

The integral is represented by the shaded areas in Figure 10-1. The only difference between the two models is in implementation: With constant λ , eqn. (10-2) can easily be solved for x , whereas a numerical integration or a look-up table may be required if λ is a function of x ¹.

The eddy size is a function of position in the pipe flow model. Once an eddy location has been selected, the eddy size is fixed. The unsteady state model, on the other hand, incorporates Kolmogorov scaling, which requires a second random PDF sampling (eqn. 9-1). For this equation, an analytical solution is possible, and no table is required. In addition to these "technical details", there is a conceptual consequence to the difference in eddy size selection: The Kolmogorov scaling incorporates Re dependence: at higher Re , the Kolmogorov length scale is smaller (eqn 2-26). A model without Kolmogorov scaling has no Re dependence (other than the combined effect of Re and Sc , expressed as the Péclet number), and should therefore not be used for Re extrapolation.

¹ A look-up table was used in the pipe-flow model. This table, created prior to the actual simulations, lists the location that corresponds to each random number. When simulations are performed, in the case of a stirring event, a random number is drawn, and the corresponding location is determined from the table.

The information obtained from the pipe flow model consists of radial profiles of average scalar and RMS scalar fluctuations. These are obtained from statistical analysis of multiple realizations. In every realization, the entire radial profile is saved at selected times. In the unsteady state model, for the purpose of calculating average scalar, RMS fluctuations and PDFs, we consider the concentration of a single point of the simulation domain (at a large number of times, and in multiple realizations). Other points of the simulation domain are saved only for the purpose of calculating spectra and correlation functions.

CHAPTER 11

CONCLUSIONS AND RECOMMENDATIONS - EPA KILN MIXING

11.1 Mixing Mechanisms in the Cold Flow Model

We have identified three different mixing mechanisms in the cold flow model: jet mixing in the cavity, mixing in recirculation zones, and shear turbulence in the transition section. The same mechanisms are likely to be present in the EPA kiln.

Interaction between the main air jet and the puff in the cavity causes significant micro-mixing¹ of the puff. This is indicated most clearly by the intensity of segregation measurements in the horizontal transition section: in the absence of micro-mixing, the intensity of segregation would be unity; instead, we find values below 0.03. On the other hand, concentration PDFs display a large peak at zero concentration, indicating that some air has not mixed with the puff. In the scalar spectra, a transient micro-scale can be observed. This suggests poor macro-mixing in the cavity. The simultaneous presence of micro-mixed fluid and a transient micro-scale insinuates a two-stage mixing mechanism in the kiln.

Recirculation zones are present in both the cavity and the transition section. These

¹ Here, micro-mixing is not molecular mixing, but mixing at a scale, smaller than the probe size.

cause a spread in residence time, which has a profound effect on the average concentration profiles. Concentration fluctuations are much less affected by the recirculation zones, as demonstrated by comparison between linear eddy simulations with and without recirculation zone.

Linear eddy simulations suggest that shear turbulence in the transition section has a minor effect on the average concentration profiles, but is important for the local mixing, which is characterized with the scalar spectra, concentration PDFs and fluctuation profiles. All observations indicate improved mixing in the vertical, compared to the horizontal, transition section.

11.2 Prediction of Puffs

Occurrence of failure modes depends not only on the average concentration at any time, but also on the concentration fluctuations. In Chapter 8.4, concentration PDFs were used to assess the probability that a critical concentration limit was exceeded at a particular time (Figure 8-11). We found that the probability of failure modes was substantial.

An alternative approach is based on the average concentration and RMS fluctuations (or intensity of segregation), assuming Gaussian concentration PDFs. Experimental results suggest that this is a reasonable assumption in the vertical transition section (Figures 7-10, D-13 to D-16). The methodology for this approach

was presented earlier in Chapter 2.8. Essentially, we calculated what fraction of waste would be unburnt for a given stoichiometric ratio (equivalent to average concentration) and intensity of segregation, assuming a Gaussian concentration PDF. The same procedure can be applied to experimental data. Table 11-1 gives stoichiometric ratio, and fraction unburnt, for toluene with the same average concentration and intensity of segregation as the experimental data from the vertical transition section, $Re = 3.4 \times 10^3$. A stoichiometric coefficient (v_a) of 92 was assumed, based on $v_o = 9$, and an oxygen mole fraction in the primary flame flue gas of 0.09775 (Wendt and Linak, 1988). The same data are presented graphically in Figure 11-1.

Table 11-1: Stoichiometric ratio and fraction unburnt for toluene with same mixing characteristics as cold flow experiments. $Re = 3.4 \times 10^3$.

t (sec)	C	$\mathcal{S}$	SR	ϕ_{unburnt}
14	0.0024	0.0075	4.51	0.003
16	0.0074	0.0084	1.45	0.098
20	0.0117	0.0039	0.92	0.173
25	0.0121	0.0044	0.89	0.190
30	0.0158	0.0028	0.68	0.292
35	0.0140	0.0024	0.76	0.233
40	0.0117	0.0024	0.92	0.156
50	0.0077	0.0029	1.40	0.049
60	0.0055	0.0029	1.95	0.013

Figure 11-1: Fraction unburnt vs. stoichiometric ratio for partially mixed toluene. Development of a puff with same mixing characteristics as cold flow experiments, assuming a Gaussian concentration PDF.

Figure 11-1 has several interesting aspects. First of all, the intensity of segregation is sufficiently large to cause a substantial fraction unburnt, even at high stoichiometric ratios, as occur at short and long times. The largest fraction unburnt coincides with the lowest stoichiometric ratio (highest concentration of waste). Because the stoichiometric ratio is less than unity ($UOD > 0$), the fraction unburnt is large, also for total micro-mixing ($\mathfrak{S} = 0$). In fact, at the peak concentration, the fraction unburnt is quite insensitive to the intensity of segregation. This has an important consequence: in the absence of macro-mixing that brings the stoichiometric ratio above unity ($UOD = 0$), improved micro-mixing will not substantially reduce the fraction unburnt.

In conclusion, large scale unmixedness (lack of macro-mixing) is the most important factor in the occurrence of failure modes. Linear eddy simulation of mixing in the EPA kiln incinerator has indicated that for a typical puff, the maximum in average UOD decreases by circa 25% due to mixing in the transition section.

11.3 Shortcomings of the Present Work

In the course of this research, we have pointed out a number of sources for error in the experiments: In Chapter 6.5, we assessed the effects of sample size (i.e. number of observations) and of variation in sampling time. The inaccuracy due to sample size is quite large, as can be seen from the 95% confidence intervals in Figures 7-5 and 7-6. Having more identical runs would reduce the size of

confidence intervals. The cross-stream variations in the horizontal transition section lead to poor correlation between concentration and integral pixel value (Chapter 7.4). This caused uncertainty in the calibration procedure, and forced us to determine "renormalized" concentration profiles (Chapter 8.2).

There are a number of additional shortcomings in the cold flow model experiments and linear eddy simulations, when they are to be compared to EPA kiln data.

Most importantly, the present work is isothermal, while the incinerator clearly is not. The temperature of the gas and air at the main burner (before reaction), and of the waste evaporating from the kiln bottom is much lower than the temperature elsewhere. Thermal expansion is likely to have an effect on the turbulence structure in the kiln cavity. This could be verified by linear eddy modeling.

No detailed information is available about the puff release. A characteristic time was estimated from the evaporation model of Wendt and Linak (1988). In cold flow experiments, we took the puff shape to be square, because other puff shapes are hard to realize. Clearly, this is not the most probable puff shape in a rotary kiln. The area over which the waste is released is another parameter that is unknown. This may not be important in terms of turbulent energy input, because most of the initial turbulent energy is supplied by the main burner, but it is likely to affect the path of the puff (see Chapter 8.1).

Chemical reaction has not been taken into account. This has two consequences. First of all, the heat of reaction causes temperature fluctuations, not only in the cavity, but also in the transition section. This results in density fluctuations, which interact with turbulent fluid motion. Secondly, chemical reactions change the local concentration of species, and thus affect the driving force for molecular diffusion.

11.4 Comparison between EPA Kiln and Full Scale Kilns

The present study helps in determining, to what extent test results in EPA's incinerator are representative for full scale rotary kilns.

The Reynolds number differs greatly between the EPA kiln and a full scale unit; however, the smallest turbulent length scales do not (see Table 5-1). For the full scale unit presented in Table 5-1, the large eddy turnover time ($\sim d/2u'$) is of the same order of magnitude as that of the EPA kiln. The residence times are also approximately equal. Therefore, in spite of the large difference in Re , both units have similar mixing characteristics. This confirms the Reynolds number similarity (Chapter 10.3), which suggests that the difference in Re may not be a determining factor for the mixing structure.

The recirculation zones in the cold flow model cause a spread in residence time. Therefore, at low Strouhal number, the maximum concentration in the vertical transition section does not reach its steady state value ($C/C_0 < 1$; see Figure 8-5).

Linear eddy simulation suggested a 25% decrease in the peak in average UOD, due to macro-mixing (Chapter 9.8). We concluded that recirculation zones were the main cause of this abatement, which is therefore specific to the EPA kiln. In full scale units without recirculation zones, the puff intensity is expected to be larger.

One issue that has been all but ignored in the present study is stratification. No stratification has been observed in the EPA rotary kiln incinerator simulator; however, it has been observed in full scale kilns (e.g. Cundy *et al.*, 1989a). Stratification can be induced by temperature differences or concentration differences, the magnitude of which is expressed in non-dimensional form by the Grashof number:

$$Gr_t = \frac{d^3 g \beta \Delta T}{\nu^2} \quad Gr_c = \frac{d^3 g \zeta \Delta C}{\nu^2} \quad (11-1)$$

where β and ζ are defined by:

$$\rho = \bar{\rho} (1 - \beta(T - \bar{T}) - \zeta(C - \bar{C}) + \dots) \quad (11-2)$$

Eqn. (11-1) clearly indicates that stratification is very sensitive to the kiln diameter, explaining why it is more important in full scale kilns than in the EPA simulator. We suspect that stratification should be taken into account, when data from the EPA kiln are to be compared to full scale units.

11.5 Mixing Enhancement

The present study has identified three basic mixing mechanisms in the EPA kiln: mixing between two jets in the cavity, mixing due to recirculation zones, and mixing by shear turbulence. Any of these mechanisms can be enhanced, to obtain improved mixing.

For improving the primary mixing, the main burner could be modified. A burner that provides a higher turbulence intensity is unlikely to have a major effect, because the scales in the cavity are already sufficiently small (as is apparent from the decrease in the intensity of segregation). We expect a more noticeable effect from a modified design that improves the macro-mixing (spread in residence time), allowing more of the primary air to mix with the puff. An asymmetrically positioned burner or a flow obstruction placed in front of the burner might have the desired effect.

Recirculation zones only help improve the mixing under two conditions. (1) The residence time of a recirculation zone needs to be sufficiently large (i.e. larger than the duration of a typical puff). If puff times are long compared to the residence time (large Strouhal number), the average concentration in the recirculation zone will reach a steady state, equal to that in the main flow, and there will no longer be an effect on the average concentration downstream. (2) There needs to be sufficient turbulent mixing downstream of a recirculation zone, to ensure that the reduction

in average concentration also results in a reduction in maximum instantaneous concentration.

Shear turbulence can be enhanced most effectively by modifying the shape of the kiln. At constant volumetric flowrate, $U \sim 1/D^2$. The turnover time of a large eddy ($t = L/u(L)$) is proportional to D^3 , while the residence time is proportional to D^2 . Consequently, in spite of a shorter residence time, a narrow kiln is expected to have better micro-mixing than a wide kiln, because turbulent time scales are more sensitive to the kiln diameter. Other ways to improve mixing intensity include the use of narrow turbulent jets or turbulence generating grids in the kiln. From an operational standpoint, these may not be very practical solutions.

Based on the earlier observation that large-scale unmixedness is the most important factor in the occurrence of failure modes, we expect that an increase in shear turbulence, without simultaneous improvements in macro-mixing, will not substantially reduce the intensity of puffs.

11.6 Project Evaluation

In the introduction, we posed ourselves several questions (Chapter 1.4). At this point, we should determine to what extent those questions have been answered.

(1) How should "puff integrity" be defined and quantified? Puff integrity is primarily

determined by macro-mixing, which is described adequately by the (cross-stream) average concentration. In the course of this dissertation, two alternative parameters have been presented, that are related to the average concentration: stoichiometric ratio and (average) unsatisfied oxygen demand. These parameters have the advantage that they include a reference to the consequence a certain average concentration has for the occurrence of failure modes. A disadvantage is that they are specific to a particular waste and oxygen mole fraction in the primary flame flue gas. Therefore, for a general treatment of the issue, average concentration is favorable.

(2) What parameters are important in determining the lifetimes and local mixing characteristics of puffs ? In Lagrangian sense, the lifetime of a puff is larger than the residence time in the cold flow model, because macro-mixing is limited. Consequently, the Eulerian lifetime (i.e. the time during which puff material passes an observation point at any downstream location) is determined primarily by the duration of waste release from the kiln bed. The mixture at the exit of the cavity (measurements in the horizontal transition section) is primarily determined by the interaction between the main air jet and the ascending transient stream. This process has been analyzed qualitatively only. A quantitative investigation (including a parametric study) should be considered. The main problem in relating results from a well-defined experiment or model predictions to mixing in the EPA kiln would be, that the exact flow rate and release area for waste evaporation from the

kiln bed are unknown, and can not easily be measured.

(3) What are the predominant mixing mechanisms, and what model best describes the observed transient mixing phenomenon ? Three mechanisms were identified: mixing between two jets in the cavity, macro-mixing in recirculation zones, and shear turbulence. A linear eddy model was employed to describe the combined effect of the second and third mechanisms. Its main advantage over alternative modeling techniques is, that it allows the prediction of excursions from average behavior, by generating concentration PDFs.

(4) Which aspects of the gas phase mixing process that occurs in the EPA kiln are unique, and which aspects are more general and occur in all rotary kilns ? Linear eddy simulations have indicated that macro-mixing is determined largely by recirculation zones. This process is therefore specific to the EPA kiln. Local mixing is expected to be similar in the EPA kiln and full scale units, based on Reynolds number similarity. One aspect of local mixing that is absent in the EPA kiln, but important in full scale kilns, is stratification. If experimental data from the EPA kiln are to be compared to full scale rotary kilns, there is a definite need to assess the effect of stratification on mixing.

11.7 Future Work I. Cold Flow Experiments

All the experiments were completed in a full scale cold flow model of the EPA kiln, having approximately the same geometry. The main difference was a compromise in axisymmetry (Figure 5-3). Mixing in this model was characterized, and divided into separate mechanisms. As a logical extension of this work, in order to fully understand the contribution of each mechanism (and possible interactions between them) we recommend a modular setup, in which different geometric components (contraction, dead end, 90° bend) can be evaluated separately. Special attention should be paid to the mechanisms in the cavity. We also recommend that the experiments be done in water, rather than in air, for two reasons. First of all, the kinematic viscosity of water is roughly a factor 10 lower than that of air, allowing smaller geometric scales at the same Re . Consequently, the light intensity of the measurements would be larger; this would possibly allow the use of a laser sheet for quantitative studies. Secondly, dye seeding in water has several advantages over the present use of $TiCl_4$: it can be metered more exactly (also when the puff flowrate is changed) and it is non-corrosive. Finally, we recommend the design to be such that an entire diameter of the model can be observed, so that true cross-stream averages are obtained, also when there are cross-stream variations in the mixture.

11.8 Future Work II. Linear Eddy Modeling

The present linear eddy model can be used to investigate, how sensitive the results are to the input signal. As the input into the EPA kiln (evaporation of waste material) is not well defined, it would be useful to know how important this is for downstream mixture characteristics. If the input signal turns out to be very important, a more detailed look into the waste evaporation process may be required.

When better experimental data from the horizontal transition section become available, the input signal for the linear eddy model can be modified, to include the experimental inlet PDF. This would require an additional length scale¹. The new input signal might consist of blocks of zero concentration, and blocks of randomly fluctuating concentration (Figure 11-2); the large length scale (transition section diameter) would control the large scale periodicity, and the randomly fluctuating part of the input signal should match both the smaller length scale and the PDF (with zero concentration subtracted) of the experiments.

In Chapter 11.3, we indicated two fundamental differences between the EPA kiln and our cold flow model: variable temperature vs. isothermal flow, and reacting vs.

¹ A choice for the second length scale could be the experimentally determined scale of segregation, or the "Taylor type micro-scale for concentration", defined by Corrsin (1964).

Figure 11-2: Input signal (left) and corresponding PDF (right) of linear eddy model with proposed modifications.

non-reacting flow. In linear eddy modeling, both chemical reaction and temperature effects can be incorporated. Including chemical reaction would give us an opportunity to verify Toor's hypothesis (Chapter 2.7). This extension of the present model will give more accurate predictions of mixing in the EPA kiln.

11.9 Future Work III. Scale Up

As mentioned earlier, we suspect that stratification constitutes a fundamental difference between the EPA simulator and full scale kilns. Linear eddy modeling can be used to model stratified flow. We will presently suggest a methodology for this.

In its simplest form, stratified flow consists of two co-current phases, with different composition and temperature. In a linear eddy model, each phase can be represented by a separate streamline, as shown schematically in Figure 11-3. Cells in each phase interact through convection, diffusion and turbulent motion, similar to the model presented in Chapter 9¹; The two phases interact through large scale turbulent motion (vertical stirring). The last can be modeled by simply placing a block of cells from one phase in the other, and vice versa. Like stirring within a phase, turbulent motion between phases should be a random process. Vertical

¹ In the simplest form, convection and diffusion would be equal in top and bottom phases, and turbulent motion would have the same frequency and PDF for eddy size. As a further refinement, these processes could differ quantitatively between the two phases.

Figure 11-3: Schematic of linear eddy model for stratified flow.

stirring causes a transfer from turbulent kinetic energy to potential energy. In addition to scalar concentration, the contents of each cell has a potential energy (proportional to the density) and a turbulent kinetic energy associated with it. These parameters also get transferred between cells, due to convection, diffusion and stirring. The frequency of stirring events (both within a phase and between phases) should be determined from the local turbulent kinetic energy, and is therefore dependent on the occurrence of vertical stirring events upstream.

Since many aspects of the proposed model are somewhat speculative, modeling should not be attempted without simultaneous experimental investigations. It would be impractical to perform experiments at the same geometric length scale as a full scale kiln. Eqn. (11-1) suggests two alternatives: (1) Using liquids (instead of gases) decreases ν . In that case, density differences should be created with variations in concentration, since β is small for liquids. (2) If air is used in the experiments, the Grashof number can be maintained at a smaller length scale by increasing the temperature differences.

APPENDIX A

OPTICAL PROPERTIES OF PARTICLES

A.1 Introduction

All aerosol particles scatter radiation. Some can also absorb it. The combination of scattering plus absorption is called extinction. In the following, optical properties of particles are presented, following Reist (1993). Relevant parameters are calculated for the particles in our flow visualization studies.

A.2 Light Scattering

Light scattering depends on particle size (d) and shape, refractive index (m) and wavelength of incident light (λ). The particle size and light wavelength are related through the dimensionless factor α , defined as:

$$\alpha = \frac{\pi d}{\lambda} \quad (\text{A-1})$$

A scattering intensity coefficient $q(\theta)$ can be defined as the flux of light, scattered into an angle θ , divided by the incident flux. Determination of the value of $q(\theta)$ as a function of the refractive index (m) can be accomplished through the use of the Mie theory of radiation scattering, for any value of α . Unfortunately, solutions of Mie's equations do not lend themselves readily to numerical computation. Manageable solutions other than Mie theory exist for the cases where $\alpha < 0.3$ (Rayleigh scattering) or $\alpha > 1$ (geometrical optics). For the intermediate region,

representing particle sizes from about 0.1 to 10 μm in visible light, Mie solutions must be used. For a monodisperse aerosol, Mie theory predicts very large fluctuations in scattering intensity with scattering angle. However, as an aerosol becomes more polydisperse, there is a tendency for the scattering patterns to become smoother.

A.3 Light Extinction by a Particle Cloud

The amount of light extinguished in a thin section of a particle-containing medium is proportional to the luminous flux (F). In integral form, this is described by Bouguer's law (also known as Beer's law):

$$F = F_0 e^{-\gamma L} \quad (\text{A-2})$$

where L is the path length from source to receptor, and γ is the extinction coefficient, which, for spherical particles, is defined as:

$$\gamma = n A_p Q_{\text{ext}} = \frac{6m Q_{\text{ext}}}{\rho_p d_p} \quad (\text{A-3})$$

The term Q_{ext} represents an efficiency factor, and is generally assumed to be 2. Several assumptions are implicit in Bouguer's law, the main one being that a maximum of one scatter per photon is allowed. This assumption implies that eqn. (A-2) is only valid for thin clouds or low concentrations; the product γL should not exceed 0.1.

A.4 Conclusions

To a first approximation, the pixel value in a video frame is proportional to the local particle number density (or "particle concentration"). Both scattering and extinction may cause deviations from proportionality.

Light scattering by TiO_2 particles in our flow visualization studies is described by Mie theory. Scattered light intensity is a strong function of scattering angle for a monodisperse aerosol. Since different points on a video frame correspond to different scattering angles, the proportionality constant is not necessarily the same at different points in a video frame. However, particle size measurements for TiO_2 in a similar system (Freymuth *et al.*, 1985) indicate considerable spread in particle size. Therefore, angular dependence of scattered light intensity can be neglected.

An estimate for the extinction coefficient γ in our experiments, from eqn. (A-3), is 2.9 to 5.8 m^{-1} , based on a particle diameter of 0.5 to $1.0 \text{ }\mu\text{m}$, a density of TiO_2 of $4.17 \cdot 10^3 \text{ kg/m}^3$, and a mass density of 0.001 kg/m^3 (see Chapter 5.4). This value is representative for the puff; since the puff stream makes up between 0.8% and 7.1% of the total flow under all experimental conditions (Tables 5-1, 7-1, 7-2), the average extinction coefficient is at least a factor 14 lower. The path length L is different, depending on the location along the laser line. A representative value is the diameter of the duct (0.46 m). Thus, an estimate for the product γL is between 0.09 and 0.19 at the lowest main air flowrate ($\text{Re} = 1.7 \cdot 10^3$), and less for higher

main air flowrates. Therefore, the assumption of single scattering is accurate for all but the lowest Re , but may be somewhat inaccurate at $Re = 1.7 \cdot 10^3$.

APPENDIX B

STATISTICAL METHODS

B.1 Statistical Inference

Both the experimental data and the results of the linear eddy simulations are made up of multiple observations. For independent observations, the laws of statistical inference (Bethea *et al.*, 1975) can be applied, to find the accuracy of estimates for mean and variance.

A normal population with unknown mean value μ and standard deviation σ (variance σ^2) is sampled N times. The value of a particular sample is x_n . Estimates for the mean value and standard deviation of the population are given by the sample mean $\bar{x}$ and the sample standard deviation s, defined as:

$$\bar{x} = \sum_{n=1}^N \frac{x_n}{N} \quad (B-1)$$

$$s = \sqrt{\sum_{n=1}^N \frac{(x_n - \bar{x})^2}{N - 1}} \quad (B-2)$$

How good the sample mean and standard deviation represent the true (population) mean and standard deviation, can be expressed with confidence intervals. A $(1-\alpha)$ confidence interval for the population mean (i.e. an interval that includes the mean with a probability of $(1-\alpha)*100\%$) is given by:

$$\bar{x} - \frac{s}{\sqrt{N}} t_{N-1, 1-\frac{\alpha}{2}} < \mu < \bar{x} + \frac{s}{\sqrt{N}} t_{N-1, 1-\frac{\alpha}{2}} \quad (\text{B-3})$$

Here, $t_{N-1, 1-\alpha/2}$ is that value of the t distribution with (N-1) degrees of freedom that has an area (1- $\alpha/2$) to the left. Tables for the t distribution can be found in Weast (1986). For large values of N, the t distribution approaches the normal distribution. For $\alpha = 0.95$, and large N, $t_{N-1, 1-\alpha/2} = 1.960$.

A (1- α) confidence interval for the variance is :

$$\frac{(N-1)s^2}{\chi^2_{N-1, 1-\frac{\alpha}{2}}} < \sigma^2 < \frac{(N-1)s^2}{\chi^2_{N-1, \frac{\alpha}{2}}} \quad (\text{B-4})$$

$\chi^2_{N-1, 1-\alpha/2}$ and $\chi^2_{N-1, \alpha/2}$ are the values of the χ^2 distribution that have areas (1- $\alpha/2$) and ($\alpha/2$) respectively to their left. The χ^2 distribution is also tabulated in Weast (1986). An approximate value for large N is (Weast, 1986):

$$\chi^2_{N-1, \frac{\alpha}{2}} = (N-1) \left(1 - \frac{2}{9(N-1)} + z_{\alpha/2} \sqrt{\frac{2}{9(N-1)}} \right)^3 \quad (\text{B-5})$$

where $z_{\alpha/2}$ is the normal deviate, or that value of x for which F(x) is the desired percentile. $z_{0.975} = 1.960$, and $z_{0.025} = -1.960$.

B.2 Analysis of Variance

Consider M groups of observations, the number of observations per group being N . Then, there are three different types of sample variance (Bethea *et al.*, 1975): within groups, between groups (variance of group means around grand mean) and total.

The pooled sample variance or mean square for within groups is given by:

$$\sigma_W^2 = \frac{SS_W}{M(N-1)} = \frac{\sum_m \left(\sum_n (x_{mn} - \bar{x}_m)^2 \right)}{M(N-1)} \quad (B-6)$$

The variance of group means or mean square for between groups is given by:

$$\sigma_B^2 = \frac{SS_B}{M-1} = \frac{N \sum_m (\bar{x}_m - \bar{x})^2}{M-1} \quad (B-7)$$

The total sum of squares is given by:

$$\sum_m \sum_n (x_{mn} - \bar{x})^2 = N \sum_m (\bar{x}_m - \bar{x})^2 + \sum_m \sum_n (x_{mn} - \bar{x}_m)^2 \quad (B-8)$$

which leads to the following expression for the total corrected variance:

$$\sigma_T^2 = \frac{SS_T}{MN-1} = \frac{SS_B + SS_W}{MN-1} \quad (B-9)$$

In other words, the total variance is partitioned into two components, one reflecting variation between groups, and the other fluctuations within groups.

APPENDIX C

COMPUTER PROGRAM LISTINGS

C.1 Linear Eddy Model for Turbulent Pipe Flow

Fortran source code for linear eddy model of Chapter 4. Compiled and vectorized with Convex Fortran compiler.

```

program lined
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c      This program simulates radial mixing in fully developed pipeflow,
c      using a triplet map or block inversion.
c      Axisymmetry is not incorporated in linear eddies or in diffusion;
c      however, total amount of scalar is calculated for axisymmetrical
c      geometry.
c
c      Multiple simulations, giving statistical properties:
c      total amount of scalar, and average and rms profiles.
c      Local eddy size: L=K*y (single eddy size)
c      minimum eddy size: L_min = 20R/Re* (wall region only)
c
c      Last revised: December, 1993
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

parameter (nn=3000, nomax=4, diffac=.2, nyout=500)
dimension y(nn), yini(nn), ynew(nn), xout(nomax),
& tout(nomax), tlo(nn/2), is(5), ytot(nomax),
& yav(nyout,nomax), ysq(nyout,nomax), yfl(nyout,nomax)
data is /72834091, 19287349, 25766547, 48767163, 87787183/
common /random/ iseed
common /eddy/ q, ied, nmin
common /outstat/ ys(nyout,nomax)
resol = 1./(float(nn)+1.)
open (unit= 1, file='input.dat', status='old')
open (unit=11, file='aver.dat', status='new')
open (unit=12, file='fluc.dat', status='new')

c
c      read input parameters, location of outputs, and initial profile
c
read (1,*) nsim
print *, nsim
iseed = is(1)
read (1,*) rey, sc, nout
write (11,*) '# gridpints =', nn
write (11,*) '# simulations =', nsim, 'average scalar profile'
write (11,*) 'Re =', rey
write (11,*) 'Sc =', sc
write (12,*) '# gridpints =', nn
write (12,*) '# simulations =', nsim, 'diffusivity profile: D_T/nu'
write (12,*) 'Re =', rey

```

```

        write (12,*) 'Sc =', sc
        do 10 i=1,nout
            read (1,*) xout(i)
c          note: xout is non-dimensionalized by d(=2*r)
10      continue
        do 20 i=1,nn
            read (1,*) yini(i)
20      continue
c
c      calculate Re*, times for stirring, diffusion, output
c
        reys = .226*rey/log(rey/7.)
        tdeld= 4.*diffac*resol**2*reys*sc
        do 30 i=1,nout
            tout(i) = 4.*xout(i)*reys/rey
30      continue
        tend = tout(nout)
        print *, 'reys =', reys
        print *, 'tdeld=', tdeld
        print *, 'tend =', tend
c
c      determine time between stirrings and
c      make lookup tables for blockcenter PDF
c
        call stirini(tlo,tdels,reys)
c
c      initialize statistical quantities
c
        n0 = 0
        do 45 iout=1,nout
            do 44 i=1,nyout
                yav(i,iout) = 0.
                ysq(i,iout) = 0.
44      continue
45      continue
c
c      do simulations
c      add results of each simulation to average quantities
c
        do 100 isim=1,nsim
            do 50 i=1,nn
                y(i)=yini(i)
50      continue
            print *, 'simulation', isim
            call sim(diffac, tdels, tdeld, tout,
&            tend, tlo, y, ynew, reys)
            do 55 iout=1,nout
                do 54 i=1,nyout/2
                    yav(i,iout) = yav(i,iout) +
&                    ys(i,iout) + ys(nyout+1-i,iout)
                    ysq(i,iout) = ysq(i,iout) +
&                    ys(i,iout)**2 +
&                    ys(nyout+1-i,iout)**2
54      continue
55      continue
100     continue
c
c      calculate statistics;
c      give output and end program
c

```

```

do 110 iout = 1, nout
    ytot(iout) = 0.
    do 104 i=1,nyout/2
        x = (float(i)-.5)*2./float(nyout)
        yav(i,iout) = yav(i,iout)/float(nsim)/2.
        ysq(i,iout) = ysq(i,iout)/float(nsim)/2.
        ytot(iout) = ytot(iout) + abs(1.-x)*yav(i,iout)
104     continue
    ytot(iout) = ytot(iout)*2./float(nyout/2)
110 continue
write (11,*) '          ',
& tout(1), tout(2), tout(3), tout(4)
write (12,*) '          ',
& tout(1), tout(2), tout(3), tout(4)
do 115 i=1,nyout/2
    do 112 iout=1, nout
        x = (float(i)-.5)*2./float(nyout)
        yfl(i,iout) = ysq(i,iout)-yav(i,iout)**2
        yav(i,iout) = yav(i,iout)/ytot(iout)
        yfl(i,iout) = yfl(i,iout)/ytot(iout)**2
112     continue
    write (11,*) x, yav(i,1), yav(i,2),
& yav(i,3), yav(i,4)
    write (12,*) x, yfl(i,1), yfl(i,2),
& yfl(i,3), yfl(i,4)
115 continue
close (1)
close (11)
close (12)
stop
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      subroutine sim(diffac, tdels, tdeld, tout, tend,
& tlo, y, ynew, reys)
C
C   do actual simulation
C
parameter (nn = 3000, nomax=4)
dimension tout(nomax), tlo(nn/2), y(nn), ynew(nn)
C
C   initialize variables
C
clock = 0.
tnexts= tdels
tnextd= tdeld
iout = 1
tnexto= tout(iout)
C
C   determine type of event implemented next and update
C   scalar field accordingly;
C   keep going until the clocktime reaches tend
C
do while (clock .lt. tend)
    call nextev(tnexts, tnextd, tnexto, next)
    goto (11,12,13) next
11    clock = tnexts
    call stir(tlo, y, ynew, nc, nlo, nhi, reys)
    tnexts= clock + tdels

```



```
c      subsequent routine half, a (random) choice between right
c      and left half of domain is made.
c
c      parameter (nn=3000)
c      common /random/ iseed
c      common /eddy/ q, ied, nmin
c      dimension tlo(nn/2)
c      r=ran(iseed)
c      nc = nmin
c      do while (r .gt. tlo(nc))
c          nc = nc+1
c      enddo
c      return
c      end
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c      subroutine bounds (nn, nc, nlow, nhigh, reys)
c
c      determine upper and lower boundaries of block;
c
c      common /eddy/ q, ied, nmin
c      c = float(nn+1)/2.
c      xi = float(nc)/c
c      blm = .4*float(nc)*q
c      if (blm .lt. float(2*nmin)) blm = float(2*nmin)
c      nlow = nc - nint(blm/2.)
c      if (nlow .le. 0) nlow = 1
c      nhigh= nlow + nint(blm)
c      return
c      end
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c      subroutine half (nn, nc, nlow, nhigh)
c
c      determine whether inversion is in right or left half of domain
c
c      common /random/ iseed
c      r = ran(iseed)
c      if (r .gt. .5) then
c          nc     = nn+1-nc
c          ntemp  = nlow
c          nlow   = nn+1-nhigh
c          nhigh  = nn+1-ntemp
c      endif
c      return
c      end
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c      subroutine triplet (nlow, nhigh, y, ynew)
c
c      apply triplet mapping to the region (nlow, nhigh);
c      no axisymmetry in this routine
c
c      parameter (nn=3000)
c      dimension y(nn), ynew(nn)
c      ntrip = nint(float(nhigh-nlow)/3)
c      nmap = 3*ntrip
```

```

do 10 i=1, ntrip
    i1 = nlow + 3*(i-1)
    i2 = nlow + 3*(i-1) + 1
    i3 = nlow + 3*(i-1) + 2
    j1 = nlow + i - 1
    j2 = nlow + 2*ntrip - i
    j3 = nlow + 2*ntrip + i - 1
    ynew(j1) = y(i1)
    ynew(j2) = y(i2)
    ynew(j3) = y(i3)
10 continue
do 20 i=1, nmap
    j = nlow + i - 1
    y(j) = ynew(j)
20 continue
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      subroutine blocki (nlow, nhigh, y, ynew)
c
c      apply blockinversion to region (nlow, nhigh)
c      no axisymmetry in this routine
c
      parameter (nn=3000)
      dimension y(nn), ynew(nn)
      do 10 i=nlow, nhigh
          ynew(i) = y(nhigh+nlow-i)
10  continue
      do 20 i=nlow, nhigh
          y(i) = ynew(i)
20  continue
      return
      end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      subroutine diffuse (diffac, y, ynew)
c
c      apply Fick's law for molecular diffusion (planar geometry)
c      boundary conditions: dy/dx = 0 ==> y(0)=y(1); y(nn+1)=y(nn)
c
      parameter (nn=3000)
      dimension y(nn), ynew(nn)
c
c      boundaries
c
      ynew(1) = y(1) + diffac*(y(2)-2.*y(1)+y(1))
      ynew(nn) = y(nn) + diffac*(y(nn-1)-2.*y(nn)+y(nn))
c
c      region between boundaries
c
      do 10 i=2, nn-1
          ynew(i)=y(i)+diffac*(y(i+1)-2.*y(i)+y(i-1))
10  continue
c
c      implement diffusion step
c
      do 20 i=1, nn

```



```

        write (12,*) 'block inversions'
    endif
    write (11,*) 'q=', q, 'a1=', a1, 'a2=', a2
    write (12,*) 'q=', q, 'a1=', a1, 'a2=', a2
c
c    determine laminar/buffer layer;
c    smallest possible eddy size;
c    position closest to wall
c
    xbl = ch/reys
    sez = q*vk*xbl
    xmin= sez/2.
    nmin= nint(xmin*float(nn+1)/2.)
    nbl = nint(xbl*float(nn+1)/2.)
c
c    determine eddy frequency in boundary layer
c    and integral
c
    frf = 6.*vk/sez**3
    if (ied .eq. 1) frf = frf*27./12.
    i = 1
    tlo(i)= 0.
    do while (i .lt. nbl)
        i = i+1
        xi = float(2*i)/float(nn+1)
        freq = frf*xi
        tlo(i) = tlo(i-1)+freq
    enddo
c
c    calculate frequency and integral outside boundary layer
c
    do 10 i=nbl+1,nn/2
        xi = float(2*i)/float(nn+1)
        freq = a1/xi/xi + a2/xi
        tlo(i) = tlo(i-1)+freq
10    continue
c
c    calculate time between stirrings;
c    normalize look-up table
c
    tdels = float(nn+1)/4./tlo(nn/2)
    print *, 'tdels=', tdels
    do 20 i=1,nn/2
        tlo(i)=tlo(i)/tlo(nn/2)
20    continue
    return
end

```

263

This section contains the Fortran source code for the linear eddy model of Chapter 9. The program was compiled and vectorized with the Convex Fortran compiler. Input files for the program are also included. Explanation of these files is given, following the source code.

```

program streamwise
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c      Implementation of linear eddy model in streamwise direction,
c      developed for simulation of cold flow model experiments.
c      A recirculation zone is added, halfway between the input
c      and the output locations.
c
c      Input signal consists of pulse with periodicity, equal to
c      large eddy size, and concentration 0 or C_1. C_1 and phi
c      (fraction of time when C = C_1) are calculated from C and c'
c      at the inlet (input condition), which are functions of time.
c
c      Output signal consists of five files:
c      (1) INX.DAT, containing C/C_0, c'/C_0 as functions of time
c      at first grid point.
c      (2) MIX.DAT, containing C/C_0, c'/C_0, S(tot) and S(+)
c      as functions of time, at output location x_out.
c      (3) SPE.DAT, containing a time-average scalar spectrum.
c      (4) PDF.DAT, containing concentration PDFs at different times.
c      (5) ACF.DAT, containing time-average correlation function.
c
c      Domain of simulations extends one large eddy size beyond
c      the output location.
c
c      last revised: May, 1994
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

parameter ( nn=200000, ne=70000, ntmax=100, nbins=40,
& nsm=100, nim=20, ncym=1000, pi=3.1416)
dimension cav(ntmax), csq(ntmax), cor(ne,ntmax), ks(5),
& pdf(ntmax,nbins), wn(nsm), sp(nsm), tin(nim), cl(nim), phi(nim),
& bav(ntmax), bsq(ntmax), rav(ne)
data ks /879304583, 91735608, 29576910, 73289105, 44719378/
external cpa, fli
common /random/ iseed
common /times/ dtstir, dtdiff, dtconv, dtout, tomax,
& tup(ncym), tdn(ncym)
common /scaling/ rel, ql, qh
common /diffnum/ diffac
common /recbp/ pbp, iconv, nconv, jump
common /outstat/ bs(ntmax), cs(ntmax), rs(ne,ntmax), lout, nr
common /probe/ np
common /dimen/ dz, nrc, nj
common /insig/ ntin,nin,ncy,dtcycl,nshift
ksarg = 1
kseed = ks(ksarg)

```

```

diffac = 0.2

c
c
c   open input files;
c       read:   number of simulations
c               fitting parameters: qf, ql, qh;
c               output specifications: z_out/D, dt_out, d_probe/D
c               length recirculation zone:
c               zrc/D and fraction of by-pass: pbp
c               experimental conditions: Re, Sc, tau, t_out,max, S_in/D
c               input profiles of C_1 and phi_1
c   note: all times non-dimensionalized with tau.
c
c   open (unit=1, file='do.dat', status='old')
c   open (unit=2, file='in.dat', status='old')
c   read (1,*) qf, ql, qh
c   read (1,*) zout, dtout, dp
c   read (1,*) zrc, pbp
c   read (1,*) nsim
c   read (2,*) re, sc, tau, tomax, sin
c   read (2,*) ntin
c   if (ntin .gt. nim) call prostop (10)
c   do 10 itin=1,ntin
c       read (2,*) tin(itin), cl(itin), phi(itin)
10 continue
c   ntout = nint(tomax/dtout)
c   if (ntout .gt. ntmax) call prostop (4)
c
c   calculate domain size, max. distance correlation,
c   Re(L), L_min, # gridpoints for probe
c   check for full resolution (L_min > 6*delz)
c   check array size for correlation function
c   check that smallest eddies are smaller than large eddies;
c   otherwise adjust q_H to obtain single eddy size
c
c   z = zout + sin + zrc
c   dz = z/float(nn)
c   nrc= nint(zrc/z*float(nn))
c   nj = (nn-nrc)/2
c   nr = nint(1.5*sin/dz)
c   lout = nint((zout+zrc)/dz)
c   res = .226*re/log(re/7.)
c   rel = 2.*res*ql
c   sez = qh*ql*rel**(-3./4.)
c   np = nint(dp/dz)
c   if (np .eq. 0) then
c       np = 1
c       print *, 'probe size smaller than resolution'
c   endif
c   if (sez .lt. 6.*dz) call prostop (1)
c   if (nr .gt. ne) call prostop (5)
c   if ((nj+nrc) .ge. lout) call prostop (8)
c   if (sez .gt. ql) then
c       qh = rel**(3./4.)
c       print *, 'single eddy size'
c   endif
c
c   calculate times for stirring, diffusion and input cycle;
c   convection time should be smaller than input cycle time
c   and smaller than output time;

```

```

c      print all times.
c
      if (qh .lt. rel**(3./4.)) then
          fl = 24./5.*(rel**(5./4.)*qh**(-5./3.))-1.)/
&      (1.-rel**(-1.)*qh**(4./3.))
      else
          fl = 6.
      endif
      dtstir = 1./(tau*rel*ql**(-3.)*z*qf*fl)
      dtstir = dtstir*12./27.
      dtdiff = diffac*z*z*sc/float(nn*nn)/tau
      dtcycl = sin/re/tau
      dtconv = dtcycl/5.
      do while (dtconv .gt. dtout)
          dtconv = dtconv/2.
      enddo
      print *, 'dtstir =', dtstir
      print *, 'dtdiff =', dtdiff
      print *, 'dtconv =', dtconv
      print *, 'dtcycl =', dtcycl
      print *, 'dtout =', dtout
      print *, 'toutmx =', tomax
      print *, 'tinmx =', tin(ntin)
c
c      calculate shift cycle size (nshift)
c      input cycle size (nin)
c      number of input cycles (ncy)
c      and cycle counter recirculation zone (nconv)
c
      nshift = nint (dtconv*re*tau*float(nn)/z)
      if (nshift .gt. nj) call prostop (9)
      nin = nint (sin*float(nn)/z)
      ncy = nint(tomax/dtcycl)
      if (ncy .gt. ncym) call prostop (10)
      if (nin .gt. ne) call prostop (3)
      nconv = nint(ql/dz/float(nshift))
      if (nconv .eq. 0) nconv = 1
c
c      open output files and write headers
c
      open (unit=10, file='inx.dat', status='new')
      open (unit=11, file='mix.dat', status='new')
      open (unit=12, file='spe.dat', status='new')
      open (unit=13, file='pdf.dat', status='new')
      open (unit=14, file='acf.dat', status='new')
      write (10,*) 'input profiles'
      write (11,*) 'mixing vs. time profiles'
      write (12,*) 'Scalar Spectrum'
      write (13,*) 'Probability Density Function'
      write (13,*) '(C_max/C_0 = 2)'
      write (14,*) 'spatial correlation function'
      do 30 i=10,14
          write (i,*) 'Re =', re
          write (i,*) 'Sc =', sc
          write (i,*) 'Z/D =', zout
          write (i,*) 'tau =', tau, '(non-dimensional)'
          write (i,*) 'dz/D=', dz
          write (i,*) '# gridpoints probe =', np
          write (i,*) '# simulations =', nsim
          write (i,*) '# gridpoints =', nn

```

```

        write (i,*) 'q_f =', qf
        write (i,*) 'q_L =', ql
        write (i,*) 'q_h =', qh
        write (i,*) 'z_recirc/D =', zrc
        write (i,*) 'u_recirc/U =', 1.-pbp
        write (i,*) ' '
30  continue
    write (10,*) 't/tau      C/C_0      cp/C_0 '
    write (11,*) 't/tau      C/C_0      cp/C_0      S(units dz/D)'
    write (12,*) 'k(1/gridpoints)      F(k)'
c
c  generate wavenumbers for spectral calculations
c  initialize variables
c
    wn(1) = 5.
    if (wn(1) .gt. 10./float(np)) wn(1) = 10./float(np)
    is = 1
    do while ((is .lt. nsm) .and. (wn(is) .gt. 1./float(ne)))
        wn(is+1) = wn(is)/1.1
        is = is+1
    enddo
    ns = is
    do 60 itout=1,ntout
        bav(itout) = 0.
        bsq(itout) = 0.
        cav(itout) = 0.
        csq(itout) = 0.
        do 40 ir=1,ne
            cor(ir,itout) = 0.
40         continue
            do 50 ibin=1,nbin
                pdf(itout,nbin) = 0.
50         continue
60     continue
        do 70 is = 1,ns
            sp(is) = 0.
70     continue
        do 80 ir = 1, nr
            rav(ir) = 0.
80     continue
c
c  do individual realizations;
c  add results to statistical quantities
c  and to bin-count for PDF
c  start each realization at random time in input cycle
c
    do 199 isim=1,nsim
        r = ran(iseed)
        npin = nint(r*float(nin))
        if (npin .le. 0) npin = 1
        npbp = 1
        call exin (tin,c1,phi,npin)
        call sim ()
        print *, 'simulation', isim
        do 120 itout=1,ntout
            bav(itout) = bav(itout) + bs(itout)
            bsq(itout) = bsq(itout) + bs(itout)**2
            cav(itout) = cav(itout) + cs(itout)
            csq(itout) = csq(itout) + cs(itout)**2
            do 110 ir = 1,nr

```

```

&
110      cor(ir,itout) = cor(ir,itout) +
      rs(ir,itout)
      continue
      ibin = nint(cs(itout)*float(nbin)/2.)
      if (ibin .eq. 0) ibin=1
      if (ibin .gt. nbin) ibin=nbin
      pdf(itout,ibin) = pdf(itout,ibin) +1.
120      continue
199  continue
c
c      for each output time:
c      calculate mixing parameters and write to file
c
      icspe=0
      do 299 itout=1,ntout
          tout = float(itout)*dtout
c
c      average, standard deviation
c
          bc0 = bav(itout)/float(nsim)
          bpr = (bsq(itout)/float(nsim) - bc0*bc0)**(0.5)
          cc0 = cav(itout)/float(nsim)
          cpr = (csq(itout)/float(nsim) - cc0*cc0)**(0.5)
c
c      spatial correlation, scale of segregation, spectrum
c      check against divide by zero for normalization
c
          if (cpr .lt. 0.01 .or. tout .lt. 0.7) then
              cnorm = 0.
          else
              cnorm = 1./cpr/cpr
              icspe = icspe+1
          endif
          ssl = csq(itout)/float(nsim) - cav(itout)**2/
&          float(nsim)**2
          ss2 = ssl
          do 210 ir=1,nr
              cr = cor(ir,itout)/float(nsim) - cav(itout)**2/
&              float(nsim)**2
              ssl = ssl + cr
              rav(ir) = rav(ir)+cr*cnorm
              if (cr .gt. 0) then
                  ss2 = ss2 + cr
                  do 205 is = 1,ns
                      sp(is) = sp(is) + cnorm*
&                      cos(wn(is)*float(ir))*cr
205                  continue
              endif
210      continue
          ssl = ssl*cnorm
          ss2 = ss2*cnorm
c
c      write average, fluctuation, scale to file
c
          write (10,*) tout, bc0, bpr
          write (11,*) tout, cc0, cpr, ssl, ss2
c
c      normalize PDF and write to file
c
          write (13,*) 't/tau =', tout

```



```
subroutine exin (tin,cl,phi,npin)
```

```

c
c calculate C_1 and phi_1 for each input time,
c by interpolation of the experimental input profile.
c determine times signal goes up and down.
c ensure maximum times are not shorter than simulation time.
c

```

[illegible]

```
subroutine sim()
```

```

c
c      do actual simulation (single realization)
c
c      parameter (nn=200000, ne=70000, ncym=1000)
c      dimension c(nn)
c      common /times/ dtstir, dtdiff, dtconv, dtout, tomax,
c      & tup(ncym), tdn(ncym)

```

```

common /dimen/ dz, nrc, nj
common /inpro/cin(ncym)
common /recbp/ pbbp, iconv, nconv, jump

c
clear domain;
initialize all variables

do 10 i=1,nn
    c(i) = 0.
10 continue
tnextc = 0.
tnexts = dtstir
tnextd = dtdiff
tnexto = dtout
icy = 1
clock = 0.
itout = 0
iconv = 1

c
determine type of event implemented next and update
keep going until clock = t_out,max

do while (clock .lt. tomax)
    call nextev (tnexts,tnextd,tnextc,tnexto,
        & tup(icy),tdn(icy),next)
    goto (11,12,13,14,15,16) next
11      clock = tnexts
        call stir (c)
        tnexts = tnexts + dtstir
        goto 20
12      clock = tnextd
        call diffuse (c)
        tnextd = tnextd + dtdiff
        goto 20
13      clock = tnextc
        call convect (c, cit)
        tnextc = tnextc + dtconv
        goto 20
14      clock = tnexto
        itout = itout + 1
        call output (c,itout)
        tnexto = tnexto + dtout
        goto 20
15      clock = tup(icy)
        cit = cin(icy)
        tup(icy) = tdn(icy)+1.
        goto 20
16      clock = tdn(icy)
        cit = 0.
        icy = icy+1
20      continue
enddo
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

subroutine nextev (tnexts,tnextd,tnextc,tnexto,
& tnextu,tnextn,next)

```

[illegible]

```

c
c      implement stirring event
c      equal likelihood of eddies anywhere, including
c      recirculation zone
c

```

[illegible]

```

c
c      determine lower and upper boundaries of stirring event
c

```

```
c
c      random placement for lower boundary
c
c      r = ran(iseed)
```

```

nlow = nint(r*float(nn))
c
c      kolmogorov scaling for eddy size
c
r = ran(iseed)
blm = ql/dz
blw = blm*(r+(1.-r)*rel**1.25*qh*(-5./3.))**-0.6
nmap = 3*nint(blw/3.)
c
c      ensure that eddy does not exceed simulation domain
c
if (nlow .eq. 0) nlow = 1
if (nlow+nmap .gt. nn) then
    nmap = 3*int(float(nn-nlow)/3.)
endif
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      subroutine triplet (nlow,nmap,c)
c
c      apply triplet map to area [nlow..nlow+nmap]
c
parameter (nn=200000)
dimension c(nn), cnew(nn)
ntrip = nmap/3
do 10 i=1, ntrip
    i1 = 3*(i-1) + nlow
    i2 = 3*(i-1) + nlow + 1
    i3 = 3*(i-1) + nlow + 2
    j1 = i + nlow - 1
    j2 = 2*ntrip - i + nlow
    j3 = 2*ntrip + i + nlow - 1
    cnew(j1) = c(i1)
    cnew(j2) = c(i2)
    cnew(j3) = c(i3)
10 continue
do 20 i=nlow, nlow+nmap
    c(i) = cnew(i)
20 continue
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      subroutine diffuse (c)
c
c      apply Fick's law for molecular diffusion
c      boundary conditions: no flux at inlet, outlet
c
parameter (nn=200000)
dimension c(nn), cnew(nn)
common /diffnum/ diffac
common /dimen/ dz, nrc, nj
c
c      boundaries
c
cnew(1) = c(1) + diffac*(c(2)-2.*c(1)+c(1))
cnew(nn)= c(nn)+ diffac*(c(nn-1)-2.*c(nn)+c(nn))

```

```
c      adjust junction point
c
c      cj = (c(nj)+c(nj+nrc))/2.
c      c(nj) = cj
c      c(nj+nrc) = cj
c
c      region between boundaries
c
c      do 10 i=2,nn-1
c          cnew(i) = c(i) + diffac*(c(i-1)-2.*c(i)+c(i+1))
10 continue
c
c      update profile
c
c      do 20 i=1,nn
c          c(i) = cnew(i)
20 continue
c      return
c      end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      subroutine convect (c, cit)
c
c      apply convection to domain
c      chance of (1-pjump) that recirculation zone is included
c      length of bypass/inclusion event is equal to large eddy size.
c      cells at domain entrance are filled with concentration cit
c
c      parameter (nn=200000, ne=70000)
c      dimension c(nn)
c      common /random/  iseed
c      common /dimen/   dz, nrc, nj
c      common /recbp/   pbb, iconv, nconv, jump
c      common /insig/   ntin,nin,ncy,dtcycl,nshift
c
c      determine whether or not recirculation zone will be included
c      in convection event; new draw every (nconv) cycles
c
c      if (iconv .eq. 1) call bypass (pbb,jump)
c      iconv = iconv + 1
c      if (iconv .gt. nconv) iconv = 1
c
c      shift profile, beginning at downstream end
c
c      if (jump .eq. 0) then
c          n1 = nn
c          n2 = nshift+1
c          call shift(n1,n2,nshift,c)
c      else
c          n1 = nn
c          n2 = nj+nrc+nshift+1
c          call shift (n1,n2,nshift,c)
c          n1 = nj+nrc+nshift
c          n2 = nj+nrc+1
c          nst = nshift+nrc
c          call shift (n1,n2,nst,c)
c          n1 = nj
c          n2 = nshift+1
```



```
&      cpa(lout-ir/2,c)
      rs(ir,itout) = cpa(lout+ir/2,c)*cpa(lout-ir/2,c)
10 continue
   return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

function cpa(i,c)
c
c calculate average concentration over probe size
c
parameter (nn=200000)
dimension c(nn)
common /probe/ np
cpa = 0.
do 10 j=1, np
    cpa = cpa + c(i-1+j)
10 continue
cpa = cpa/float(np)
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

function fli (x,xl,xh,y1,yh)
c
c calculate the y value at location x, by linear interpolation
c between xl and xh, with corresponding y values yl and yh.
c
dx1 = (x-xl)/(xh-xl)
dx2 = (xh-x)/(xh-xl)
fli = dx2*y1 + dx1*yh
return
end
```

The input file DO.DAT contains information about the simulation domain. It contains the following parameters:

- line 1: q_f, q_l, q_h : Three proportionality constants, relating eddy frequency and eddy size to flow parameters. Values 1, 0.5, 20 were used throughout; $q_h = 20$ corresponds to Hill's observation (see Chapter 2.6).
- line 2: $z_{out}/d, \Delta t_{out}/\tau, d_{probe}/d$: Distance between input and output locations, excluding recirculation zone; time between outputs; probe size.
- line 3: $z_{rc}/d, p_{bp}$: Size of recirculation zone; fraction of flow that bypasses recirculation zone.
- line 4: n_{sim} : number of realizations.

For all simulations of cold flow model experiments, with recirculation zone included, the following file was used; the same file served to predict mixing in the EPA kiln:

```

1.000000      0.500000      20.00000
5.000000      5.0000001E-02  1.5435000E-03
2.000000      0.6000000
      500

```

The input file IN.DAT contains information about flow parameters and the input signal for the simulation. It is set up as follows:

line 1: Re , Sc , $\tau v/d^2$, $t_{out,max}/\tau$, S_{in}/d
line 2: number of input points
lines 3 ff: t_{in}/τ , C_1/C_0 , ϕ_1 : Time of input point, and corresponding concentration, and volume fraction of that concentration; a description of how C_1/C_0 and ϕ_1 are chosen is given in Chapter 9.3.

The following files were used for simulation of the cold flow model experiments:

```

2012.000      500000.0      4.9500000E-03      4.000000      1.000000
      15
      0.          0.          0.
      0.          0.          0.2570000
7.5000003E-02  0.2920000      0.2570000
0.1050000      0.3720000      0.3520000
0.1500000      0.4550000      0.4400000
0.2260000      0.5060000      0.6740000
0.3010000      0.5530000      0.6710000
0.4510000      0.4080000      0.6570000
0.6020000      0.3520000      0.4840000
0.9030000      0.2770000      0.3870000
1.354000      0.2290000      0.3800000
1.805000      0.1740000      0.3150000
2.708000      0.1380000      0.3480000
6.169500          0.          0.3480000
100.0000          0.          0.

```

3360.000	500000.0	2.9300000E-03	5.000000	1.000000
15				
0.	0.	0.		
0.	0.	0.3380000		
7.5999998E-02	1.138000	0.3380000		
0.1270000	1.242000	0.4970000		
0.2540000	1.038000	0.5010000		
0.3810000	1.064000	0.5380000		
0.5080000	1.058000	0.5770000		
0.5850000	1.060000	0.5780000		
0.6350000	0.8730000	0.2710000		
0.7620000	0.6260000	0.2670000		
1.017000	0.5650000	0.3340000		
1.525000	0.3740000	0.2910000		
2.287000	0.2390000	0.1630000		
3.636022	0.	0.1630000		
100.0000	0.	0.		

5516.000	500000.0	1.7900000E-03	5.000000	1.000000
15				
0.	0.	0.		
0.	0.	0.2610000		
8.2999997E-02	1.180000	0.2610000		
0.1240000	1.494000	0.4660000		
0.2070000	1.444000	0.5040000		
0.4150000	1.437000	0.5860000		
0.6220000	1.392000	0.6980000		
0.8300000	1.535000	0.7440000		
0.9130000	1.317000	0.3790000		
1.037000	0.5440000	0.1670000		
1.245000	0.3690000	0.1340000		
1.660000	0.2440000	0.2290000		
2.490000	0.1300000	0.2130000		
3.436491	0.	0.2130000		
100.0000	0.	0.		

16836.00	500000.0	5.9000001E-04	5.000000	1.000000
12				
0.	0.	0.		
0.	0.	0.1760000		
0.2540000	3.592000	0.1760000		
0.6350000	3.374000	0.1160000		
1.271000	5.369000	0.1610000		
1.906000	5.027000	0.2650000		
2.542000	2.997000	0.2400000		
3.177000	0.6720000	0.3780000		
3.812000	0.4200000	0.4210000		
5.083000	0.1870000	0.3210000		
6.103073	0.	0.3210000		
100.0000	0.	0.		

C.3 Image Analysis

This section contains the Fortran source code for three image analysis programs (described in Chapter 6): PROPERTIES, CORRELATION and PDF. All programs were compiled with Microsoft Fortran compiler, and run on a 486DX/33 personal computer. Subroutines and functions that are used by more than one program are only listed in the first program in which they appear.

The nomenclature of computer files in image analysis is as follows:

- * Raw data files are named HXY_{YY}_ZZ.RDF or VXY_{YY}_ZZ.RDF, where H or V stands for horizontal or vertical (location), X is the setup number¹, YY is the run number, and ZZ the time (in seconds). For times over 99 seconds, ZZ is replaced by 1ZZ, etc. For example, the file H311_20.RDF contains the digitized image of setup 3 in the horizontal transition section ($Re = 5.5 \cdot 10^3$), run 11, at 20 seconds. V406240.RDF contains the image of vertical setup 4 ($Re = 1.7 \cdot 10^3$), run 6, at 240 seconds.
- * Processed data files are named LINHX_ZZ.DAT or LINVX_ZZ.DAT. So, the processed pixel values of setup 1 in the vertical transition section, at 60 seconds (from all runs), can be found in the file LINV1_60.DAT. The corresponding file with ensemble average pixel values and ensemble standard deviation is named STAHX_ZZ.DAT or STAVX_ZZ.DAT.
- * Files containing pixel value histograms, correlation curves and scales of segregation, or scalar spectra, have the same naming convention as processed data files, with one letter signifying the information being contained, as follows:

C	spatial correlation curve and scale of segregation
P	pixel value histogram
S	scalar spectrum (positive correlation only)
T	scalar spectrum (total, including negative correlation. Results not presented in dissertation)

Example: PV3_20.DAT contains the pixel value histogram of setup 3, vertical, at 20 seconds.

Setup (run) numbers and times of input files to any program are entered interactively when running the program. Names for corresponding output files are created by the programs. For change between vertical and horizontal transition section, and for times over 99 seconds, it is necessary to modify the appropriate characters in the program listing and re-compile.

¹ The relation between setup number and Re is given in Tables 7-1 and 7-2.

idir direction of laser line in image; idir = 2 always.
i1 i_{min},
j1 j_{min},
i1 i_{max},
j1 j_{max}, all from Table 7-3.
itype type of processed pixel value (maximum or total); itype = 1 always.

```

c cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c This program copies columns (or rows) from NFILE input files
c (raw data files VXYY_ZZ.RDF) into the output file LINVX_ZZ.DAT.
c The elements that get transferred to the output file are maxima
c or totals in a specified window of each row (column).
c Each raw data file is filtered prior to the copying process.
c The average and standard deviation of every point along the
c line and the total average and standard deviation are written
c to the file STAVX_ZZ.DAT.
c
c last revised: October, 1993
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c Declarations; clear arrays.
c
c     external int chr, filpv
c     parameter (nfilemax = 20)
c     common /window/ idir, mlo, mhi, itype
c     character*2 filenr
c     character*12 infile, outfile, stafile
c     dimension pav(320), psq(320)
c
c Specify raw data files
c open output file and statistics file.
c
c     infile = 'VXYY_ZZ.RDF'
c     outfile= 'LINVX_ZZ.DAT'
c     stafile= 'STAVX_ZZ.DAT'
c     print *, 'specify raw data files:'
c     print *, 'number of files = (max 20)'
c     read *, nfile
c     print *, 'setup number (X)'
c     read *, nsetup
c     print *, 'timenumber (ZZ)'
c     read *, ntime
c     filenr = int_chr(nsetup)
c     infile(2:2) = filenr(2:2)
c     outfile(5:5) = filenr(2:2)
c     stafile(5:5) = filenr(2:2)
c     filenr = int_chr(ntime)

```

```

        infile (6:7) = filenr
        outfile(7:8) = filenr
        stafile(7:8) = filenr
        open (unit=20, file=outfile, status='new')
        open (unit=21, file=stafile, status='new')
c
c      Initialize parameters:
c      specify region of interest and filter options.
c      Write headers of output files.
c      clear arrays for statistics.
c
        call domini (nlo, nhi)
        ncell = nhi-nlo+1
        write (20,1000) nfile, ncell, nlo
        write (21,1100) nfile
        do 10 icell = nlo, nhi
            pav(icell) = 0.
            psq(icell) = 0.
10      continue
        ptav = 0.
        ptsq = 0.
c
c      For every raw data file, every cell (along line):
c      determine maximum (or total) in window;
c      write to output file;
c      add to average and variance.
c
        do 100 ifile = 1, nfile
            print *, 'run # (YY)'
            read *, irun
            filenr = int_chr(irun)
            infile (3:4) = filenr
            open (unit=10, file=infile, status='old', recl=1,
&             form='binary', access='direct')
            print *, infile, ' now opened'
            do 50 icell = nlo, nhi
                call value (icell, cv)
                nv = nint(cv)
                write (20,*) nv
                pav(icell) = pav(icell) + cv
                psq(icell) = psq(icell) + cv*cv
                ptav = ptav + cv
                ptsq = ptsq + cv*cv
50          continue
            close (10)
100      continue
c
c      Write out statistics.
c      End of main program.
c
        ktot=0
        do 110 icell = nlo, nhi
            pav(icell) = pav(icell)/float(nfile)
            psq(icell) = (psq(icell) - float(nfile)
&             *pav(icell)**2) / float(nfile-1)
            psq(icell) = sqrt(psq(icell))
            write (21,1300) icell, pav(icell), psq(icell)
110      continue
        ptav = ptav/float(nfile*(nhi-nlo+1))
        ptsq = ptsq/float(nfile*(nhi-nlo+1))

```

```

c      subroutine domini (nlo, nhi)
c
c      Specify region of interest in raw data files:
c      horizontal or vertical lines;
c      first and last location along line: NLO, NHI;
c      first and last location across line
c      ("window"): MLO, MHI
c      Specifications are read from file WINDOW.DAT
c
      common /window/ idir, mlo, mhi, itype
      open (unit = 2, file='window.dat', status='old')
      read (2,*) idir
      read (2,*) i1
      read (2,*) j1
      read (2,*) i2
      read (2,*) j2
      read (2,*) itype
      close (2)
      if (idir .eq. 1) then
         nlo = j1
         nhi = j2
         mlo = i1
         mhi = i2
      else
         nlo = i1
         nhi = i2
         mlo = j1
         mhi = j2
      endif
      return
      end

```

```

c      subroutine value (icell, cv)
c
c      Determine the value of element ICELL in the currently
c      open raw data file. This value is the maximum over the
c      specified window (after filtering), or the total,
c      depending on the value of itype.
c
c      common /window/ idir, mlo, mhi, itype
c      cv = 0.
c      do 100 iwin = mlo, mhi
c      .      if (idir .eq. 1) then
c              jp = icell
c              ip = iwin

```

```

        else
            ip = icell
            jp = iwin
        endif
        cvc = filpv(ip,jp)
        if (itype .eq. 1) then
            cv = max(cv, cvc)
        else
            cv = cv + cvc
        endif
    continue
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

function filpv(ip,jp)
C
C Return the filtered pixelvalue at location (ip,jp)
fpv = pv(i,j) + pv(i,j+1) + pv(i,j+2) + pv(i,j+3) -
      pv(i,j-3) - pv(i,j-2) -pv(i,j+5) - pv(i,j+6)
C
dimension n(8)
do 2 k=1,4
call getpix(10,ip,jp+k-1,n(k))
2 continue
call getpix(10,ip,jp-3,n(5))
call getpix(10,ip,jp-2,n(6))
call getpix(10,ip,jp+5,n(7))
call getpix(10,ip,jp+6,n(8))
filpv = float(n(1) + n(2) + n(3) + n(4)
& - n(5) - n(6) - n(7) - n(8))
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

subroutine getpix (nunit, i, j, npix)
C
C This subroutine gets the pixelvalue at location (i,j) in a
C 320 X 200 raw data file (1 byte numbers)
integer*1 nraw
loc = i+320*j+1
read(nunit, rec=loc) nraw
npix = int2(nraw)
if (npix .lt. 0) npix=npix+256
return
end

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

function int_chr(nn)
C
C This function translates an integer number
C (00 < nn < 99) into a character*2 variable.
character*2 cv
nh = nn/10
nl = nn-10*nh
```



```

sav = 0.
do 50 icol = 1, ncol
    do 40 irow = 1, nrow
        read (1,*) npv(icol,irow)
        sav = sav + npv(icol,irow)
40    continue
50    continue
sav = sav/float(ncol*nrow)
print *, 'average pixelvalue =', sav

c
c    calculate correlation coefficient for each distance,
c    and integral, scale of segregation
c    write results to output file, and store
c

    cint1 = 0.
    cint2 = 0.
    call corco(0, cc, icount)
    r0 = cc
do 150 idis = 0,mdis
    call corco(idis, cc, icount)
    cint1 = cint1 + cc
    cp = cc
    if (cp .lt. 0.) cp = 0.
    cint2 = cint2 + cp
    write (10,1300) idis, cc
    ct(idis) = cc
150    continue
    write (10,*) 'time=', ntime
    write (10,*) 'S =', cint1/r0
    write (10,*) 'Sp=', cint2/r0

c
c    calculate scalar spectra, both from total and positive-only
c    correlation functions
c

    print *, 'calculating spectra...'
    wn = 0.005
    do while (wn .lt. 2*pi)
        call spectrum (wn, ct, st, sp)
        write (11,*) wn, st
        write (12,*) wn, sp
        wn = wn*1.1
    enddo

c
c    formats and end of program
c
1000 format (2i5)
1300 format (i10,'          ',f10.4, i10)
    close (1)
    close (10)
    close (11)
    close (12)
    stop
end

cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

    subroutine corco(idis, cc, icount)

c
c    determine the correlation coeff. at spacing of IDIS pixels
c    in every column, with spacing of NSKIP between samples

```



```

c      parameter (nrmax=320, ncmax=100, nskip=1)
common /pix/ npv(ncmax,nrmax), sav, ncol, nrow
icount = 0
cc = 0.
do 100 icol = 1, ncol
    irow = 1
    do while (irow .lt. (nrow-idis))
        icount = icount + 1
        s1 = npv(icol,irow)
        s2 = npv(icol,irow+idis)
        cc = cc + (s1-sav)*(s2-sav)
        irow = irow + nskip
    enddo
100 continue
if (icount .eq. 0) icount = 1
cc = cc/float(icount)
return
end

cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      subroutine spectrum (wn, ct, st, sp)
c
c      calculate value of 1-D spectrum for current wavenumber
c
      parameter (mdis=200)
      dimension ct(0:mdis)
      st = 0.
      sp = 0.
      do 10 idis=1,mdis
          ds = ct(idis)/ct(0)*cos(wn*idis)
          st = st + ds
          if (ct(idis) .gt. 0) sp = sp + ds
10      continue
      return
      end

*****

      program PDF

cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c
c      This program calculates a PDF for pixelvalue, from
c      input file LINVX_ZZ.DAT. The number of bins (NBIN)
c      and number of pixels per bin (NPB) are specified in
c      the parameter declaration. The calculated PDF is
c      written to the file PVX_ZZ.DAT
c
c      Last revised: February 1994
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c
c      declaration of parameters, etc.
c
      parameter (nbin=40, npb=10)
      character*12 infile, outfile
      character*2 filenr

```

```

        dimension npdf(nbin)
c
c      open files;
c      read input parameters
c
        infile = 'LINVX ZZ.DAT'
        outfile = 'PVX ZZ.DAT'
        print *, 'setup number ?'
        read *, nsetup
        print *, 'time number ?'
        read *, ntime
        filenr = int_chr(nsetup)
        infile(5:5) = filenr(2:2)
        outfile(3:3) = filenr(2:2)
        filenr = int_chr(ntime)
        infile(7:8) = filenr(1:2)
        outfile(5:6) = filenr(1:2)
        open (unit=1, file=infile, status='old')
        open (unit=10, file=outfile, status='new')
        print *, 'created file', outfile
        read (1,1000) ncol, nrow
        print *, ncol, nrow
c
c      clear PDF array
c
        do 10 ibin=1,nbin
            npdf(ibin) = 0
10      continue
c
c      read elements and do bin count
c
        do 30 icol=1,ncol
            do 20 irow=1,nrow
                read (1,*) npv
                ibin = npv/npb
                if (ibin .gt. nbin) ibin = nbin
                if (ibin .eq. 0) ibin = 1
                npdf(ibin) = npdf(ibin) + 1
20          continue
30      continue
c
c      print out results
c      formats and end of program
c
        do 50 ibin=1,nbin
            write (10,*) ibin*npb, npdf(ibin)
50      continue
1000  format (2i5)
        close (1)
        close (10)
        stop
        end

```

APPENDIX D

EXPERIMENTAL DATA

D.1 Cross-stream Average Pixel Value and Standard Deviation

Table D-1: Cross-stream average pixel value and standard deviation.
Horizontal transition section, $Re = 2.0 \times 10^3$.

time (sec)	PV	pv'	dPV/dt	pv' corrected
5	47	70	47	69
7	75	94	13	94
10	110	119	13	119
15	182	124	9	124
20	197	136	-2	136
30	145	102	-5	102
40	95	93	-3	93
60	63	72	-1	72
90	53	60	0	60
120	37	45	0	45
180	33	37	0	37

Table D-2: Cross-stream average pixel value and standard deviation.
Horizontal transition section, $Re = 3.4 \times 10^3$

time (sec)	PV	pv'	dPV/dt	pv' corrected
3	81	107	81	104
5	124	120	4	120
10	106	101	-1	101
15	115	103	2	103
20	122	101	1	101
23	123	102	-14	101
25	53	76	-12	76
30	40	55	-1	55
40	44	54	0	54
60	29	36	-1	36
90	16	20	0	20

Table D-3: Cross-stream average pixel value and standard deviation.
Horizontal transition section, $Re = 5.5 \cdot 10^3$

time (sec)	PV	pv'	dPV/dt	pv' corrected
2	70	108	70	106
3	146	151	28	151
5	152	146	4	146
10	175	144	5	144
15	201	130	6	130
20	234	136	-13	136
22	107	130	-41	130
25	27	44	-11	44
30	19	29	0	29
40	20	24	0	24
60	14	14	0	14

Table D-4: Cross-stream average pixel value and standard deviation.
Horizontal transition section, $Re = 1.7 \cdot 10^4$.

time (sec)	PV	pv'	dPV/dt	pv' corrected
2	35	61	35	60
5	25	48	1	48
10	44	85	4	85
15	64	95	-1	95
20	38	56	-4	56
25	19	17	-2	17
30	16	13	-1	13
40	11	8	0	8

Table D-5: Cross-stream average pixel value and standard deviation.
Vertical transition section, $Re = 1.7 \times 10^3$.

time (sec)	PV	pv'	dPV/dt	pv' corrected
20	20	25	20	24
22	27	38	6	38
25	48	63	6	63
30	74	82	6	82
35	106	91	5	91
40	128	101	3	101
50	150	83	0	83
60	134	75	-2	75
90	81	58	-1	58
120	59	50	0	50
180	38	39	0	39
240	29	34	0	34

Table D-6: Cross-stream average pixel value and standard deviation.
Vertical transition section, $Re = 3.4 \times 10^3$.

time (sec)	PV	pv'	dPV/dt	pv' corrected
14	42	63	42	62
16	112	112	22	112
20	171	96	7	96
25	178	103	6	103
30	229	95	3	95
35	205	83	-6	83
40	172	77	-6	77
50	116	68	-4	68
60	85	59	-2	59
90	49	44	-1	44
120	32	34	0	34
180	18	23	0	23

Table D-7: Cross-stream average pixel value and standard deviation.
Vertical transition section, $Re = 5.5 \times 10^3$.

time (sec)	PV	pv'	dPV/dt	pv' corrected
8	17	21	17	21
10	54	53	18	52
12	90	60	13	60
15	120	65	9	65
20	165	66	4	66
30	181	61	-4	61
35	101	54	-11	54
40	71	47	-3	47
50	54	40	-2	40
60	40	36	-1	36
90	21	21	0	21
120	14	13	0	13

Table D-8: Cross-stream average pixel value and standard deviation.
Vertical transition section, $Re = 1.6 \times 10^4$.

time (sec)	PV	pv'	dPV/dt	pv' corrected
5	15	12	15	11
6	21	17	6	17
8	31	24	6	24
10	43	27	5	27
15	67	31	5	31
20	90	35	2	35
25	85	35	-3	35
30	57	29	-5	29
35	37	24	-3	24
40	29	20	-1	20
50	18	12	-1	12
60	13	9	0	9

D.2 Ensemble Average Pixel Value and Standard Deviation

The following figures contain ensemble average pixel values and ensemble standard deviations, as functions of both time and cross-stream position. Each figure represents a setup. In the horizontal transition section, location 0 is closest to the top of the duct, and 300 near the bottom. In the vertical transition section, location 0 is facing away from the kiln cavity (see Figure 7-3).

Figure D-1: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 2.0 \cdot 10^3$.

Figure D-2: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 3.4 \cdot 10^3$.

Figure D-3: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 5.5 \cdot 10^3$.

Figure D-4: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Horizontal transition section, $Re = 1.7 \cdot 10^4$.

Figure D-5: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 1.7 \cdot 10^3$.

Figure D-6: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 3.4 \cdot 10^3$.

Figure D-7: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 5.5 \cdot 10^3$.

Figure D-8: Ensemble average pixelvalue (top); ensemble standard deviation (bottom). Vertical transition section, $Re = 1.6 \times 10^4$.

D.3 Probability Density Functions

The following figures contain experimentally determined pixel value histograms. Each figure consists of eight histograms, representing different times in a single setup. A single histogram contains the processed pixel values (Chapter 6.2) of all runs and all cross-stream locations, for a given setup and time. Each bin in the histograms represents ten adjacent pixel values; values over 400 have been discarded. A height of 10 mm corresponds to a count of 200; counts over 800 are not shown. To convert from pixel value to concentration, use eqn. (7-1). To determine probability, multiply the bin height (in mm) by 20, and divide by the total number of observations, given in Table D-9.

Figure D-9: Pixel value histograms. Horizontal transition section, $Re = 2.0 \times 10^3$.

Figure D-10: Pixel value histograms. Horizontal transition section, $Re = 3.4 \times 10^3$.

Figure D-11: Pixel value histograms. Horizontal transition section, $Re = 5.5 \times 10^3$.

Figure D-12: Pixel value histograms. Horizontal transition section, $Re = 1.7 \times 10^4$.

Figure D-13: Pixel value histograms. Vertical transition section, $Re = 1.7 \times 10^3$.

Figure D-14: Pixel value histograms. Vertical transition section, $Re = 3.4 \times 10^3$.

Figure D-15: Pixel value histograms. Vertical transition section, $Re = 5.5 \cdot 10^3$.

Figure D-16: Pixel value histograms. Vertical transition section, $Re = 1.6 \cdot 10^4$.

D.4 Spatial Correlation Functions and Scale of Segregation

The following figures contain experimentally determined spatial correlation curves and scales of segregation (in pixels), at different times in each setup. All correlation curves have been normalized with $R(0)$, the RMS pixelvalue fluctuations for that particular setup and time.

Figure D-17: Spatial correlation function and scale of segregation. Horizontal transition section, $Re = 2.0 \cdot 10^3$.

Figure D-18: Spatial correlation function and scale of segregation. Horizontal transition section, $Re = 3.4 \times 10^3$.

Figure D-19: Spatial correlation function and scale of segregation. Horizontal transition section, $Re = 5.5 \times 10^3$.

Figure D-20: Spatial correlation function and scale of segregation. Horizontal transition section, $Re = 1.7 \cdot 10^4$.

Figure D-21: Spatial correlation function and scale of segregation. Vertical transition section, $Re = 1.7 \times 10^3$.

Figure D-22: Spatial correlation function and scale of segregation. Vertical transition section, $Re = 3.4 \times 10^3$.

Figure D-23: Spatial correlation function and scale of segregation. Vertical transition section, $Re = 5.5 \cdot 10^3$.

Figure D-24: Spatial correlation function and scale of segregation. Vertical transition section, $Re = 1.6 \times 10^4$.

Table D-9: Characteristics of mixing, including 95% confidence intervals for average concentration and RMS fluctuations

horizontal transition section; Re = 2.0e+3				3906 observations			tau = 66.48 sec.			
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
5	0.08	16.20	21.50	182	0.083	0.061	0.105	0.1404	0.1273	0.1565
7	0.11	4.16	16.21	241	0.144	0.119	0.170	0.1951	0.1791	0.2143
10	0.15	21.94	29.01	135	0.220	0.177	0.265	0.2485	0.2219	0.2823
15	0.23	17.02	27.51	142	0.375	0.331	0.420	0.2606	0.2334	0.2951
20	0.30	32.32	35.86	109	0.408	0.353	0.464	0.2857	0.2521	0.3296
30	0.45	25.08	26.50	147	0.295	0.260	0.331	0.2129	0.1911	0.2405
40	0.60	27.31	30.29	129	0.187	0.153	0.223	0.1934	0.1723	0.2204
60	0.90	19.88	26.55	147	0.118	0.093	0.144	0.1483	0.1331	0.1675
90	1.35	14.73	19.72	198	0.096	0.078	0.114	0.1223	0.1113	0.1357
120	1.81	9.59	15.37	254	0.060	0.049	0.072	0.0887	0.0816	0.0971
180	2.71	5.19	12.06	324	0.053	0.045	0.062	0.0721	0.0669	0.0781
horizontal transition section, Re = 3.4e+3				4336 observations			tau = 39.35 sec.			
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
3	0.08	32.23	35.93	121	0.260	0.193	0.329	0.3640	0.3231	0.4167
5	0.13	24.76	30.22	143	0.418	0.349	0.489	0.4201	0.3764	0.4752
10	0.25	10.75	21.52	201	0.352	0.303	0.402	0.3509	0.3196	0.3889
15	0.38	10.93	17.89	242	0.387	0.342	0.434	0.3587	0.3294	0.3939
20	0.51	-1.05	14.37	302	0.412	0.372	0.454	0.3534	0.3273	0.3841
23	0.58	21.59	27.24	159	0.415	0.360	0.472	0.3541	0.3190	0.3980
25	0.64	5.18	17.09	254	0.160	0.127	0.194	0.2622	0.2412	0.2873
30	0.76	4.32	20.71	209	0.113	0.087	0.140	0.1871	0.1707	0.2070
40	1.02	17.73	26.16	166	0.128	0.100	0.158	0.1804	0.1629	0.2022
60	1.52	6.13	11.37	381	0.074	0.062	0.087	0.1151	0.1074	0.1239
90	2.29	15.38	20.86	208	0.026	0.018	0.036	0.0596	0.0544	0.0660

Table D-9 (continued)

horizontal transition section; Re = 5.5e+3 4950 observations tau = 24.10 sec.										
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
2	0.08	7.35	22.15	224	0.355	0.275	0.438	0.5975	0.5467	0.6587
3	0.12	33.48	38.64	128	0.803	0.654	0.956	0.8592	0.7653	0.9796
5	0.21	32.16	32.68	151	0.839	0.706	0.975	0.8322	0.7479	0.9382
10	0.41	26.34	27.68	179	0.972	0.852	1.095	0.8161	0.7394	0.9107
15	0.62	17.45	20.69	239	1.121	1.027	1.217	0.7366	0.6760	0.8093
20	0.83	14.41	25.66	193	1.318	1.209	1.430	0.7722	0.7021	0.8581
22	0.91	64.31	67.53	73	0.575	0.405	0.749	0.7363	0.6333	0.8795
25	1.04	16.59	26.27	188	0.105	0.072	0.142	0.2343	0.2128	0.2607
30	1.24	7.86	20.03	247	0.057	0.039	0.078	0.1450	0.1333	0.1591
40	1.66	7.58	17.14	289	0.065	0.051	0.081	0.1184	0.1094	0.1289
60	2.49	15.84	17.12	289	0.032	0.025	0.042	0.0613	0.0567	0.0668
horizontal transition section; Re = 1.7e+4 5040 observations tau = 7.87 sec.										
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
2	0.25	13.53	31.21	161	0.463	0.306	0.632	1.0041	0.9052	1.1274
5	0.64	19.25	29.83	169	0.289	0.169	0.419	0.7950	0.7183	0.8902
10	1.27	22.47	37.73	134	0.635	0.389	0.893	1.4498	1.2943	1.6481
15	1.91	32.57	50.31	100	0.978	0.659	1.311	1.6296	1.4309	1.8928
20	2.54	11.31	29.79	169	0.528	0.387	0.681	0.9403	0.8497	1.0528
25	3.18	8.83	21.67	233	0.187	0.156	0.227	0.2395	0.2195	0.2635
30	3.81	18.41	21.84	231	0.130	0.110	0.159	0.1525	0.1398	0.1679
40	5.08	8.62	13.99	360	0.044	0.037	0.058	0.0641	0.0597	0.0691

Table D-9 (continued)

vertical transition section; Re = 1.7e+3				2835 observations			tau = 77.12 sec.			
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
20	0.26	17	18	157	0.011	0.008	0.014	0.0208	0.0187	0.0234
22	0.29	10	13	212	0.018	0.014	0.023	0.0347	0.0317	0.0384
25	0.32	31	32	89	0.040	0.027	0.052	0.0609	0.0531	0.0714
30	0.39	25	27	105	0.067	0.052	0.082	0.0805	0.0709	0.0932
35	0.45	24	27	105	0.100	0.083	0.117	0.0896	0.0789	0.1037
40	0.52	25	27	104	0.123	0.104	0.142	0.1004	0.0883	0.1163
50	0.65	18	20	144	0.146	0.133	0.159	0.0814	0.0730	0.0920
60	0.78	24	24	117	0.130	0.116	0.143	0.0729	0.0646	0.0837
90	1.17	17	18	153	0.075	0.066	0.084	0.0554	0.0498	0.0624
120	1.56	7	12	235	0.051	0.045	0.057	0.0475	0.0436	0.0523
180	2.33	3	10	280	0.030	0.026	0.034	0.0364	0.0336	0.0397
240	3.11	3	7	399	0.021	0.017	0.024	0.0314	0.0293	0.0337
vertical transition section; Re = 3.4e+3				4410 observations			tau = 39.35 sec.			
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
14	0.36	16.17	19.79	223	0.067	0.051	0.082	0.1159	0.1061	0.1278
16	0.41	23.20	42.27	104	0.207	0.165	0.249	0.2164	0.1905	0.2505
20	0.51	17.23	19.43	227	0.326	0.302	0.351	0.1854	0.1698	0.2042
25	0.64	32.89	32.94	134	0.339	0.305	0.373	0.1999	0.1785	0.2272
30	0.76	14.34	18.80	235	0.443	0.420	0.467	0.1826	0.1675	0.2009
35	0.89	5.41	10.24	431	0.393	0.378	0.408	0.1588	0.1489	0.1702
40	1.02			200	0.328	0.307	0.350	0.1465	0.1334	0.1624
50	1.27	18.31	19.37	228	0.215	0.198	0.232	0.1285	0.1177	0.1416
60	1.52	6.97	9.59	460	0.154	0.144	0.164	0.1102	0.1035	0.1178
90	2.29	1.48	6.04	730	0.081	0.075	0.087	0.0796	0.0757	0.0839
120	3.05	3.26	7.46	591	0.046	0.042	0.051	0.0604	0.0571	0.0641
180	4.57	4.95	10.04	439	0.017	0.014	0.021	0.0376	0.0353	0.0403

Table D-9 (concluded)

vertical transition section; Re = 5.5e+3				4410 observations			tau = 24.10 sec.			
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
8	0.33	22	22	197	0.025	0.017	0.032	0.0536	0.0488	0.0595
10	0.41	32	34	128	0.144	0.117	0.171	0.1563	0.1393	0.1782
12	0.50	14	20	219	0.262	0.238	0.286	0.1812	0.1657	0.2000
15	0.62	21	26	171	0.358	0.329	0.387	0.1963	0.1775	0.2196
20	0.83	14	22	201	0.504	0.476	0.531	0.2000	0.1822	0.2217
30	1.24	28	29	155	0.556	0.526	0.585	0.1856	0.1670	0.2089
35	1.45	15	16	277	0.299	0.279	0.318	0.1617	0.1492	0.1764
40	1.66	4	9	510	0.199	0.187	0.211	0.1375	0.1295	0.1465
50	2.07	8	10	430	0.146	0.134	0.157	0.1175	0.1102	0.1260
60	2.49	-0	5	805	0.102	0.095	0.109	0.1040	0.0991	0.1093
90	3.73	3	7	637	0.039	0.035	0.043	0.0559	0.0530	0.0592
120	4.98	3	9	498	0.015	0.013	0.018	0.0281	0.0265	0.0300
vertical transition section; Re = 1.6e+4				4410 observations			tau = 8.13 sec.			
time sec.	t/tau	scale of segregation		# indep. observ.	C/C_0			c'/C_0		
		(total)	(pos.)		estimate	low	high	estimate	low	high
5	0.61	12	13	328	0.057	0.049	0.065	0.0677	0.0629	0.0734
6	0.74	13	15	288	0.112	0.098	0.126	0.1230	0.1138	0.1340
8	0.98	28	28	159	0.217	0.187	0.247	0.1908	0.1719	0.2144
10	1.23	18	19	236	0.331	0.302	0.360	0.2241	0.2055	0.2464
15	1.84	8	11	389	0.561	0.535	0.587	0.2595	0.2425	0.2792
20	2.46	5	11	390	0.779	0.749	0.808	0.3010	0.2812	0.3238
25	3.07	3	10	450	0.733	0.705	0.761	0.3035	0.2849	0.3247
30	3.69	7	11	417	0.463	0.440	0.486	0.2417	0.2264	0.2594
35	4.30	2	8	529	0.272	0.256	0.289	0.1970	0.1858	0.2097
40	4.92	2	7	593	0.195	0.182	0.207	0.1518	0.1436	0.1610
50	6.15	2	6	706	0.085	0.080	0.090	0.0731	0.0694	0.0771
60	7.38	1	7	633	0.043	0.039	0.047	0.0486	0.0460	0.0514

APPENDIX E

CALIBRATION ROTAMETER

The rotameter that controls the flow of the puff into the cold flow model was calibrated, by monitoring the flowrate at different rotameter readings and different pressures. A stopwatch and wet test meter were used in the calibration process. The results are presented in Table E-1.

From regression of the data, we determined the following relation (see Figure E-1):

$$Q = 0.01156(\text{rotameter reading})\sqrt{p+13.5} + 0.426 \quad (\text{E-1})$$

where Q is in scfm, and p in psig.

Table E-1: Calibration data.

p (psig)	rotameter reading	Q (scfm)
40	5	0.92
73	4	1.11
40	11	1.22
79	12	1.97
59	22	2.55
79	25	3.24
58	30	3.53
97	30	4.14
76	40	3.83
55	50	5.00
73	55	6.49
92	60	7.83
70	70	8.00

Figure E-1: Calibration curve for rotameter puff flow.

APPENDIX F

LIST OF SYMBOLS AND ABBREVIATIONS

C	concentration (mol/m^3); mol fraction
c	concentration fluctuation
D	diffusivity (without subscript: molecular diffusivity)
d	diameter
Da	Damköhler number = $L/\tau u'$
F	one-dimensional scalar spectrum
FPV	filtered pixel value
Gr	Grashof number
g	gravitational acceleration
$\mathfrak{S}$	intensity of segregation
K	proportionality constant, relating concentration to pixel value
k	kinetic energy of fluctuations (m^2s^{-2}); wave number (m^{-1} or pix^{-1}); Boltzmann constant
L	large eddy size
l	(small) eddy size or length scale
M	number of runs in a setup; number of groups (Appendix B)
m	molar flux; ratio of flowrates or momentum flowrates; particle mass density
N	step frequency (s^{-1}); number of points along laser line; number of observations in group (Appendix B)
n	particle number density
P	probability in probability density function
p	pressure
PDF	probability density function
PPV	processed pixel value
Pr	Prandtl number = ν/α
PV	cross-stream average (processed) pixel value
pv'	cross stream standard deviation (processed) pixel value
Q	volumetric flowrate
q	empirical fitting parameter in eddy size
R	radius; auto-correlation function

r	radial position; separation distance in spatial correlation function; random number ($0 < r < 1$)
Re	Reynolds number = Ud/ν
RMS	root mean square
RPV	raw (i.e. un-processed) pixel value
S	scale of segregation (m or pix)
Sc	Schmidt number = ν/D
SR	stoichiometric ratio
St	Strouhal number = t_{puff}/τ
T	temperature
t	time
U	velocity
u	velocity fluctuation or eddy velocity
UOD	unsatisfied oxygen demand
V	volume
ν	radial velocity fluctuation
W	window for tapering auto-correlation function
x	position; dimensionless radial position
Z	downstream position; length of simulation domain
z	step size
α	thermal diffusivity
β	thermal coefficient of expansion
γ	extinction coefficient
ϵ	energy dissipation rate (m^2s^{-3})
ζ	concentration coefficient of expansion
κ	Von Karman constant
Λ	dimensionless linear eddy frequency
λ	linear eddy frequency ($\text{m}^{-1}\text{s}^{-1}$)
μ	dynamic viscosity
ν	kinematic viscosity; stoichiometric coefficient
ξ	position
ρ	density
σ	standard deviation
τ	specific time or residence time
ϕ	volume fraction

Superscripts:

—	average
'	root mean square
l	derivative

Subscripts:

*	friction
0	initial or inlet
a	air
B	Batchelor; Brownian; between groups (Appendix B)
b	block inversions
C	Corrsin
c	concentration
i	coordinate index; inertia
j	coordinate index
K	Kolmogorov
L	large eddy
o	oxygen
p	particle
R	recirculation zone
s	settling
T	turbulent total (Appendix B)
t	temperature
W	within groups (Appendix B)

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