Contents

Preface XIX List of Contributors XXI

- **1 Computational Fluid Dynamics: the future in safety technology!** *1 Jürgen Schmidt*
- 2 Organized by ProcessNet: Tutzing Symposion 2011 CFD its Future in Safety Technology' 5 Norbert Pfeil

2.1 ProcessNet – an Initiative of DECHEMA and VDI-GVC 5

- 2.1.1 The ProcessNet Safety Engineering Section 6
- 2.2 A Long Discussed Question: Can Safety Engineers Rely on Numerical Methods? 7

3 CFD and Holistic Methods for Explosive Safety and Risk Analysis 9

- Arno Klomfass and Klaus Thoma
- 3.1 Introduction 9
- 3.2 Deterministic and Probabilistic Design Tasks *11*
- 3.3 CFD Applications on Explosions and Blast Waves 12
- 3.4 Engineering Methods: The TNT Equivalent 22
- 3.5 QRA for Explosive Safety 25
- 3.6 Summary and Outlook 27 References 28

Part One CFD Today – Opportunities and Limits if Applied to Safety Techology 31

- 4 Status and Potentials of CFD in Safety Analyses Using the Example of Nuclear Power 33 Horst-Michael Prasser
- 4.1 Introduction 33
- 4.2 Safety and Safety Analysis of Light Water Reactors 33
- 4.3 Role and Status of Fluid Dynamics Modeling 36

IX

X Contents

4.4	Expected Benefits of CFD in Nuclear Reactor Safety 37
4.5	Challenges 40
4.6	Examples of Applications 42
4.6.1	Deboration Transients in Pressurized Water Reactors 42
4.6.2	Thermal Fatigue Due to Turbulent Mixing 47
4.6.3	Pressurized Thermal Shock 49
4.7	Beyond-Design-Based Accidents 53
4.7.1	Hydrogen Transport, Accumulation, and Removal 53
4.7.2	Aerosol Behavior 59
4.7.3	Core Melting Behavior 60
	References 66
Part Two	Computer or Experimental Design? 69
5	Sizing and Operation of High-Pressure Safety Valves 71
	Jürgen Schmidt and Wolfgang Peschel
5.1	Introduction 71
5.2	Phenomenological Description of the Flow through a
	Safety Valve 71
5.3	Nozzle/Discharge Coefficient Sizing Procedure 72
5.3.1	Valve Sizing According to ISO 4126-1 73
5.3.2	Limits of the Standard Valve Sizing Procedure 74
5.3.3	Valve Sizing Method for Real Gas Applications 74
5.3.4	Numerical Sizing of Safety Valves for Real Gas Flow 77
5.3.5	Equation of State, Real Gas Factor, and Isentropic Coefficient
	for Real Gases 78
5.3.6	Comparison of the Nozzle Flow/Discharge Coefficient
	Models 80
5.4	Sizing of Safety Valves Applying CFD 82
5.4.1	High Pressure Test Facility and Experimental Results 82
5.4.2	Numerical Model and Discretization 86
5.4.3	Numerical Results 87
5.5	Summary 90
	References 93
6	Water Hammer Induced by Fast-Acting Valves – Experimental Studies, 1D
	Modeling, and Demands for Possible Future CFX Calculations 95
	Andreas Dudlik and Robert Fröhlich
6.1	Introduction 95
6.2	Multi-Phase Flow Test Facility 97
6.3	Extension of Pilot Plant Pipework PPP for Software
	Validation 99
6.4	Experimental Set-Up 99
6.5	Experimental Results 100
6.5.1	Experimental Results – Thermohydraulics 100

Contents XI

- 6.6 2 Case Studies of Possible Future Application of CFX 103
- 1D Modeling of Kaplan Turbine Failure 105 6.6.1
- Simulation Results Closing Time 10 s, Linear 105 6.6.2
- Possible Chances and Difficulties in the Use of CFX for 6.7 Water Hammer Calculations 106
- Benchmark Test for Influence of Numerical Diffusion in 6.7.1 Water Hammer Calculations 107
- CFD The Future of Safety Technology? 109 6.8 References 110
- CFD-Modeling for Optimizing the Function of 7 Low-Pressure Valves 113 Frank Helmsen and Tobias Kirchner References 119

Part Three Fire and Explosions – are CFD Simulations Really Profitable? 121

8	Consequences of Pool Fires to LNG Ship Cargo tanks 123
	Benjamin Scholz and Gerd-Michael Wuersig
8.1	Introduction 123
8.2	Evaluation of Heat Transfer 125
8.2.1	Simplified Steady-State Model (One-Dimensional) 125
8.2.2	Different Phases of Deterioration 126
8.2.3	Possibility of Film Boiling 127
8.2.4	Burning Insulation 128
8.3	CFD-Calculations 128
8.3.1	Buckling Check of the Weather Cover 129
8.3.2	Checking the CFD Model 129
8.3.3	Temperature Evaluation of Weather Cover/Insulation 131
8.3.3.1	Temperature Distribution inside the Insulation 131
8.3.3.2	Hold Space Temperature Distribution During Incident 132
8.3.4	Results of CFD Calculation in Relation to Duration of Pool
	Fire Burning According to the Sandia Report 133
8.3.5	CFD – the Future in Safety Technology? 136
8.4	Conclusions 136
	References 137
9	CFD Simulation of Large Hydrocarbon and Peroxide Pool Fires 139
	Axel Schönbucher, Stefan Schälike, Iris Vela, and Klaus-Dieter Wehrstedt
9.1	Introduction 139
9.2	Governing Equations 139
9.3	Turbulence Modeling 140
9.4	Combustion Modeling 141
9.5	Radiation Modeling 142
9.6	CFD Simulation 144

XII Contents

9.7 9.7.1 9.7.2 9.7.3 9.7.4 9.8 9.9	Results and Discussion 145 Flame Temperature 145 Surface Emissive Power (SEP) 147 Irradiance 149 Critical Thermal Distances 150 Conclusions 154 CFD – The Future of Safety Technology? 154 References 155
10	Madeling Fire Conversion and Smalls Mignation in Churcharas 150
10	Modeling Fire Scenarios and Smoke Migration in Structures 139
10.1	Introduction 159
10.1	Hierarchy of Fire Models 161
10.3	Balance Equations for Mass, Momentum, and Heat
	Transfer (CFD Models) 162
10.4	Zone Models 164
10.5	Plume Models 164
10.6	Computational Examples 166
10.6.1	Isothermal Turbulent Flow through a Room with
	Three Openings 166
10.6.2	Buoyant Non-Reacting Flow over a Heated Surface 168
10.6.3	Simulation of an Incipient Fire in a Trailer House 170
10.6.4	Simulation of Smoke Migration 174
10.7	Conclusions 175
10.8	CFD – The Future of Safety Technology? 175
	References 177
Dant Carry	CED Tomorrow The Wey to CED as a Standard Tablin
Part Four	Safety Technology 170
	Salety recimology 179
11	The ERCOFTAC Knowledge Base Wiki – An Aid for Validating
	CFD Models 181
	Wolfgang Rodi
11.1	Introduction 181
11.2	Structure of the Knowledge Base Wiki 182
11.2.1	Application Challenges (AC) 182
11.2.2	Underlying Flow Regimes (UFR) 183
11.3	Content of the Knowledge Base 184
11.4	Interaction with Users 185
11.5	Concluding Remarks 185
10	CED at its limiter Carling Lawren Hannatain Data
12	CrD at its Limits: Scaling issues, Uncertain Data, and the
	Users Rule 107 Matthias Münch and Punart Klain
10.1	Numerics and Under Resolved Simulations 100
1/1	INVESTIGATION AND A DEPENDENCIAL AND ADDRESS AND ADDRE

- 12.1.1 Numerical Discretizations and Under-Resolution 190
- 12.1.2 Turbulence Modeling 191
- 12.1.2.1 Reynolds-Averaged Navier-Stokes (RANS) Models 192
- 12.1.2.2 Large Eddy Simulation (LES) Models 194
- 12.2 Uncertainties 196
- 12.2.1 Dependency of Flow Simulations on Uncertain Parameters: Basic Remarks 196
- 12.2.2 Polynomial Chaos and Other Spectral Expansion Techniques 198
- 12.3 Theory and Practice 199
- 12.3.1 Reliability of CFD Program Results 200
- 12.3.1.1 Verification and Validation 200
- 12.3.1.2 The User's Influence 200
- 12.3.2 Examples 201
- 12.3.2.1 User's Choice of Submodels 201
- 12.3.2.2 Influence of a Model's Limits of Applicability 202
- 12.3.2.3 The Influence of Grid Dependency 206
- 12.3.2.4 Influence of Boundary Conditions 207
- 12.4 Conclusions 208 References 210
- 13Validation of CFD Models for the Prediction of Gas Dispersion
in Urban and Industrial Environments213

Michael Schatzmann and Bernd Leitl

- 13.1 Introduction 213
- 13.2Types of CFD Models214
- 13.3 Validation Data 215
- 13.3.1 Validation Data Requirements 215
- 13.3.2 Analysis of Data from an Urban Monitoring Station 218
- 13.4 Wind Tunnel Experiments 227
- 13.5 Summary 229
 - References 231
- 14 CFD Methods in Safety Technology Useful Tools or Useless Toys? 233 Henning Bockhorn
- 14.1 Introduction 233
- 14.2 Characteristic Properties of Combustion Systems 234
- 14.2.1 Ignition of Flammable Mixtures 234
- 14.2.2 Ignition Delay Times 237
- 14.2.3 Laminar Flame Velocities 239
- 14.2.4 Turbulent Flame Velocities 242
- 14.3 Practical Problems 247
- 14.3.1 Mixing of Fuels with Air in Jet-In-Cross-Flow Set-ups 247
- 14.3.2 Chemical Reactors for High-Temperature Reactions 251
- 14.4 Outlook 256 References 257

XIV Contents

Part Five	Dynamic Systems – Are 1D Models Sufficient? 259
15	Dynamic Modeling of Disturbances in Distillation Columns 261 Daniel Staak, Aristides Morillo, and Günter Wozny
15.1	Introduction 261
15.2	Dynamic Simulation Model 262
15.2.1	Column Stage 263
15.2.1.1	Balance Equations 264
15.2.1.2	Phase Equilibrium 265
15.2.1.3	Incoming Vapor Flow 265
15.2.1.4	Outgoing Liquid Flow 265
15.2.1.5	Additional Equations 266
15.2.2	Relief Device 266
15.3	Case Study 268
15.4	CFD- The Future of Safety Technology? 269
15.5	Nomenclature 272
	References 274
16	Dynamic Process Simulation for the Evaluation of Upset Conditions in Chemical Plants in the Process Industry 275
16.1	Introduction 275
16.1.1	Dynamic Process Simulation for Process Safety 276
16.2	Application of Dynamic Process Simulation 277
16.2.1	Rectification Systems 277
16.2.1.1	General 277
16.2.1.2	Verification of the Dynamic Process Simulation 278
16.2.1.3	Process Safety-Related Application of a Dynamic Process Simulator 284
1622	Hydrogen Plant 288
16221	General 288
16.2.2.2	Model Building and Verification of the Dynamic Process
	Simulation 289
16.3	Conclusion 293
16.4	Dvnamic Process Simulation – The Future of Safety
	Technology? 293
17	The Process Safety Toolbox – The Importance of Method Selection for Safety-Relevant Calculations 295 Andy Jones
17.1	Introduction – The Process Safety Toolbox 295
17.2	Flow through Nitrogen Piping During Distillation Column
	Pressurization 296
17.2.1	Initial Design Based on Steady-State Assumptions 296
17.2.2	Damage to Column Internals 297

1723	
17.2.3	Dynamic Model of Nitrogen Flow Rates and Column
172	Tube Failure in a Wined Film Evenerator 201
17.3	Tube Failure A Dotentially Dangerous Overpressurization
17.3.1	Scenario 301
1737	Dequired Policying Date Rased on Steam Flow An Unsafe
17.3.2	Assumption 202
1722	Assumption 505 Decuired Policying Data Paged on Water Flow An Expansive
17.5.5	Assumption 202
1734	Dynamic Simulation of Wined Film Evaporator An Optimal
17.3.4	Solution 204
17 /	Dhanal Formaldohude Uncontrolled Evothermic Deaction 306
17.4	Assumptions Degarding Single Dhace Venting 306
17.4.1	Will Two-Phase Venting Occur? 306
17.4.2	Effect of Disengagement Behavior on Required Believing Bate
17.4.5	and Area 307
175	Computational Eluid Dynamics – Is It Ever Necessary) 308
17.5	Design of Storage Tanks for Thermally Sensitive Liquids 308
17.5.1	Dispersion of Sprayed Droplets during Application of a Surface
17.5.2	Costing 308
1753	Dispersion of Heat and Chemical Substances 309
17.5.5	Computational Fluid Dynamics – The Future of Safety
17.0	Technology? 309
	Technology. 509
	References 311
	References 311
18	References 311 CFD for Reconstruction of the Buncefield Incident 313
18	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson
18 18.1	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson Introduction 313
18 18.1 18.2	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson 313 Introduction 313 Observations from the CCTV Records 314
18 18.1 18.2 18.2.1	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson 313 Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314
18 18.1 18.2 18.2.1 18.2.2	References311 CFD for Reconstruction of the Buncefield Incident 313Simon E. Gant and G.T. Atkinson111Introduction313Observations from the CCTV Records314Progress of the Mist314Wind Speed317
18 18.1 18.2 18.2.1 18.2.2 18.2.3	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson 313 Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3	References311CFD for Reconstruction of the Buncefield Incident313Simon E. Gant and G.T. AtkinsonIntroduction313Introduction313Observations from the CCTV Records314Progress of the Mist314Wind Speed317Wind Speed317Final Extent of the Mist318CFD Modeling of the Vapor Cloud Dispersion318
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2 18.3.3	References 311 CFD for Reconstruction of the Buncefield Incident 313 Simon E. Gant and G.T. Atkinson Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2 18.3.3 18.3.4	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320 Sensitivity Tests 320
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2 18.3.3 18.3.4 18.3.4.1	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320 Sensitivity Tests 320 Grid Resolution 321
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2 18.3.3 18.3.4 18.3.4.1 18.3.4.1 18.3.4.2 	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320 Sensitivity Tests 320 Grid Resolution 321 Turbulence 321
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2 18.3.3 18.3.4 18.3.4.1 18.3.4.2 18.3.4.3 	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320 Sensitivity Tests 320 Grid Resolution 321 Turbulence 321 Ground Topology 322
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2 18.3.3 18.3.4 18.3.4.1 18.3.4.2 18.3.4.3 18.3.4.3 18.3.4.4 	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320 Sensitivity Tests 320 Grid Resolution 321 Turbulence 321 Ground Topology 322 Hedges and Obstacles 323
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3 18.3.1 18.3.2 18.3.3 18.3.4 18.3.4.1 18.3.4.2 18.3.4.3 18.3.4.4 18.3.4.5 	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320 Sensitivity Tests 320 Grid Resolution 321 Turbulence 321 Ground Topology 322 Hedges and Obstacles 323 Ground Surface Roughness 324
18 18.1 18.2 18.2.1 18.2.2 18.2.3 18.2.4 18.3.1 18.3.2 18.3.4 18.3.4.1 18.3.4.2 18.3.4.3 18.3.4.4 18.3.4.5 18.3.4.6 	References 311 CFD for Reconstruction of the Buncefield Incident 313 <i>Simon E. Gant and G.T. Atkinson</i> Introduction 313 Observations from the CCTV Records 314 Progress of the Mist 314 Wind Speed 317 Final Extent of the Mist 317 What Was the Visible Mist? 318 CFD Modeling of the Vapor Cloud Dispersion 318 Initial Model Tests 318 Vapor Source Term 319 CFD Model Description 320 Sensitivity Tests 320 Grid Resolution 321 Turbulence 321 Ground Topology 322 Hedges and Obstacles 323 Ground Surface Roughness 324 Summary of Sensitivity Tests 325

XVI Contents

18.4	Conclusions 328
18.5	CFD: The Future of Safety Technology? 328
	References 329
Part Six	Contributions for Discussion 331
10	
19	Do we really want to Calculate the wrong Problem as Exactly as Possible?
	The Relevance of Initial and Boundary Conditions in Treating the
	Consequences of Accidents 333
10.1	Unich Hauptmanns
19.1	Introduction 333
19.2	Models 334
19.2.1	Leaks 334
19.2.1.1	Leak Size 334
19.2.1.2	Geometry of the Aperture 335
19.2.2	Discharge of a Gas 335
19.2.2.1	Filling Ratio 336
19.2.2.2	Duration of Release 336
19.2.2.3	Ambient Temperature and Pressure 336
19.2.3	Atmospheric Dispersion 337
19.2.3.1	Wind Speed 337
19.2.3.2	Eddy Coefficient 337
19.2.4	Health Effects 338
19.3	Case Study 339
19.3.1	Deterministic Calculations 339
19.3.2	Sensitivity Studies 339
19.3.3	Probabilistic Calculations 342
19.4	Conclusions 345
	References 346
20	Con Coffman French Coff) 240
20	Can Software Ever De Safer 349 Erank Schiller and Ting Matter
20.1	Fruit Schlief und Thin Mattes
20.1	Pagica 250
20.2	Definitions 250
20.2.1	Conoral Strataging 251
20.2.2	Derfect Systems 251
20.2.2.1	Ferret Systems 551
20.2.2.2	Fault-Tolerant Systems 352
20.2.2.3	Error-Tolerant Systems 355
20.2.2.4	Fail-Safe Systems 354
20.3	Software Errors and Error Handling 334
20.3.1	Software Development Errors 555
20.3.1.1	Errors III Software Development 355
20.3.1.2	Process models for Software Development 355
20.5.2	Errors and Methods concerning Errors in Source Code 358

- 20.3.2.1 Errors in Source Code 358
- 20.3.2.2 Methods for Preventing Software Errors 362
- 20.4 Potential Future Approaches 366
- 20.5 CFD The Future of Safety Technology? 367 References 367
- 21 CFD Modeling: Are Experiments Superfluous? 369 B. Jörgensen and D. Moncalvo References 371

Index 373