Contents

Preface XIX
List of Contributors XXI

1 Computational Fluid Dynamics: the future in safety technology
   Jürgen Schmidt 1

   Norbert Pfeil 5
   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
   Arno Klomfass and Klaus Thoma 9
   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 Technology 31

4 Status and Potentials of CFD in Safety Analyses Using the Example of Nuclear Power
   Horst-Michael Prasser 33
   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
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.4</td>
<td>Expected Benefits of CFD in Nuclear Reactor Safety</td>
<td>37</td>
</tr>
<tr>
<td>4.5</td>
<td>Challenges</td>
<td>40</td>
</tr>
<tr>
<td>4.6</td>
<td>Examples of Applications</td>
<td>42</td>
</tr>
<tr>
<td>4.6.1</td>
<td>Deboration Transients in Pressurized Water Reactors</td>
<td>42</td>
</tr>
<tr>
<td>4.6.2</td>
<td>Thermal Fatigue Due to Turbulent Mixing</td>
<td>47</td>
</tr>
<tr>
<td>4.6.3</td>
<td>Pressurized Thermal Shock</td>
<td>49</td>
</tr>
<tr>
<td>4.7</td>
<td>Beyond-Design-Based Accidents</td>
<td>53</td>
</tr>
<tr>
<td>4.7.1</td>
<td>Hydrogen Transport, Accumulation, and Removal</td>
<td>53</td>
</tr>
<tr>
<td>4.7.2</td>
<td>Aerosol Behavior</td>
<td>59</td>
</tr>
<tr>
<td>4.7.3</td>
<td>Core Melting Behavior</td>
<td>60</td>
</tr>
<tr>
<td></td>
<td>References</td>
<td>66</td>
</tr>
<tr>
<td></td>
<td><strong>Part Two  Computer or Experimental Design?</strong></td>
<td>69</td>
</tr>
<tr>
<td>5</td>
<td>Sizing and Operation of High-Pressure Safety Valves</td>
<td>71</td>
</tr>
<tr>
<td>5.1</td>
<td>Introduction</td>
<td>71</td>
</tr>
<tr>
<td>5.2</td>
<td>Phenomenological Description of the Flow through a Safety Valve</td>
<td>71</td>
</tr>
<tr>
<td>5.3</td>
<td>Nozzle/Discharge Coefficient Sizing Procedure</td>
<td>72</td>
</tr>
<tr>
<td>5.3.1</td>
<td>Valve Sizing According to ISO 4126-1</td>
<td>73</td>
</tr>
<tr>
<td>5.3.2</td>
<td>Limits of the Standard Valve Sizing Procedure</td>
<td>74</td>
</tr>
<tr>
<td>5.3.3</td>
<td>Valve Sizing Method for Real Gas Applications</td>
<td>74</td>
</tr>
<tr>
<td>5.3.4</td>
<td>Numerical Sizing of Safety Valves for Real Gas Flow</td>
<td>77</td>
</tr>
<tr>
<td>5.3.5</td>
<td>Equation of State, Real Gas Factor, and Isentropic Coefficient</td>
<td>78</td>
</tr>
<tr>
<td>5.3.6</td>
<td>Comparison of the Nozzle Flow/Discharge Coefficient Models</td>
<td>80</td>
</tr>
<tr>
<td>5.4</td>
<td>Sizing of Safety Valves Applying CFD</td>
<td>82</td>
</tr>
<tr>
<td>5.4.1</td>
<td>High Pressure Test Facility and Experimental Results</td>
<td>82</td>
</tr>
<tr>
<td>5.4.2</td>
<td>Numerical Model and Discretization</td>
<td>86</td>
</tr>
<tr>
<td>5.4.3</td>
<td>Numerical Results</td>
<td>87</td>
</tr>
<tr>
<td>5.5</td>
<td>Summary</td>
<td>90</td>
</tr>
<tr>
<td></td>
<td>References</td>
<td>93</td>
</tr>
<tr>
<td>6</td>
<td>Water Hammer Induced by Fast-Acting Valves – Experimental Studies, 1D Modeling, and Demands for Possible Future CFX Calculations</td>
<td>95</td>
</tr>
<tr>
<td>6.1</td>
<td>Introduction</td>
<td>95</td>
</tr>
<tr>
<td>6.2</td>
<td>Multi-Phase Flow Test Facility</td>
<td>97</td>
</tr>
<tr>
<td>6.3</td>
<td>Extension of Pilot Plant Pipework PPP for Software Validation</td>
<td>99</td>
</tr>
<tr>
<td>6.4</td>
<td>Experimental Set-Up</td>
<td>99</td>
</tr>
<tr>
<td>6.5</td>
<td>Experimental Results</td>
<td>100</td>
</tr>
<tr>
<td>6.5.1</td>
<td>Experimental Results – Thermohydraulics</td>
<td>100</td>
</tr>
</tbody>
</table>
6.6  Case Studies of Possible Future Application of CFX  103
6.6.1  1D Modeling of Kaplan Turbine Failure  105
6.6.2  Simulation Results – Closing Time 10 s, Linear  105
6.7  Possible Chances and Difficulties in the Use of CFX for Water Hammer Calculations  106
6.7.1  Benchmark Test for Influence of Numerical Diffusion in Water Hammer Calculations  107
6.8  CFD – The Future of Safety Technology?  109
References  110

7  CFD-Modeling for Optimizing the Function of 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
9.7 Results and Discussion 145
9.7.1 Flame Temperature 145
9.7.2 Surface Emissive Power (SEP) 147
9.7.3 Irradiance 149
9.7.4 Critical Thermal Distances 150
9.8 Conclusions 154
9.9 CFD – The Future of Safety Technology? 154
References 155

10 Modeling Fire Scenarios and Smoke Migration in Structures 159

Ulrich Krause, Frederik Rabe, and Christian Knaust

10.1 Introduction 159
10.2 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

Part Four CFD Tomorrow – The Way to CFD as a Standard Tool in Safety Technology 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

12 CFD at its Limits: Scaling Issues, Uncertain Data, and the User’s Role 189

Matthias Münch and Rupert Klein

12.1 Numerics and Under-Resolved Simulations 190
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

13 Validation of CFD Models for the Prediction of Gas Dispersion in Urban and Industrial Environments 213
Michael Schatzmann and Bernd Leitl
13.1 Introduction 213
13.2 Types of CFD Models 214
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
<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>Dynamic Modeling of Disturbances in Distillation Columns</td>
<td>261</td>
</tr>
<tr>
<td></td>
<td><em>Daniel Staak, Aristides Morillo, and Günter Wozny</em></td>
<td></td>
</tr>
<tr>
<td>15.1</td>
<td>Introduction</td>
<td>261</td>
</tr>
<tr>
<td>15.2</td>
<td>Dynamic Simulation Model</td>
<td>262</td>
</tr>
<tr>
<td>15.2.1</td>
<td>Column Stage</td>
<td>263</td>
</tr>
<tr>
<td>15.2.1.1</td>
<td>Balance Equations</td>
<td>264</td>
</tr>
<tr>
<td>15.2.1.2</td>
<td>Phase Equilibrium</td>
<td>265</td>
</tr>
<tr>
<td>15.2.1.3</td>
<td>Incoming Vapor Flow</td>
<td>265</td>
</tr>
<tr>
<td>15.2.1.4</td>
<td>Outgoing Liquid Flow</td>
<td>265</td>
</tr>
<tr>
<td>15.2.1.5</td>
<td>Additional Equations</td>
<td>266</td>
</tr>
<tr>
<td>15.2.2</td>
<td>Relief Device</td>
<td>266</td>
</tr>
<tr>
<td>15.3</td>
<td>Case Study</td>
<td>268</td>
</tr>
<tr>
<td>15.4</td>
<td>CFD- The Future of Safety Technology?</td>
<td>269</td>
</tr>
<tr>
<td>15.5</td>
<td>Nomenclature</td>
<td>272</td>
</tr>
<tr>
<td></td>
<td>References</td>
<td>274</td>
</tr>
<tr>
<td>16.1</td>
<td>Introduction</td>
<td>275</td>
</tr>
<tr>
<td>16.1.1</td>
<td>Dynamic Process Simulation for Process Safety</td>
<td>276</td>
</tr>
<tr>
<td>16.2</td>
<td>Application of Dynamic Process Simulation</td>
<td>277</td>
</tr>
<tr>
<td>16.2.1</td>
<td>Rectification Systems</td>
<td>277</td>
</tr>
<tr>
<td>16.2.1.1</td>
<td>General</td>
<td>277</td>
</tr>
<tr>
<td>16.2.1.2</td>
<td>Verification of the Dynamic Process Simulation</td>
<td>278</td>
</tr>
<tr>
<td>16.2.1.3</td>
<td>Process Safety-Related Application of a Dynamic Process Simulator</td>
<td>284</td>
</tr>
<tr>
<td>16.2.2</td>
<td>Hydrogen Plant</td>
<td>288</td>
</tr>
<tr>
<td>16.2.2.1</td>
<td>General</td>
<td>288</td>
</tr>
<tr>
<td>16.2.2.2</td>
<td>Model Building and Verification of the Dynamic Process Simulation</td>
<td>289</td>
</tr>
<tr>
<td>16.3</td>
<td>Conclusion</td>
<td>293</td>
</tr>
<tr>
<td>16.4</td>
<td>Dynamic Process Simulation – The Future of Safety Technology?</td>
<td>293</td>
</tr>
<tr>
<td>17</td>
<td>The Process Safety Toolbox – The Importance of Method Selection for Safety-Relevant Calculations</td>
<td>295</td>
</tr>
<tr>
<td></td>
<td><em>Andy Jones</em></td>
<td></td>
</tr>
<tr>
<td>17.1</td>
<td>Introduction – The Process Safety Toolbox</td>
<td>295</td>
</tr>
<tr>
<td>17.2</td>
<td>Flow through Nitrogen Piping During Distillation Column Pressurization</td>
<td>296</td>
</tr>
<tr>
<td>17.2.1</td>
<td>Initial Design Based on Steady-State Assumptions</td>
<td>296</td>
</tr>
<tr>
<td>17.2.2</td>
<td>Damage to Column Internals</td>
<td>297</td>
</tr>
</tbody>
</table>
## 17.2.3 Dynamic Model of Nitrogen Flow Rates and Column Pressurization 297

17.3 Tube Failure in a Wiped-Film Evaporator 301

17.3.1 Tube Failure – A Potentially Dangerous Overpressurization Scenario 301

17.3.2 Required Relieving Rate Based on Steam Flow – An Unsafe Assumption 303

17.3.3 Required Relieving Rate Based on Water Flow – An Expensive Assumption 303

17.3.4 Dynamic Simulation of Wiped-Film Evaporator – An Optimal Solution 304

17.4 Phenol-Formaldehyde Uncontrolled Exothermic Reaction 306

17.4.1 Assumptions Regarding Single-Phase Venting 306

17.4.2 Will Two-Phase Venting Occur? 306

17.4.3 Effect of Disengagement Behavior on Required Relieving Rate and Area 307

17.5 Computational Fluid Dynamics – Is It Ever Necessary? 308

17.5.1 Design of Storage Tanks for Thermally Sensitive Liquids 308

17.5.2 Dispersion of Sprayed Droplets during Application of a Surface Coating 308

17.5.3 Dispersion of Heat and Chemical Substances 309

17.6 Computational Fluid Dynamics – The Future of Safety Technology? 309

References 311

## 18 CFD for Reconstruction of the Buncefield Incident 313

*Simon E. Gant and G.T. Atkinson*

18.1 Introduction 313

18.2 Observations from the CCTV Records 314

18.2.1 Progress of the Mist 314

18.2.2 Wind Speed 317

18.2.3 Final Extent of the Mist 317

18.2.4 What Was the Visible Mist? 318

18.3 CFD Modeling of the Vapor Cloud Dispersion 318

18.3.1 Initial Model Tests 318

18.3.2 Vapor Source Term 319

18.3.3 CFD Model Description 320

18.3.4 Sensitivity Tests 320

18.3.4.1 Grid Resolution 321

18.3.4.2 Turbulence 321

18.3.4.3 Ground Topology 322

18.3.4.4 Hedges and Obstacles 323

18.3.4.5 Ground Surface Roughness 324

18.3.4.6 Summary of Sensitivity Tests 325

18.3.5 Final Dispersion Simulations 325
18.4 Conclusions 328
18.5 CFD: The Future of Safety Technology? 328
References 329

Part Six Contributions for Discussion 331

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
Ulrich 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 Can Software Ever be Safe? 349
Frank Schiller and Tina Mattes
20.1 Introduction 349
20.2 Basics 350
20.2.1 Definitions 350
20.2.2 General Strategies 351
20.2.2.1 Perfect Systems 351
20.2.2.2 Fault-Tolerant Systems 352
20.2.2.3 Error-Tolerant Systems 353
20.2.2.4 Fail-Safe Systems 354
20.3 Software Errors and Error Handling 354
20.3.1 Software Development Errors 355
20.3.1.1 Errors in Software Development 355
20.3.1.2 Process Models for Software Development 355
20.3.2 Errors and Methods concerning Errors in Source Code 358