Contents

1 **Introduction** 1

1.1 The Importance of DDT for Containment Integrity 1

1.2 State of Research -Prior to Commencement of this Project 3

1.2.1 ReactionKinetics 3

1.2.2 Detailed Mechanisrns and Global Behaviour of DDT 3

1.2.3 Modelling and Numerical Simulation. 3

1.2.4 Validation Status of Existing Codes. 4

1.2.5 Mitigation 4

1.3 SummaryofthePresentProject 5

1.3.1 Goals and Potential Applications of Results 5

1.3.2 Summary of the Work Packages 7

1.4 A **Remark on Uncertainties, Errors and Error Bounds** 7

2 **Experimental Investigations 11**

2.1 Reaction Kinetics and Reignition 11

2.1.1 Auto-ignition Characteristics 12

2.1.2 DDT Induced by a **Single Obstacle 23**

2.2 Flame Acceleration and DDT in Obstacle Arrays 39

2.2.1 Summary of Experimental Methods 40

2.2.2 Results of Idealised DDT Mode A **Experiments. 40**

2.2.3 Results of Prototypic DDT Mode A **Experiments. 57**

2.2.4 Results of DDT Mode B **Experiments. 62**

3 **Modelling and Numerics 73**

3.1 Modelling, Scaling Relations, Derivation of Criteria 73

3.1.1 Critical Conditions for Detonations Initiation in Nonuniformly Heated Re- active Pockets 74

3.1.2 DDT within the Turbulent Flame Brush -Scaling Analysis. 78

3.2 NumericalTechniques 83
3.2.1 The Argument for Flame Front Tracking 85
3.2.2 The Basic Capturing/Tracking Hybrid Scheme 86
3.2.3 Tracking Flames with Unsteady Internal Flame Structure 89
3.2.4 Incorporation of a **pdf-based Turbulent Combustion Model 92**
3.2.5 Criteria-EnforcedDDT-Transition 98
3.2.6 Demonstration of a **DDT-Switch in Sample Computations 100**

4 **Validation 103**
4.1 MotivationandOverview 105
4.2 Computer Codes for DDT-Related Simulations. 105
4.3 The FZJ High-Performance Computing Infrastructure 107
4.4 Vectorization, Parallelization and Code Developments 109
4.5 DDT Simulations and Code Verification vs. Validation. 112
4.6 Further Developments and Interactions 123
4.7 Conclusions 125

5 **Mitigation 127**
5.1 DDT-RelatedMitigation ..127
5.1.1 TheTONUSCode[l] 128
5.1.2 Combustion models. 131
5.2 Improved PSA strategies for DDT risk assessment 150
5.2.1 SafetyCasePhilosophies 150
5.2.2 Inclusion of New DDT Research Results in Extended PSA 151
5.3 Remarks on Mitigation Measures 153

6 **Further Deliverabies 155**
6.1 SWL/RWTH-Aachen: Code Validation Data Base. 155
6.2 FUB: Flame Tracking with Dynamic Internal Structure 159
6.3 FZJ: ParallelizationManuals 159
6.3.1 Performance Analysis and Optimization Tools 159
6.3.2 AutoTasking:DETonT90 159
6.3.3 High-Performance Fortran: DET on T3E 160
6.3.4 Domain Decomposition: CFX-4/5 on T90/T3E 160
6.3.5 Domain Decomposition: AIXCO on T90/T3E ...160

7 **Summary** & **Conclusions 163**

7.1 WP1: Experimental Investigations 163
7.1.1 Chemical Kinetics and Detailed DDT Mechanisms 163
7.1.2 Prototypical DDT Mode A **and Mode** B **Experiments. 164**
7.2 WP 2: Modelling and Numerical Techniques 164
7.2.1 Modeling of Detailed DDT Mechanisms 164
7.2.2 Numerical Techniques for DDT Simulation. 165
7.3 WP3:VerificationandValidation 165
7.4 WP4:Mitigation 166
7.4.1 DDT-Related Mitigation 166
7.4.2 Advanced PSA Methods 167
7.4.3 Recommendations for Future Work 167

References 169