EXECUTIVE SUMMARY

This report concerns the key issue of hydrogen combustion that may occur as a result of severe accidents in nuclear power plants, namely to predict which type of combustion will occur: a slow flame, a fast turbulent flame, or a detonation. This question is crucial because the combustion mode governs the amplitude and time scale of the containment pressure load.

Chapter 1 introduces the phenomena of flame acceleration (FA) and deflagration-to-detonation transition (DDT) with respect to the relevance of these processes in severe accidents, the basic physical phenomena that define the detonation limits involved in these processes, and options for control and mitigation of these processes.

Chapter 2 describes the basic elements of FA and DDT, which have been understood for many years. Both these phenomena are basically due to the intrinsic instability of flame surfaces. Depending on the mixture composition, the initial pressure and temperature conditions, the geometrical configuration and, most importantly, the physical size (or scale) of the reactive system, FA and detonation on-set may or may not occur What has been missing up until now are quantitative predictions of FA and DDT for given conditions.

Chapter 3 outlines the significant advances that have been made in this field during the last decade (1990-1999). Two criteria were derived from a large new experimental database. The first criterion predicts the potential for spontaneous FA to supersonic flame speeds. This criterion controls the formation of shocks that have sufficient strength to trigger a secondary local explosion. The second criterion governs the amplification and transmission of this local explosion to a stable detonation in the undisturbed mixture. For this step, the effective geometrical size of the reactive mixture must be greater than 7 times the detonation cell width of the average mixture composition. Both conditions, namely the critical flame velocity and the minimum scale requirement, are necessary for a complete DDT. The two criteria allow realistic assessments of the FA and DDT potential during an accident scenario. Rules and data for evaluation of the criteria in reactor containments are formulated.

An important property of these criteria is that they can be evaluated from the results of three dimensional (3D) computational fluid dynamics (CFD) distribution calculations, which provide all the necessary data for mixture composition and geometrical scales. Depending on these results, the criteria allow us to predict the fastest combustion regime possible, namely either slow deflagration, fast turbulent deflagration, or detonation. An approach on how to use the criteria within a lumped-parameter framework is described in Section 6.3.

Chapter 4 summarizes the state-of-the-art of the mathematical description of these 3 combustion regimes. It starts with modelling of non-reacting turbulent flames, putting major emphasis on Reynolds-averaged Navier-Stokes equations. Different types of closure approaches are discussed. An important practical issue for large-scale nuclear containments is the modelling of obstacles for which porosity models are described. Moreover, the key ideas for large eddy simulation are summarized.

For simulation of turbulent premixed combustion, three model categories are described, covering heuristic closures, flamelet models, and probability density function (PDF) approaches. The realistic representation of chemistry poses a major challenge to numerical modellers because of its wide range of inherent time scales. Chapter 4 presents heuristic models for the net effect of numerical reactions as well as for more sophisticated reduced chemistry models and the most recent developments, aiming at a systematic mathematical approach to chemistry reduction.

The particular numerical challenges posed to a numerical flow solver in the context of FA and DDT are discussed, and the current most-popular finite-difference and finite-volume approaches are presented. For numerical representation of the combustion front, essentially 2 alternatives exist: (a) detailed models for all relevant physical processes within the turbulent combustion zone, or (b) treatment of the reaction front as a discontinuous surface in space.

Chapter 5 gives examples for recent mathematical and numerical model developments and their validation by corresponding experiments. Moreover, the important question is addressed: which tool to choose for which task in practical applications. For many of the every day engineering tasks, it would be inefficient to employ the most advanced and complex modelling tools giving the currently best-possible answers. On the other hand, with increasing requirements on the precision of safety analysis, a demand for detailed and sophisticated modelling exists. Therefore, a good compromise seems to be the compilation of a hierarchy of models with increasing levels of detail, starting from coarse-grain zero-dimensional lumped-parameter models to high-resolution 3D tools. The choice of model then is primarily governed by the type of processes to be resolved and the required precision.

With respect to simulation of FA and DDT, first-level models neglecting momentum exchange have very restricted predictive value. The next level of computational complexity that allows representation of 3D global unsteady but statistically averaged flow fields provides estimates for the influence of momentum exchange and the effects from the other previously neglected terms in the Navier-Stokes equations. This level of modelling allows realistic assessments of potential structural loads that are due to high-speed combustion events. However, this kind of approach still misses events that are triggered by localized processes and can then develop into global combustion events. Examples are ignition by hot spots or detonation onset through gas-dynamic–reactive resonances. Reliable modelling of this kind of process requires an even more advanced modelling level that is able to resolve the smallest flow scales, e.g., by sophisticated dynamic mesh refinement.

Chapter 6 describes how the tested model approaches, outlined in Chapter 5, are currently applied to reactor containment analysis. Two different levels of model sophistication are currently applied. The first one is based on the mixture and geometry information available within conventional zero-dimensional lumped-parameter models. This fast and relatively easy analytical method is useful to screen a large number of different event sequences for the risk-dominating cases. However, this screening procedure requires well- experienced users who are familiar with the intrinsic uncertainties of lumped-parameter distribution calculations, in order not to miss critical accident sequences. The identified critical cases should then be investigated with the next higher level of model sophistication, using three-dimensional CFD tools.

The higher precision of CFD prediction with respect to FA and DDT potential comes first from the solved equations (3D, fully compressible Navier-Stokes equations, including momentum balance and a complete set of fluid dynamic terms); second, from the much finer spatial resolution (typically 1 m^3 versus 1000 m^3 with a lumped-parameter method); and third, from the correspondingly smaller numerical truncation errors and mixing effects. The given examples of full CFD distribution analysis with the corresponding evaluation of the FA and DDT criteria demonstrate that currently available CFD tools allow us to exam the relative merits of different mitigation schemes. For a given plant, mitigation system, accident scenario, and set of hydrogen-steam sources, the times and space regions with FA and DDT potential can be clearly identified. In case of unacceptable risk, the mitigation measure can be varied in order to reach a negligible threat for the containment integrity.

Chapter 7 summarizes the significant advances, outlined above, in the understanding of FA and DDT during this decade. In addition, the most important topics for future work on mechanistic calculations are described; these topics aim at a better definition of the initial conditions for FA and DDT (the

H_2-steam sources and the prediction of their distribution); a decreased conservatism in the currently applied FA and DDT criteria (inhomogeneous and vented mixtures); and improved numerical CFD simulation techniques for fast turbulent deflagration and detonations (advanced models, higher spatial resolution, massive parallel processing).