7. SUMMARY AND ISSUES *

7.1 Summary

This report concerns the key issue of hydrogen combustion behaviour that may occur as a result of severe accidents in NPPs. Chapter 1 gives an overview of the hydrogen combustion issue in relation to NPP safety. Mechanical (pressure) and thermal loads from hydrogen combustion are one mechanism that can result in the failure of the outermost containment structure of an NPP. The estimation of these loads and the evaluation of the potential hazards associated with various accident scenarios have been the subject of extensive investigation over the last two decades. There are many issues, but the one that is most difficult to evaluate is to determine what type of combustion will occur: slow flames, fast flames, or detonations.

Because of the non-linear feedback between fluid motion and flame propagation, determination of the boundaries separating various flame regimes is not just a matter of conducting a few experiments on selected mixtures. Not only is the mixture composition important, but experimentation has demonstrated that initial conditions, geometrical configuration, and—most importantly—the physical size or scale of the apparatus is crucial in determining the outcome of a combustion experiment. The most difficult behaviour to predict, and one of the most significant for evaluating potential hazards, is the occurrence of detonation as the result of the FA processes. As described in Chapter 2, the basic elements of FA and DDT have been understood for many years. What has been missing up until now are quantitative predictions of the criteria for FA and transition-to-detonation.

This report describes the significant advances in the understanding of FA and DDT that have been made in the last decade (1990-1999). Focused programs of experimental research—described in Chapters 3, 5, Appendices A, B, C and D, and also numerical simulation (Chapters 4 and 5)—have enabled the identification of criteria for boundaries of fast flame and detonation regimes in hydrogen-air-steam mixtures of interest to reactor safety. These criteria enable a more refined evaluation of explosion regimes than was previously possible for severe accidents in NPPs (see Chapter 6).

The significant factors in improving our understanding of FA and DDT are

1. systematic large-scale experimentation on FA and DDT using hydrogen-air-steam mixtures;

2. measurement of hydrogen-air-steam mixture properties such as detonation cell width and flame speed at elevated temperatures (100°C to 377°C) and pressures (up to 3 bar);

3. using fundamental models of flames and detonations to identify relevant non-dimensional parameters that were used to correlate experimental data;

4. multi-dimensional (3D) field-equation modelling of species transport, flame, and detonation propagation; and

5. spatially resolved visualization of chemical species during transient flame propagation.

However, it is important to note that despite these advances in our understanding of FA and DDT, our knowledge of FA and DDT is largely empirical. The current state of the art in computation is such that even with research tools, numerical simulation is unable to provide a truly predictive capability

* Professor Joseph E. Shepherd is the lead author of Chapter 7.

for DDT. What we are able to do is to provide a framework of ideas that can be used with existing engineering simulations to screen accident scenarios for situations in which FA and DDT may be possible. This framework is limited in the sense that many situations arise in which we cannot rule out the possibility of FA and DDT, but we have no means to predict whether these will actually occur. If the criteria are not satisfied, then FA and DDT are extremely unlikely in those cases, but exceptions are always possible in marginal situations.

7.1.1 Framework for Evaluating FA and DDT

First, it is important to note that only empirical necessary conditions for FA and DDT can be supplied at the present time. This limitation is due to the complexity of the processes involved, the limited database of experimental results, the lack of a theoretical foundation, and the inability to run end-to-end numerical simulations from first principles. These conditions have been culled from experiments conducted to date and are the subject of ongoing research.

1. Detonations can only be created indirectly by the processes of low-speed flame ignition, FA, and transition-to-detonation. The "direct initiation" pathways are highly unlikely because of the large amount of concentrated energy, which is required for direct initiation. Therefore, it is anticipated that in all but the most exceptional cases, FA is a prerequisite condition for DDT to occur.

2. In order for FA to occur, a sufficiently large expansion ratio $\sigma = \rho_u/\rho_b$ must exist between the burned and unburned gas. A critical magnitude can be computed based only on the properties of the mixture within the containment. There are two cases, one for lean and one for rich hydrogen mixtures. Chapter 3 discusses the experimental evidence and boundaries for these cases in detail, and Figure 7.1.1-1 plots the values of the expansion ratio for one set of thermodynamic conditions.

3. Even if the expansion ratio is sufficiently large, the flame must accelerate to sufficiently high velocities—approximately equal to the speed of sound in the burned gas—before the conditions for detonation initiation can be reached. This means that flame propagation through obstructions, channels, or interconnected rooms must occur in order to produce the fluid motions required for flame folding and stretching.

4. Once the necessary conditions for detonation onset are set up, then detonation may only occur if the physical size of the containment compartment or region is sufficiently large compared with a length that characterizes the reactivity of the mixture. The usual choice of the reactivity length scale is the detonation cell size λ. Measurements of the detonation cell width (Appendix D, Tables D.1-1 and -2) and correlation functions (Figure 7.1.1-2) are available for estimating cell size as a function of mixture composition and thermodynamic conditions.

5. Characteristic Size Evaluation

   Results of numerous FA and DDT experiments (described in Chapter 3) have demonstrated that the physical dimension, L, of the compartment or experiment has to be greater than some multiple of the cell width in order for DDT to be possible. These lead to the necessary criteria for DDT

$$L \geq \alpha\lambda$$

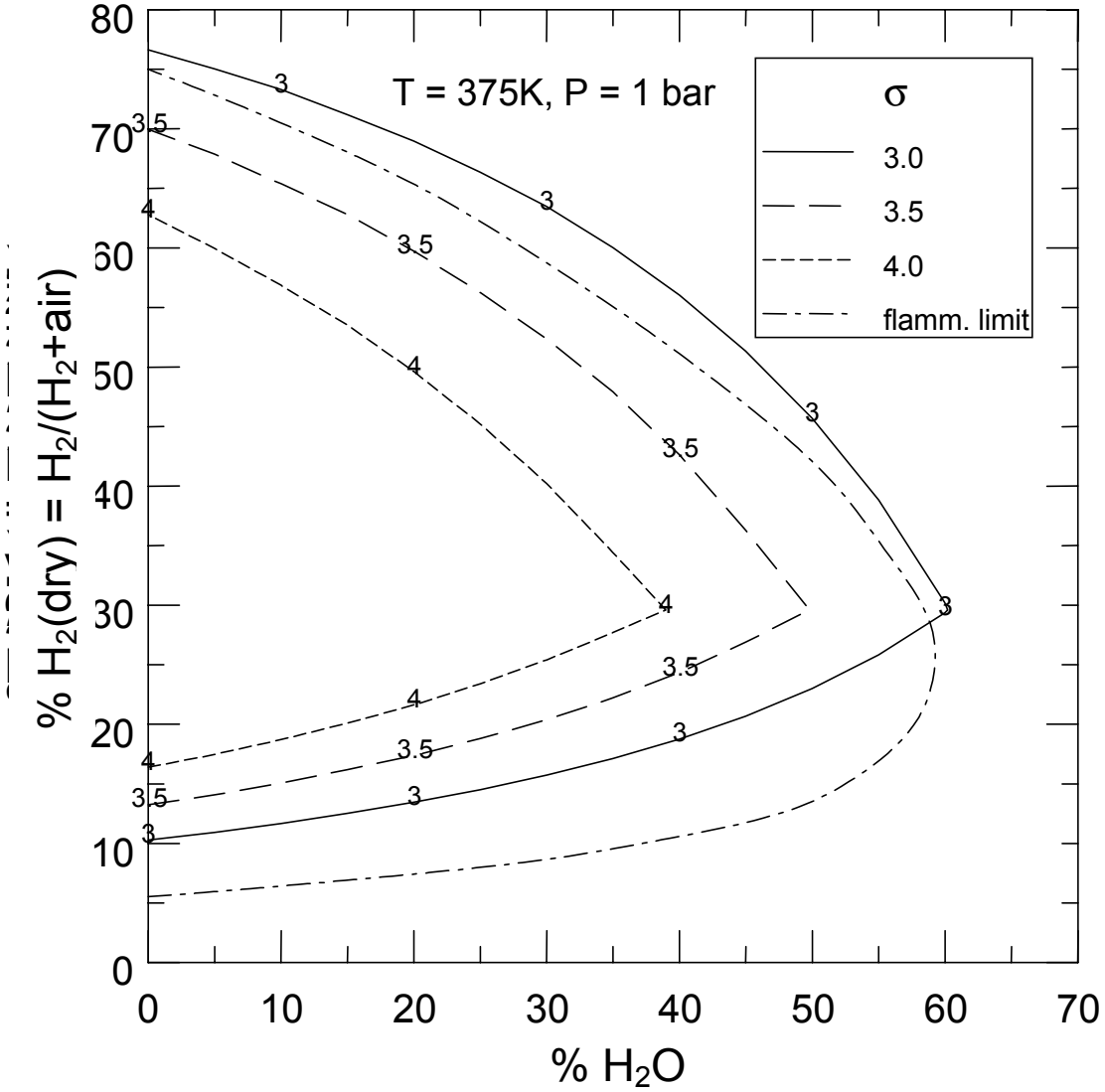

Figure 7.1.1-1 Expansion ratio σ as a function of hydrogen and steam concentration for a mixture at 375 K and 1 bar. The results shown are illustrative of the general situation; computations should be performed directly for mixtures at other temperatures and pressures

where the value of the constant α depends on the particular geometric configuration. For example, in the case of a long channel with obstructions, the minimum value of $\alpha = 1$ when L is the transverse dimension of the smallest cross-section in the channel. For large compartments or clouds, the minimum value of α is about 7 when L refers to the largest transverse extent of the cloud. In the case of turbulent jets, α is between 14 and 24 when L refers to the exit diameter of the jet. For interconnected rooms or channels with various blockage ratios, formulas for computing the effective value of L are suggested in Chapter 3.

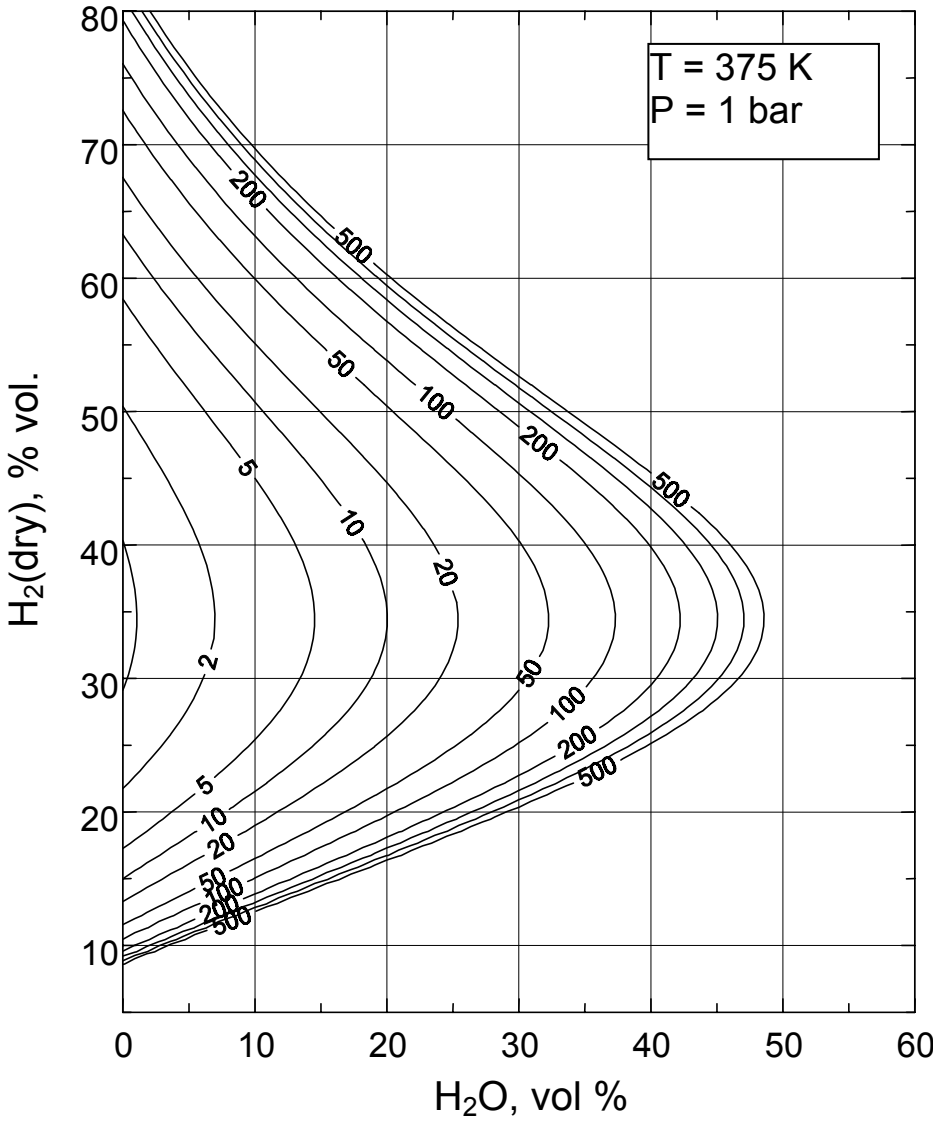

Figure 7.1.1-2 Detonation cell width λ (cm) as a function of hydrogen and steam concentration for a mixture at 375 K and 1 bar. The results shown are illustrative of the general situation, the correlation should be evaluated directly for mixtures at other temperatures and pressures

6. Combustion Regimes

The results of the previous considerations enable the construction of a combustion regime map for a particular set of thermodynamic conditions. The key parameters in this map are the amounts of hydrogen and steam in the mixture. Figure 7.1.1-3 illustrates that within the flammable regime, there is a narrow region of mixtures for which only slow flames are possible. Inside of this region, fast flames can appear once the expansion ratio is greater than the minimum values described in Chapter 3 and given in Figure 7.1.1-1. The application of the cell width of Figure 7.1.1-2 is shown for two characteristic rooms or compartment sizes, 1 and 10 m. Within the boundaries shown, DDT will be possible. It is extremely important to note that the boundaries

between combustion regimes are not simply fixed concentration values, such as some minimum hydrogen concentration as used in the past, but are a function of hydrogen and steam concentrations and also, the thermodynamic state. Not shown in the illustration, but apparent in the data, is a strong dependence of detonation cell width on initial temperature.

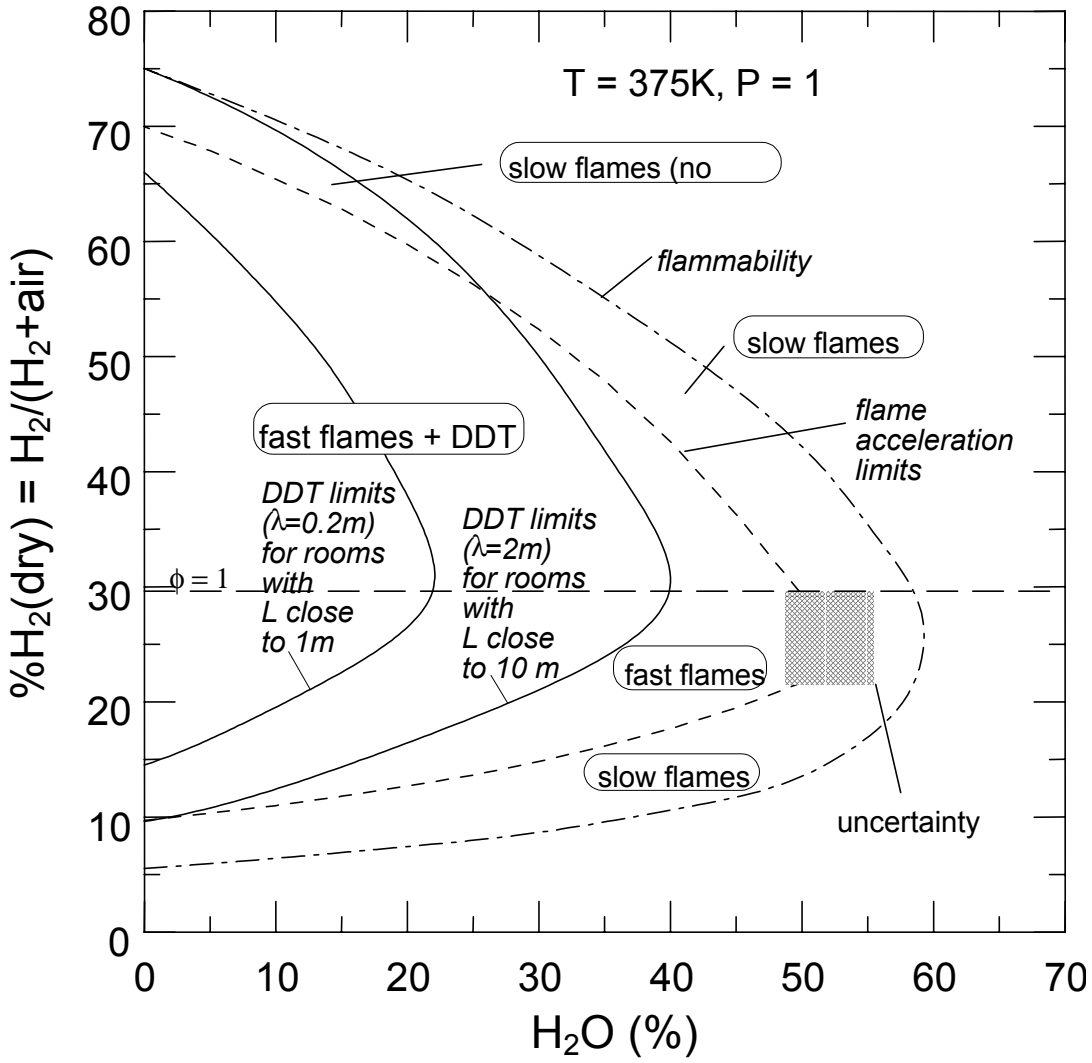

Figure 7.1.1-3 Combustion regimes possible in a hydrogen-air steam mixture at 375 K and 1 bar initial pressure. The DDT limits are based on a criteria of $L/\lambda = 5$

7. Evaluating Accident Scenarios

In order to evaluate the hazard of FA and DDT, a sequential process is suggested in Figure 7.1.1-4. The first steps are to use risk assessment methodology to define a set of accident sequences of interest, and then evaluate the hydrogen and steam source terms

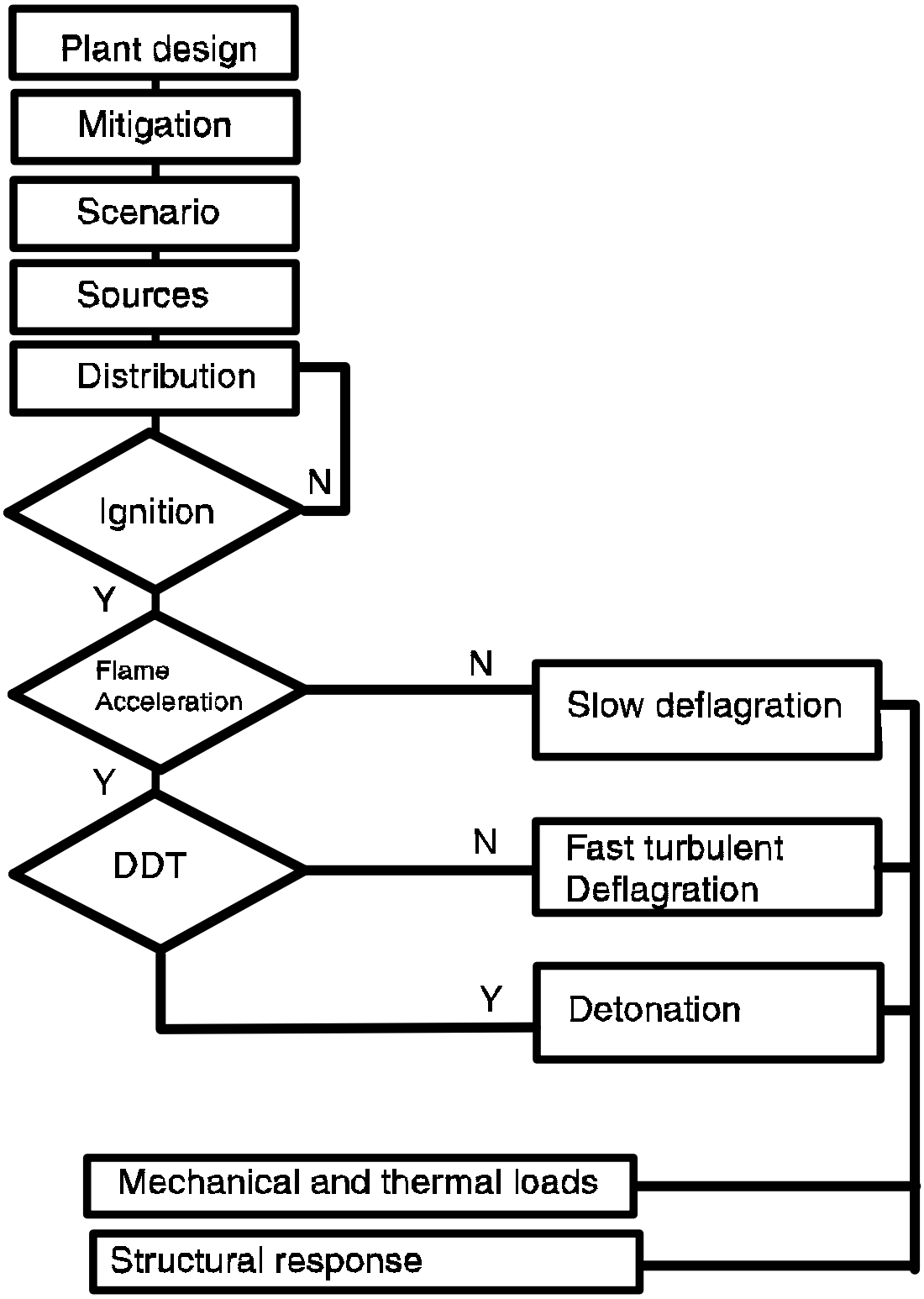

Figure 7.1.1-4 Steps in evaluating flame acceleration and deflagration-to-detonation transition hazards for severe accidents in nuclear power plants

using a system-level simulation of the postulated accident and release scenario. Once the source terms are defined, then some estimate of hydrogen distribution and mixing is needed along with predictions for the containment thermodynamic state, i.e., pressure and temperature. The framework developed above can then be applied compartment by compartment at each point in time to determine detonation and FA indices that provide a quantitative measure of the possibility of these events. In some cases, despite using mitigation schemes, some significant FA or DDT hazard may exist during some part of the transient. In those cases, closer investigation with numerical simulations of flames or detonations may be needed in order to determine whether localized fast flames or detonations pose a threat to containment integrity.

7.2 Issues

7.2.1 Combustion Modelling Appropriate to FA and DDT Events

There is a significant lack of numerical tools available to safety analysts for running approximate simulations of FA and DDT events. The existing lumped-parameter models that have been heavily used to date in reactor safety are completely inappropriate for modelling high-speed flows of any kind. Simulation of turbulent flow (without combustion) in 3D transient situations is a still-developing field without the additional complexity of combustion. In fact, at the present time, there is no single numerical method or simulation tool that can cover the entire range of phenomena in FA and DDT. Numerical models for low-speed (laminar) flames, high-speed (turbulent) flames, and detonations are distinct and, at present, there are no practical methods for running an end-to-end simulation with the goal of predicting DDT. Even at the research level, the only technique available is direct numerical simulation, albeit with a simplified chemical and transport model, and the resolution requirements of this technique make this approach impossible to apply to NPPs. This is one of the reasons why an empirical approach to FA and DDT has been so extensively explored in the last decade and will continue to be used for the foreseeable future (see the discussion of Chapter 4 on resolution requirements for numerical simulations).

An important challenge for the future is to develop approximate but reliable methods for simulating both FA and detonation in such a fashion that the simulation can be run within a single software framework. One goal would be to simply eliminate the substantial human effort that is currently required in order to transfer results between simulations and do a hand evaluation of flow fields. A more ambitious goal is to develop reliable combustion models that can be used to model DDT without the judgment and intervention of the simulator.

Progress is now being made in modelling turbulent combustion through using variations on the eddy breakup model and flame-front tracking models with empirical turbulent flame speed correlations. Although confidence is being gained in the ability of these techniques to reproduce certain features of medium- and large-scale experiments, at the core these models are empirical. Additional work is needed to validate computation results against experiments at different scales in order to gain confidence in using these methods at an NPP scale.

Further improvement in the simulation of fast turbulent deflagration will depend foremost on progress in turbulence modelling for transient flows. A current trend is to shift away from isotropic 2-equation models towards non-isotropic LES models. For chemical reaction rates, the situation is less clear. In some combustion regimes, multi-dimensional β-PDF approaches appear promising, provided fast numerical integration schemes can be found for the required multi-dimensional integrals. Future work should also address better spatial resolution or the development of sub-grid models or both for representation of unresolved structures. These models need to represent the sub-grid-scale effects on momentum balance (drag), turbulence generation, and combustion rate.

7.2.2 First-principles Modelling of DDT

At present, DDT has been modelled in a near-first-principles fashion only by research codes simulating small spatial regions of sensitive fuel-oxygen mixtures with very simplified chemical models. Because of the wide range of possible outcomes and also the sensitivity to initial and boundary conditions, it is not clear whether individual simulations would be useful for engineering evaluations of NPP safety. However, continued development of first-principles research-grade simulation tools will be very valuable in gaining insight into the mechanisms and physical-chemical parameters that are important in characterizing DDT. In particular, further exploration of the critical gradient or SWACER mechanisms is needed with detailed chemistry and multi-dimensional situations.

7.2.3 Loads and Structural Response

Ultimately, the structural response to the loads created by the combustion event is the most important measure of risk to the containment integrity. First, although it is known that the loads from fast flames can be severe, it is not clear how these compare with detonations or a DDT event. Second, work to date indicates that one must consider the details of the structural response in order to determine what is the most threatening combustion mode for a particular structure. Finally, there are at least as many uncertainties in modelling the failure of complex structures as there are in CFD and combustion modelling.

7.2.4 Experiments

7.2.4.1 FA and DDT criteria

DDT conditions are only necessary criteria and as such provide bounds that are most useful in evaluating when DDT will not occur. Combining criteria should make the boundaries sharper but at the present time, it is not possible to eliminate the essential feature of only being able to specify necessary conditions. Individual criteria also have uncertainties and in some cases are also overly bounding. Cell size uncertainty and uncertainties related to extrapolation and interpolation between distant values must be taken into account.

7.2.4.2 Minimum tube diameter

In the case of short channels or rooms, the $d/\lambda \geq 1$ criterion for detonation is probably overly restrictive as a necessary condition.

7.2.4.3 The 7-λ Criterion

Defining the physical length scale can be ambiguous in many cases. In the case of large volumes (L > 10 to 15 m), there is considerable uncertainty about cell widths greater than 2 m. No measurements are available in this regime, and no detonations have ever been observed in mixtures with cell width greater than 2 m.

7.2.4.4 Non-uniform mixtures

There are 3 issues regarding non-uniform mixtures: first, the difference in sensitivity between the mixtures as expressed by a variation in chemical length (lambda) between the most- and least-sensitive portions; second, the variation in energy content between the most-sensitive and least-sensitive mixtures; and third, how to define the characteristic physical size of a non-uniform cloud. All factors need to be taken into account, but a useful estimate of the appropriate chemical length is the cell size corresponding to the average mixture. For a non-uniform mixture within a well-defined room, the 7-λ criteria can be applied directly using the physical dimensions of the room. For a non-uniform cloud within a large volume, there are several proposals (one is discussed in Chapter 3) of how to compute the appropriate length scale. Another issue is how to determine the effective expansion ratio in a non-uniform cloud. In general, FA in non-uniform mixtures has not been investigated sufficiently to draw firm conclusions at the present time. One area of particular uncertainty is the role of the gradient dimensions and the need to investigate more realistic gradients in the hydrogen concentration.

7.2.4.5 Detonation initiation by shock focusing

It is unclear how to apply the existing data (see Appendix C) on shock focusing obtained in 50- to 350-mm-diameter shock tubes to NPP-scale situations. Shock tubes have a limited test time, and the tube walls provide confinement that will probably not be present in an NPP containment building. Although a wide range of hydrogen concentrations has been investigated, it is unclear whether the observed Mach number thresholds are independent of scale or whether the Mach number ranges investigated to date are realistic to expect in NPP severe accident conditions. Other experiments on FA and DDT show a very strong influence of system size on combustion behaviour, for example, the DDT criteria of a minimum length scale as compared to the detonation cell width. Shock focusing is now a well-established mechanism of creating critical conditions for detonation onset and will occur whenever shocks interact with concave corners. A systematic effort is needed to identify non-dimensional scaling parameters in shock-focusing experiments and to correlate these to the observed behaviour. Based on our previous experience with cell size scaling, it seems clear that it will be necessary to extend the experimental database to much larger scales before these results can be applied directly to safety analyses for NPPs.

7.2.4.6 Shock tube experiments and kinetic modelling

Detailed chemical reaction networks and modelling of flames and detonations on this basis have a role in estimating parameters such as flame speed and detonation cell width. However, there is scant data at high pressures and low temperatures with which to calibrate detailed reaction network models. The limited data that are available (see Chapter 5, Appendices A and B) suggest that there is an up to 3-order-of-magnitude discrepancy between computed and measured induction times at temperatures below 1200 K, an important regime in reactor safety applications. The direction of this discrepancy is such that computations predict much more benign conditions (longer induction times than the actual values) than may exist in practice. This may result in serious underestimation of the severity of an explosion hazard in these cases. A greater effort is needed, both in refining the experimental measurements and in investigating the reaction mechanism failures, before reaction mechanisms can be used with confidence in this regime.

7.2.4.7 Mixtures including CO and CO_2

Up to now, most of the experimental effort has been concentrated on hydrogen-air-steam mixtures. This has been appropriate since the accident scenarios predict that steam and hydrogen are the major constituents released from the primary system into the containment atmosphere. However, in some accident scenarios, significant amounts of carbon monoxide (CO) and dioxide (CO_2) may also be generated in the containment. Although some data are available (see Appendices B and C) on dilution with these components, the interaction with H_2 and H_2O has not been carefully investigated. There is a need to systematically measure parameters such as laminar and turbulent flame speed, transition limits, and detonation cell width.

7.2.4.8 Buoyancy

For lean mixtures of hydrogen, there is significant deformation of the flame and induced fluid flow resulting from the action of gravity on the hot products within the flame. This is one of the key mechanisms for accelerating very lean flames in large compartments. Lean flames generally have expansion ratios less than the critical value observed for FA in a channel geometry. For marginal situations (near the FA limit), it will be important to evaluate the influence of buoyancy at physical sizes appropriate to NPP applications. The issue of scaling is particularly crucial since the time available for buoyancy to act will vary with both physical size and hydrogen concentration. It is unclear at this time whether scale model experiments will suffice or whether large-scale experimentation is needed. An additional complexity for lean mixtures is the creation of flame instabilities (cellular structure) and the unusual influence of flame stretch in this regime; see the next subsection.

7.2.4.9 Lean hydrogen-air flame behavior

Lean hydrogen-air mixtures have Lewis numbers less than unity and negative Markstein numbers. This means that flame speed initially increases rather than decreases with positive straining motion (flame stretch) in the flow. This makes the application of standard turbulent flame speed and quenching criteria suspect in these flows. Turbulent flame speeds for lean hydrogen-air mixtures have been measured; however, the correct treatment of these data is unclear since there is no theoretical basis for treating phenomena such as quenching in these cases. There is a need for both more measurements on turbulent flame speed and quenching limits as well as an improved theoretical treatment.

7.3 Application to Safety Assessments in NPPs

There are a number of issues in applying the proposed framework to NPP safety assessment. Many of these issues are connected with reducing the uncertainty in mechanistic analysis of hydrogen behaviour.

7.3.1 Length Scales

A key issue in applying the 7-λ criterion is in determining the appropriate length scales associated with the physical compartments within the containment volume. There is a particular difficulty in evaluating this issue in conjunction with using the lumped-parameter models, which are often employed by utilities and safety agencies to screen accident sequences for potential hydrogen explosion hazards.

The lumped-parameter models can use an artificial subdivision of the physical volumes into logical volumes for the purposes of convenience in the computation. It is not obvious how to correctly ascribe a scaling length to these subvolumes in order to apply the 7-λ criteria to the results of lumped-

parameter simulations. Results of model computations (discussed in Chapter 6) indicate that although a reasonable range of length scales is obtained through a simple set of rules, the sensitivity of the results to other choices of subdivision has not been examined.

7.3.2 Source Terms

Initial conditions and distribution computations play an important role in evaluating FA and DDT potential. Although hydrogen and steam sources are highly plant- and scenario-dependent, there is a general need for better understanding of hydrogen and steam generation from certain in- and ex-vessel phenomena (in PWRs). These phenomena include fast transient sources such as reflood of an overheated core; steam explosions; hydrogen generation through steel oxidation; B4C behaviour during core-melt; and the oxidation of Zr-Ur-Oxide conglomerate; effect of fuel irradiation, and vessel failure. Core-concrete interaction can, in addition to hydrogen, also contribute important amounts of CO and CO_2. There is little information available today on flame acceleration and DDT in H_2-CO-air-steam-CO_2 mixtures.

7.3.3 Lumped-parameter Models

It is commonly assumed that lumped-parameter approaches are adequate in simulating the initial phase of the accident that determines the distribution of hydrogen and steam prior to ignition. However, there are particular cases in which this may fail. One such case occurs when large control volumes (100 to 1000 m^3) are employed that average out or mask local concentrations that may actually exist. Another case is when significant natural convection loops exist within large compartments or simultaneous inflow and outflow occur within the same opening to a compartment. Finally, since lumped-parameter codes do not conserve momentum, any situation in which the fluid momentum is significant will not be correctly computed. Examples include the prediction of peak pressure from slow flames in complex geometries. In such cases, it may be necessary to take an approach based on computational fluid dynamics (CFD), simulating the solution of the field equations of mass, momentum, and energy conservation on a fine spatial mesh.

7.3.4 Computational Fluid Dynamics

CFD is playing an increasingly important role in simulations of hydrogen distribution, FA, DDT, and detonation propagation. Modelling of turbulence and turbulent combustion is a major research area that is receiving intense study from many researchers, and all CFD codes will benefit from these efforts. For nuclear safety applications, future work is especially important with respect to improved treatment of the water phase (spray, film behaviour), modelling of radiation heat transfer, and development of improved numerical solution methods (massive parallel processing). Finally, it is important that the results of CFD simulations be carefully validated against experiments, examining both the dependence on submodels and the effects of mesh size. Several new experimental facilities are currently under construction in Western Europe that will provide the high-resolution data necessary for further validation of CFD models. A particular concern when validating CFD codes is demonstrating convergence in the face of necessarily coarse spatial meshes that are used when modelling NPP containments.

7.3.5 Ignition Predictions and Effectiveness of Mitigation Techniques

An important part of accident simulations is the prediction of the time and location of the first (and eventually subsequent) ignition of the reactive containment mixture. There is a need to develop improved criteria for ignition by spark-plug igniters as a function of spark parameters, criteria for

self-ignition by high temperatures, and a treatment of other random ignition sources (electrical sparks, hot surfaces, hot particles). The influence of high γ-radiation levels on the ignition process should also be better understood.

7.3.6 Analysis Strategies

The analysis of accident sequences and potential explosion hazards always involves evaluating complex phenomena in the face of considerable uncertainties. Often because of these uncertainties, the results of analysis are not clear-cut. In some cases, it may be necessary to use CFD or experimentation in order to sharpen the limits and provide sufficient as well as necessary conditions. As an example, if detonation cannot be completely ruled out in a particular portion of a containment, CFD simulations can be used to estimate structural loads. Computation structural simulation can then be used to see whether these loads actually pose a threat to the integrity of the containment.