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# DYNAMIC MODELING OF PHYSICAL PHENOMENA FOR PROBABILISTIC ASSESSMENT OF SPENT FUEL ACCIDENTS

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**Abstract**

If there should be an accident involving drainage of all the water from a spent fuel pool, the fuel elements will heat up until the heat produced by radioactive decay is balanced by that removed by natural convection to air, thermal radiation, and other means. If the temperatures become high enough for the cladding or other materials to ignite due to rapid oxidation, then some of the fuel might melt, leading to an undesirable release of radioactive materials. The amount of melting is dependent upon the fuel loading configuration and its age, the oxidation and melting characteristics of the materials, and the potential effectiveness of recovery actions. We have developed methods for modeling the pertinent physical phenomena and integrating the results with a probabilistic treatment of the uncertainty distributions. The net result is a set of complementary cumulative distribution functions for the amount of fuel melted.

## 1. Introduction

Over the past two decades, the moratorium on spent fuel reprocessing in the United States has resulted in an expansion of facilities that store spent fuel under water in a retrievable configuration. To accommodate the growing quantities of used fuel bundles, storage pools were enlarged and adapted to higher storage densities. In the process, storage racks evolved from widely spaced, open frame structures to tightly packed, closed frame steel containers. An example of a spent fuel pool with a vertical storage array is shown in Figure 1, and some of the storage racks that have been used in these pools are shown in Figure 2.

To assess the safety of such facilities, a range of postulated accidents may be considered, and the probability of occurrence of these accidents and the resulting consequences may be predicted. Of the various accidents, the most severe type for storage in water is one that leads to a complete drainage of the pool. For this type of accident, methods have been developed at Sandia National Laboratories to analyze: (1) the thermal-hydraulic phenomena involved when the storage racks and their contents become exposed to air, (2) the conditions that could lead to clad failure due to overheating, (3) the potential for melting of fuel that could lead to an undesirable release

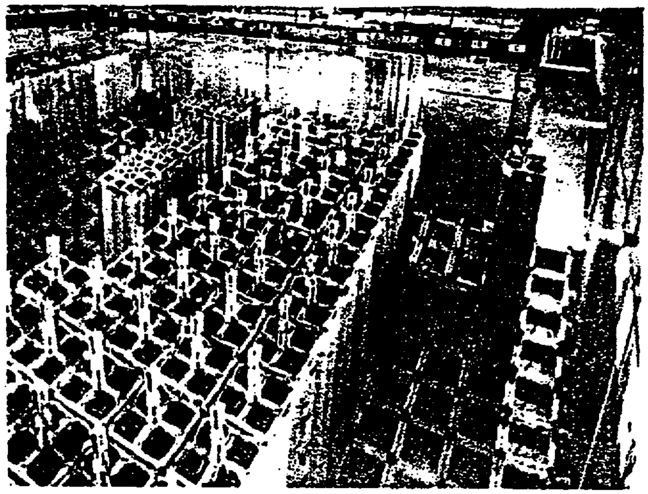


*Figure 1.* Example of an away-from reactor spent fuel storage pool (Morris, IL).

of radioactive materials, and (4) the overall uncertainty in the amount of fuel that would melt. These methods are the subject of this paper.

Aside from a few introductory comments to follow, this paper does not address accident initiation mechanisms, their probability of occurrence, the magnitude of fission product releases, or the public or environmental consequences. While these are essential factors in a complete risk assessment, they are addressed in others' work. Having said that, it should be noted that the likelihood of a severe spent fuel drainage accident has historically been judged to be very low. The Reactor Safety Study [1] evaluated the probability as being in the range of $10^{-5}$ to $10^{-7}$ per year at a typical U.S. reactor facility. Numerous design and security features are incorporated in all facilities to minimize the likelihood of a loss of pool water, including: (1) the conservative design philosophy of building the concrete pool structure, racks, cooling system, and support structures to withstand the forces that might result from a large earthquake or tornado; (2) the design of the racks to ensure that the geometry of the stored spent fuel is maintained in a subcritical configuration; (3) location of pool penetrations to prevent draining or siphoning of water through associated piping systems; (4) inclusion of mechanical interlocks and operating procedures to prevent any equipment from passing over the pool with heavy loads; (5) provision of multiple water level, water temperature, and radioactivity monitors that actuate alarms in the control room; and (6) enforcement of stringent security measures to prevent sabotage.

If there should be a complete pool drainage despite all these measures, the fuel elements will heat up. In the process, they will tend to reach a steady-state temperature distribution when the thermal power produced by radioactive decay is balanced by that removed by natural convection, thermal radiation, and other means. Undesirable releases of radioactive materials will occur only if the maximum attained temperature is

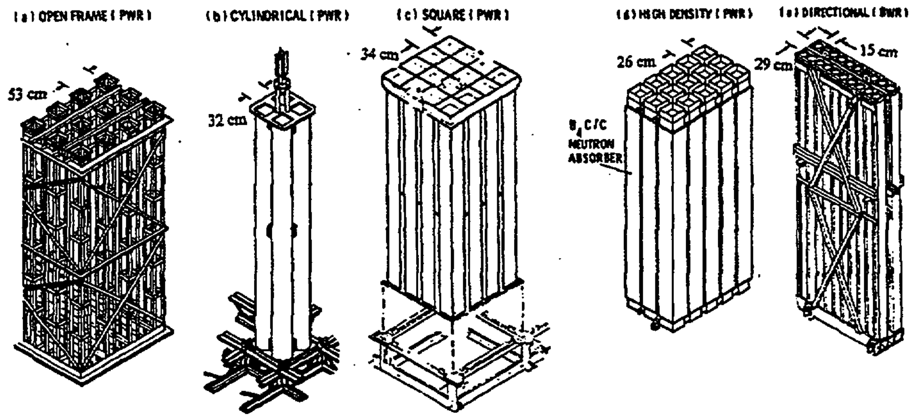



*Figure 2.* Examples of spent fuel storage racks.

high enough at some location in the pool to cause the cladding (generally a zirconium alloy) to rupture as a result of internal pressure, or to undergo rapid exothermic oxidation, leading to melting of the cladding. Coincidentally, the rupture temperature for zirconium-based cladding is quite close to the temperature at which the air oxidation reaction becomes self-sustaining, both being in the neighborhood of 850 – 950 °C [1,2]. The likelihood of reaching a deleterious temperature varies inversely with the amount of time that has elapsed since shutdown of fission power (i.e., the decay time), since longer times imply reduced decay heats.

A method for predicting the spent fuel heatup following drainage of the pool has been implemented at Sandia in a code called SFUEL [3,4]. The code can be used to assess the effects of decay time, fuel element design, storage rack design, packing density, enclosure ventilation, and other variables on the heat-up characteristics of the spent fuel, and to investigate the potential for the propagation of fuel melting across the pool. This paper provides an overview of the fluid dynamic, chemical reaction, and heat transfer models in the SFUEL code; shows some sample results; and describes a method for integrating the deterministic code results into a probabilistic framework. Although the details of the methods apply to a specific type of accident and storage option, namely, a rapid drainage of a water-filled spent fuel pool, the principles could be applied to other types of accidents and other types of storage configurations.

## 2. Phenomenological Models in the SFUEL Code

The principal models in the SFUEL code involve decay heat generation, chemical reaction, natural convection and thermal radiation within the drained spent fuel pool, heat removal from the containment enclosure, and relocation of melted materials. The following subsections describe these models.

## 2.1 DECAY HEAT GENERATION

Decay heat produced by spent fuel elements varies strongly with time since removal from the core as well as the operating conditions and burn-up experienced in the core. Figure 3 shows representative results from the ORIGEN code [5] for decay heat as a function of decay time and burn-up. The overall decay heat produced within the spent fuel pool is determined by the fuel loading configuration, and three patterns representative of U.S. facilities are shown in Table 1.

## 2.2 CHEMICAL REACTION

Oxidation of zirconium alloy cladding at elevated temperatures by air occurs primarily by the following reaction:

$$Zr + O_2 \rightarrow ZrO_2$$

which liberates approximately 262 kcal per mole of Zr. Zirconium can also react with steam to produce $ZrO_2$ and hydrogen gas, but that reaction is not considered here because of the assumption of an instantaneous pool drainage. The rate of reaction depends upon whether the reaction is rate-limited or diffusion-limited, the latter occurring when oxygen is unable to diffuse through nitrogen sufficiently fast to sustain the kinetics of the reaction.

For a rate-limited reaction, the rate of oxidation may be assumed to obey a parabolic rate law:

$$2w\frac{dw}{dt} = K_o \exp(-E_a / RT) \tag{1}$$

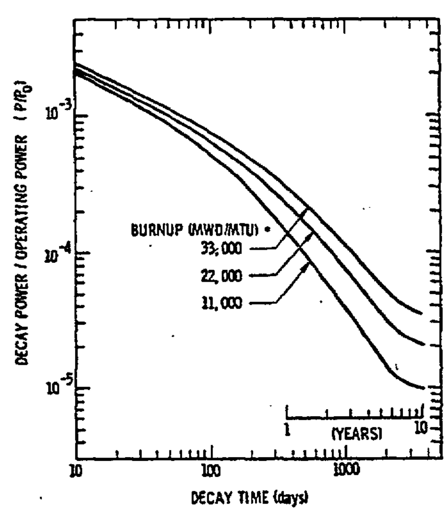
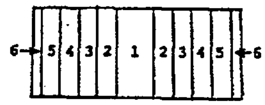



*Figure 3.* Normalized decay power versus decay time for spent fuel from a pressurized water reactor (PWR). (Note: MWD/MTU = megawatt-days per metric ton of uranium.)




| | Section of Pool | Fraction of Core | Number Of Cycles In Reactor | Burnup (MWD/MTU) | Decay Time |
|---|---|---|---|---|---|
| (A) | Full-Core PWR Discharge | | | | |
| | 1 | 1/3 | 3 | 33,000 | T |
| | 2 | 1/3 | 2 | 22,000 | T |
| | 3 | 1/3 | 1 | 11,000 | T |
| | 4 | 1/3 | 3 | 33,000 | T + 1 yr |
| | 5 | 1/3 | 3 | 33,000 | T + 2 yrs |
| | 6 | 1/12 | 3 | 33,000 | T + 3 yrs |
| (B) | Normal PWR Discharge | | | | |
| | 1 | 1/3 | 3 | 33,000 | T |
| | 2 | 1/3 | 3 | 33,000 | T + 1 yr |
| | 3 | 1/3 | 3 | 33,000 | T + 2 yrs |
| | 4 | 1/3 | 3 | 33,000 | T + 3 yrs |
| | 5 | 1/3 | 3 | 33,000 | T + 4 yrs |
| | 6 | 1/12 | 3 | 33,000 | T + 5 yrs |
| (C) | Full-Core BWR Discharge | | | | |
| | 1 | 1/8 | 4 | 30,600 | T |
| | 2 | 1/4 | 3 | 23,700 | T |
| | 3 | 1/4 | 2 | 16,300 | T |
| | 4 | 1/4 | 1 | 8,300 | T |
| | 5 | 1/8 | 4 | 27,200 | T |
| | 6 | 3/4 | 4 | 30,600 | T+1,2,3 yrs |

*Table 1.* Typical fuel loadings for spent fuel storage at a pressurized water reactor (PWR) and a boiling water reactor (BWR). (Schematic denotes postulated division of pool into sections.)

where $w$ is the weight gain per surface area, $t$ is the time since initiation of the reaction, $E_a$ is the activation energy for the reaction, $R$ is the gas constant, and $T$ is the temperature. The assumption of parabolic kinetics for air oxidation of zirconium is an approximation, since it is known that the oxidation process is more complex than would be indicated by parabolic kinetics. Figure 3 shows a reaction rate correlation for zirconium alloy based on the parabolic rate law.

When the reaction is limited by oxygen diffusion, a different model is required. The rate of reaction in this case is taken from the following equation, which is derived from the analogy between heat and mass transfer:

$$\frac{dw}{dt} = \frac{\rho_a D_{on} m_o}{x} \mathrm{Nu}(\mathrm{Re}_x, \mathrm{Gr}_x, \mathrm{Sc}) \qquad (2)$$

where $\rho_a$ is the air density, $D_{on}$ is the diffusion coefficient for air in nitrogen, $m_o$ is the mass fraction of oxygen, $x$ is the distance from the origin of the boundary layer, Nu is the Nusselt number, $\mathrm{Re}_x$ is the Reynolds number, $\mathrm{Gr}_x$ is the Grashoff number, and Sc is the Schmidt number.

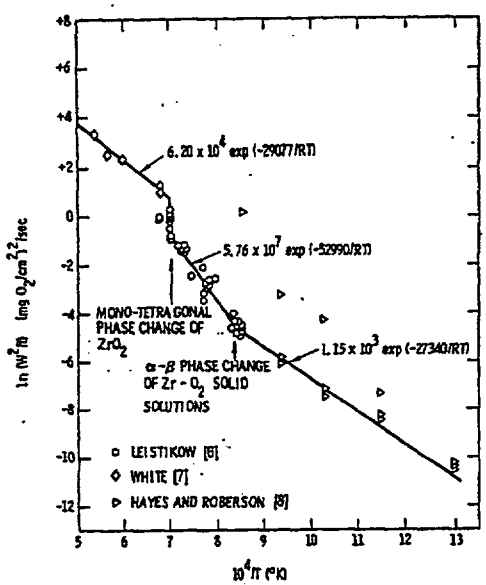



*Figure 4.* Reaction Rate Correlation for Air Oxidation of Zirconium Alloy.

## 2.3 HEAT TRANSFER MODELS

The heat removal processes for the drained spent fuel pool are considered in two parts: (1) the heat transfer problem within the confines of the pool, and (2) the removal of heat from the containment enclosure.

Schematics of the heat transfer problem for the spent fuel pool are shown in Figures 5 through 7. Heat produced by decay within the spent fuel elements and by chemical oxidation of the cladding is removed, in part, by buoyancy-driven air flows circulating in well-defined channels (Figure 5). Transport of mass, momentum, and energy for the air flows is calculated within the SFUEL code through an iterative, finite-difference solution of the appropriate conservation equations, averaged over the cross sections. Transient conduction equations are solved in the axial direction to determine the heat-up of the fuel rods as a function of time and vertical location. Thermal radiation between structural elements (i.e., fuel rods, subassembly channel walls if present, tie plates, holders or baskets, and pool liners) is accounted for, as is transient conduction into a concrete encasement (Figures 6 and 7).

To account for the containment enclosure, the SFUEL code computes the amount of heat that is removed by a combination of forced ventilation, leakage of air through the building structure, heat storage by the structural heat sinks, and radiation/natural convection from the exterior of the containment enclosure to the outside. A schematic of these processes is shown in Figure 8.

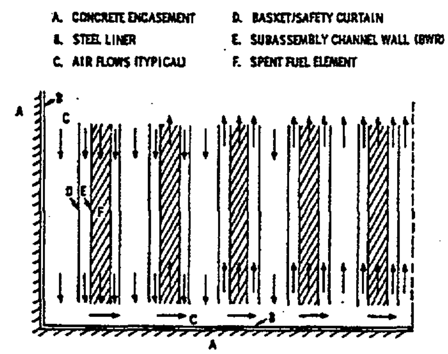



*Figure 5.* Schematic of spent fuel storage configuration and natural convection flows following a complete drainage.

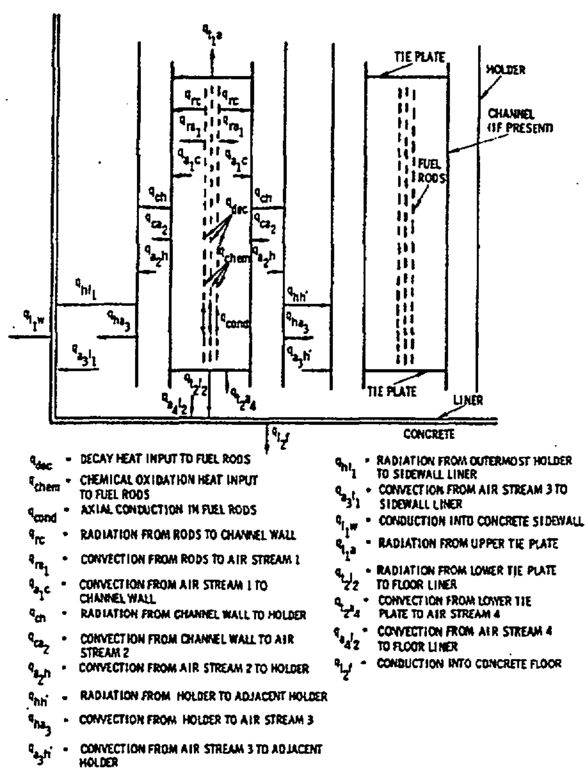
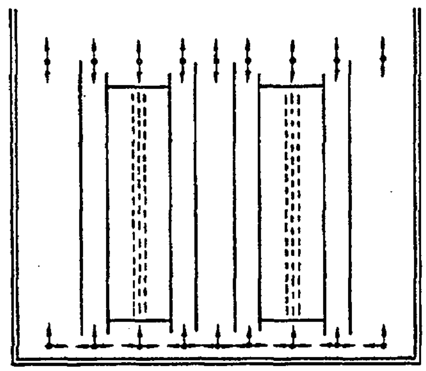



*Figure 6.* Identification of heat transfer modes considered in the pool region.



| ITEMS | SYMBOLS | SOLUTION PROCEDURE, EACH TIME STEP |
|---|---|---|
| FLOW PATHS | | SOLVE EQUATIONS OF MOMENTUM AND ENERGY CONSERVATION, ONE DIMENSION, TO DETERMINE AIR TEMPERATURE AND VELOCITY AS A FUNCTION OF POSITION. |
| JUNCTIONS | | ITERATE UNTIL (1) MASS OUTFLOW EQUALS MASS INFLOW, (2) PRESSURES ON ALL SIDES OF JUNCTION ARE EQUAL, (3) ENTHALPY OUTFLOW EQUALS ENTHALPY INFLOW. |
| FUEL RODS | | SOLVE TRANSIENT 1-D CONDUCTION EQUATION, INCLUDING INTERNAL HEAT GENERATION, TO DETERMINE FUEL ROD TEMPERATURE AS A FUNCTION OF POSITION. |
| STRUCTURAL ELEMENTS | | APPLY TRANSIENT HEAT BALANCE EQUATION TO DETERMINE STRUCTURE TEMPERATURE AS A FUNCTION OF POSITION. |
| CONTAINMENT ATMOSPHERE | (NOT SHOWN) | APPLY HEAT AND MASS BALANCES TO DETERMINE BULK TEMPERATURE OF ROOM AIR. |

*Figure 7.* Identification of solution procedures used in spent fuel heat-up problem.

## 2.4 FUEL RELOCATION MODELS

If the fuel reaches its melting temperature in some portions of the pool, the geometry of the spent fuel array will change due to relocation of the melted fuel. The degree to which fuel melting in one portion propagates to other portions of the pool is strongly dependent upon the manner in which the fuel relocates. The modeling of relocation is one of the most uncertain portions of the analysis. The SFUEL code at present has three different models, representing two limiting cases and an intermediate case. For any given run, the analyst selects one of the three models.

In the first model, the melted fuel is assumed to stay in place and no change of geometry is computed. This model leads to an upper limit for the total amount of fuel melting in the pool, because it keeps the decay heating source close to the location of highest temperature and allows the air channels to remain open to flow (thereby prolonging the cladding reaction with oxygen).

In the second model, the fuel is assumed to drop to the base plate of the spent fuel subassembly as soon as it melts. This model leads to a lower limit on the total amount of fuel melting, because it removes the decay heating source from the location of highest

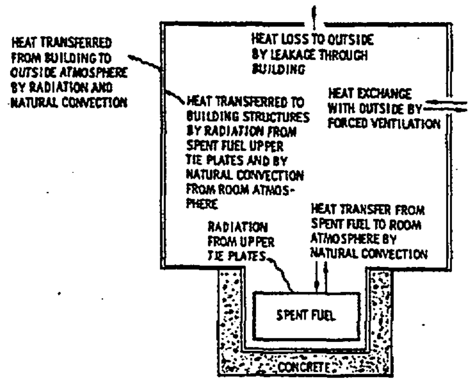



*Figure89.* Heat transfer modes for the containment enclosure.

temperature and blocks the air channels (thereby terminating the cladding reaction with oxygen).

In the third model, the melted fuel is assumed to drop beyond the base plate of the subassembly to the very bottom of the pool. This model leads to an intermediate result for the amount of fuel melting, because it removes the decay heating source but does not block the air channels (thereby allowing the cladding reaction to continue).

## 3. Example Results from SFUEL Calculations

Figure 9(a) illustrates example results for the heat-up of spent fuel in various storage configurations one year following a full-core discharge from a PWR. (This pattern corresponds to Case A in Table 1 with T = 1.0 year.) The temperatures shown are those of the fuel in the hottest location in the pool. For these calculations, it was assumed that the ventilation systems in the containment enclosure were fully operational. The highest-density storage configuration corresponds to the use of high-density racks with complete filling of the space within the pool. For that case, the cladding oxidation reaction becomes self-sustaining, as illustrated by the top dashed curve, which becomes nearly vertical. Fuel melting temperatures are attained after about 12 hours following the drainage of the water.

Figure 9(b) shows the maximum temperature attained in the pool as a function of the time since shutdown of the reactor (time T). The results are seen to be extremely sensitive to the storage configuration and to the size of the base-plate hole designed into the container at the bottom of each spent fuel subassembly. Smaller base-plate holes constrict the flow of air through the subassemblies, thereby constraining the cladding reaction.

Figure 10 illustrates how the heat-up is affected by lack of ventilation in the containment enclosure. In this case, the fuel elements heat up faster due to the rising temperature in the containment, but the depletion of the oxygen supply due to lack of ventilation causes the self-sustaining cladding reaction to terminate.

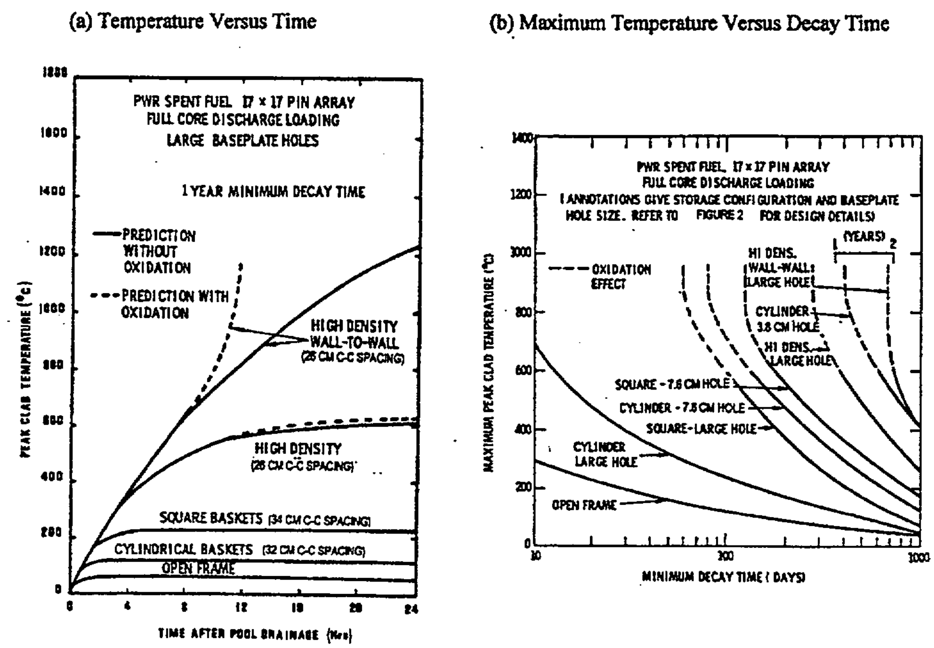



*Figure 9.* Effect of storage rack configuration on heat-up of PWR spent fuel in a well-ventilated enclosure.

Finally, Figure 11 depicts how the melting of fuel in one portion of the pool may propagate to other portions of the pool. The calculations in this figure correspond to the fuel relocation model in which the melted fuel drops to the bottom of the pool but the air channels remain open. The loading of the various pool sections and their assumed placement within the pool correspond to Case A in Table 1. The temperatures correspond to a location about two-thirds of the way up from the base of the fuel subassemblies. In this illustration, pool Section 4 encounters melting of fuel because of heat from Section 3, which has been loaded with fuel from a more recent reactor discharge.

## 4. Integration of SFUEL Results with a Probabilistic Model

Deterministic results obtained from the SFUEL code have to be interpreted realistically in the light of the uncertainties that exist in various phases of the calculation. One of the largest sources of uncertainty was discussed in Section 2.4, where it was noted that the modeling of fuel relocation has a large influence on the propagation of melting across the pool. Many other parameters in the calculation, such as heat transfer coefficients and oxidation rates, are also uncertain.

In addition, the overall probability distribution for the final result (amount of fuel melted) may depend not only upon uncertainties in the phenomenological models, but

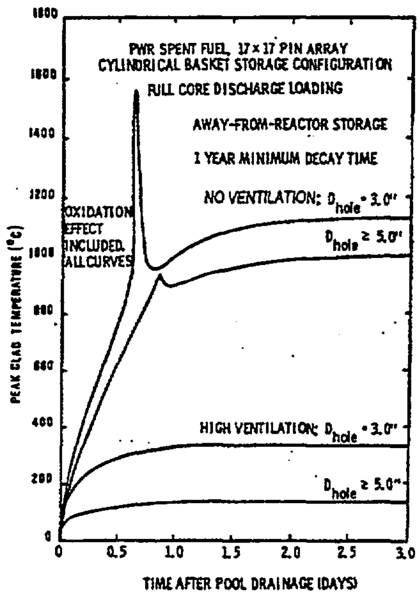



*Figure 10.* Heat-up of PWR spent fuel in an away-from-reactor storage facility with complete ventilation failure, compared to heat-up with high ventilation in the same facility.

also upon other factors not included in these models. Suppose, for example, that there are human actions available for mitigating the accident, such as providing water from alternative sources. Such actions may be either ad hoc in nature or covered by formal procedures. In either case, the recovery actions may be assumed to take time, so that there would be a race between the ability to effect recovery versus the time it takes for the fuel to melt. In addition, the success of recovery actions may be hampered if there is significant fuel melting, both because of the increased radiological hazard to the humans trying to achieve the recovery and because of the likelihood that the fuel has relocated to a less coolable configuration. Thus, the probability for recovery can be viewed as a bivariate function of time and of the amount of fuel that has melted. The functional relationship may be written as follows:

$$\frac{dP_{\text{rec}}}{dt} = F(m_f, t) \tag{3}$$

where $dP_{\text{rec}}/dt$ is the time derivative of the recovery probability at time $t$ given that the amount of melted fuel at that time is $m_f$. The algebraic form selected for $F$ will have its own set of uncertainties that should be included in the analysis.

To address uncertainties in a complex problem, methods have been developed to construct uncertainty distributions by polling experts [9]. Before conducting the polling, or elicitation, of experts, it is the responsibility of the analyst to break down the problem

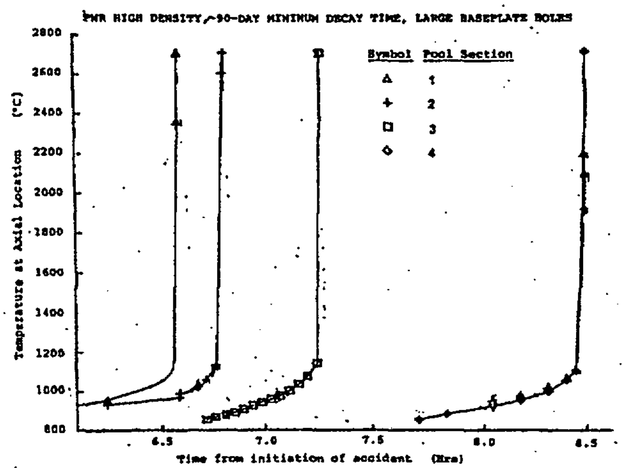



*Figure 11.* Composite view of pool-wide propagation results using intermediate fuel relocation model.

into manageable "bites." The experts are asked to render their judgments, not with respect to the final result, but with respect to various possible values of the uncertain parameters or models. In the present problem, each expert may be asked to provide a degree of belief for each of the candidate fuel relocation models and human recovery models, as well as a distribution function for the heat transfer coefficient, the chemical reaction rate constant, and other parameters that are believed to be uncertain. We refer to each distribution as an uncertainty function, rather than a probability function, because it reflects the experts' degrees of belief regarding an uncertain process rather than a realization of a stochastic process.

The process for constructing an uncertainty distribution for the final result (amount of fuel melted) is based on the following steps, which are illustrated schematically in Figure 12:

1. A Monte Carlo or Latin hypercube sampling scheme is used to set up a matrix of sample members consisting of specific values for all the uncertain parameters and models.
2. An SFUEL calculation is made for each sample member to determine the mass of fuel melted as a function of time given the parameter values and models that correspond to that sample member.
3. The probability of recovery as a function of time is determined for each sample member by integrating Equation (3), using the SFUEL prediction for $m_f(t)$ as input. The following equation applies:

$$P_{\mathrm{rec},i}(t) = \int_0^t F[m_{f,i}(t'), t']dt' \tag{4}$$

where the subscript $i$ indicates the sample member number.

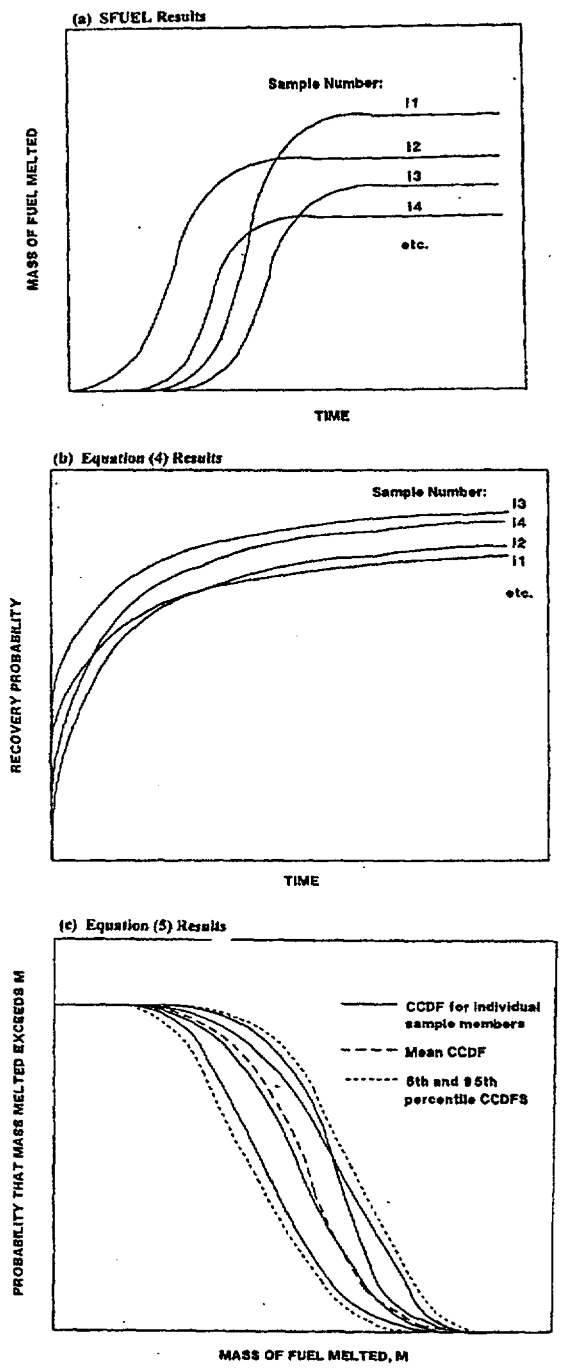



*Figure 12.* Schematic of process leading to complementary cumulative distribution functions (CCDFs) for mass of fuel melted.

4. A complementary cumulative distribution function (CCDF) for the total mass of fuel melting is constructed for each sample member. The probability that $m_{f,i} \geq M$ is equal to the probability that recovery has not been achieved by the time the mass of melted fuel reaches $M$. That is to say,

$$P(m_{f,i} \geq M) = 1 - P_{\text{rec}}(t_{M,i}) \quad \text{where} \quad t_{M,i} = m_{f,i}^{-1}(M) \tag{5}$$

5. Using the CCDFs for the individual sample members, a mean CCDF is obtained as well as CCDFs representing the 5$^{th}$ and 95$^{th}$ percentile confidence levels. These are derived by noting that the CCDF for each sample member has an associated degree of belief of $1/N$, where $N$ is the number of sample members. That each sample member has the same degree of belief results from the fact that the sampling was performed using input distributions that represent degrees of belief.

## 6. Summary

A set of deterministic and probabilistic methods has been developed for analyzing the heat-up and possible melting of spent fuel following a complete drainage of the pool. Results from these methods show the amount of fuel melting that could occur for particular storage configurations and fuel loading patterns. They also provide insights into how judicious choices of design variables, loading patterns, and human actions could mitigate the consequences of the accident. Although the details of the methods apply to a specific type of accident, namely a rapid drainage of all the water, the principles could be applied to other types of accidents and other types of storage configurations.

## 7. Acknowledgements

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## 8. References

1. Reactor Safety Study (1975) WASH-1400, U.S. Nuclear Regulatory Commission, Washington, DC.
2. Chapman, R.H. (1977) Multirod Burst Test Program, Quarterly Progress Report, ORNL/NUREG/TM-77, Oak Ridge National Laboratory, Oak Ridge, TN.
3. Benjamin, A.S., McCloskey, D.J., Powers, D.A., and Dupree, S.A. (1979) Spent Fuel Heatup Following Loss of Water During Storage, SAND77-1371, NUREG/CR-0649, Sandia National Laboratories, Albuquerque, NM.
4. Pisano, N.A. (1984) The Potential for Propagation of Spent-Fuel Overheating Following Loss of Water During Storage, Master's Thesis, Massachusetts Institute of Technology, Cambridge, MA.
5. Bell, M.J. (1973) ORIGEN – The ORNL Isotope Generation and Depletion Code, ORNL-4628, Oak Ridge National Laboratory, Oak Ridge, TN.
6. Leistikow, et al. (1976) Study on High Temperature Steam Oxidation of Zircaloy-4 Cladding Tubes, Nuclear Safety Project, Second Semiannual Report, KfK-2262, Karlsruhe, Germany.
7. White, J.H. (1967) AEC Fuels and Material Development Program, Progress report No. 67, GEMP-67, General Electric Company, Valley Forge, PA.
8. Hayes, E.T., and Roberson, A.H. (1949) Some Effects of Heating Zirconium in Air, Oxygen, and Nitrogen, *J. Electrochem. Soc.*, Vol. 96.
9. Severe Accident Risks: An Assessment for Five U.S. Nuclear Power Plants (1990), NUREG-1150, U.S. Nuclear Regulatory Commission.

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