SENSITIVITY ANALYSIS OF THE QUENCH-04 NUCLEAR SAFETY EXPERIMENT USING THE ADJOINT SENSITIVITY ANALYSIS PROCEDURE (ASAP) IN RELAP5/MOD3.2 CODE SYSTEM

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ABSTRACT

To investigate the hydrogen source term produced by water re-flooding the uncovered core of a Light Water Reactor (LWR), the Research Center Karlsruhe (FZK) has initiated the QUENCH Experimental Program. This work illustrates the use of the Adjoint Sensitivity Analysis Procedure (ASAP), recently implemented into the RELAP5/MOD3.2 reactor safety code system, for performing sensitivity analysis of the calculated temperature profiles at selected axial and radial levels in the rod bundle of the QUENCH-04 experiment at the Research Center Karlsruhe (FZK).

1. INTRODUCTION

The most important accident management measure for terminating a postulated severe accident transient in a Light Water Reactor (LWR) is the re-flooding of the uncovered, degraded core with water. During the re-flooding process, though, the immediate consequence of the contact of water and/or steam with the core material is not a cooling of this material, as would be intuitively expected, but an enhanced oxidation of the zircaloy fuel cladding, accompanied by an increase in temperature, hydrogen production, and fission product release. Since the physical and chemical processes underlying the release of hydrogen under the above circumstances are poorly known, the Research Center Karlsruhe (FZK) has initiated the QUENCH Experimental Program. The objectives of this program are to: (a) generate an extensive data base for developing detailed mechanistic fragmentation models; (b) examine the physico-chemical behavior of overheated fuel elements under various flooding conditions; (c) study the effects of water/steam insertion at various stages of core degradation; (d) develop cladding failure criteria and study the cracking of oxide layers; (e) determine the hydrogen source term for use in code systems for reactor safety analysis. In particular, Section 2 describes briefly the QUENCH-4 experiment.

The pre-test parameters for the QUENCH experiments, and the post-test analysis and interpretation of the experimental results are performed with the RELAP5/MOD3.2 safety analysis code system, using its two-fluid thermal-hydraulics and heat structure models. For both pre-test and post-test analyses, it is important to understand the sensitivities of measured and calculated results (such as temperature profiles, pressures, and hydrogen production) to parameters underlying the QUENCH experiment, such as initial and boundary conditions, geometry, and material properties. Therefore, the implementation of efficient methods to

analyze the sensitivity of results (responses) calculated with the RELAP5 code system is of considerable interest to the design and interpretation of the QUENCH experiments. Furthermore, the establishment of an efficient sensitivity analysis capability in RELAP5 would also represent a major development towards establishing a general-purpose code system for the analysis of postulated safety transient scenarios.

In practice, the most efficient procedure for deterministic local sensitivity analysis of large-scale nonlinear systems is the Adjoint Sensitivity Analysis Procedure (ASAP), originally developed by Cacuci (1981). As has been previously reported, the ASAP has been implemented for the **two-fluid model with non-condensable(s)** in RELAP5/MOD3.2, resulting in an additional code segment in RELAP5, called ASM-REL/TF (see, e.g., Cacuci and Ionescu-Bujor 2000, and Ionescu-Bujor and Cacuci, 2000). This work describes briefly the continuation of this work, namely the implementation of ASAP for the *heat structure models* in RELAP5/MOD3.2, its coupling to the extant ASM-REL/TF, and its validation using the QUENCH-04 experiment. The derivation of the Adjoint Sensitivity Model corresponding to the heat structures is described in Section 3. As will be noted there, each heat structure contributes a distinct matrix equation, which is subsequently coupled to the extant ASM-REL/TF. The resulting system of matrix equations is denoted as the ASM-REL/TFH. Section 4 presents illustrative adjoint sensitivity analysis results, using the ASM-REL/TFH, for the QUENCH-04 experiment. Finally, Section 5 presents a summary, conclusions, and a brief description of current work.

2. Brief Description of the QUENCH-04 Experiment

The QUENCH experimental facility (L. Sepold et al., 2002) comprises the following component systems: a test section with fuel rod simulators; an electric power supply for heating the test bundle; a water and steam supply system; an argon-gas supply system; hydrogen measurement devices; a process control system; a data acquisition system. The design characteristics of the test bundle are depicted in Fig. 1, while a top-view of the fuel rod simulator bundle is presented on the right side of Fig. 2. As Fig. 2 indicates, the test bundle includes four (4) unheated corner rods and 21 fuel rod simulators, each of ca. 2.5 m long. The positioning of the four corner rods helps to obtain a more uniform radial temperature profile; these rods are also used to determine the thickness of the axial oxide layer, at any given instance in time.

The central fuel rod simulator is unheated, while the others rods can be heated electrically over a length of 1024 mm. The unheated rod is filled with solid ZrO_2 pellets, while the heated rods contain centrally located tungsten heaters surrounded by annular ZrO_2 pellets. All of the rods are clad with Zircaloy-4, identical in composition and size to that used in typical Pressurized Water Reactors (PWR), namely: 10.75 mm outside diameter, and 0.725 mm wall thickness. The rods are filled with a mixture of 95% argon and 5% krypton at approx. 0.22 MPa, just slightly above the pressure in the rest of the test section. The krypton additive allows detection (using a mass spectrometer) of fuel rod failure during the experiment.

As shown in Fig.2, the test bundle is surrounded by a shroud made of Zircaloy (2.38 mm thickness), a fiber insulation of ZrO_2 (37 mm thickness), and an annular stainless steel cooling jacket. The 6.7 mm annulus of the cooling jacket is cooled by argon. To allow for higher radial heat losses, the ZrO_2 insulation extends axially only up to the 1024 mm elevation of the heated region. To reduce the magnitude of the maximum temperature in the axial direction, the top region of the cooling jacket is cooled by water.

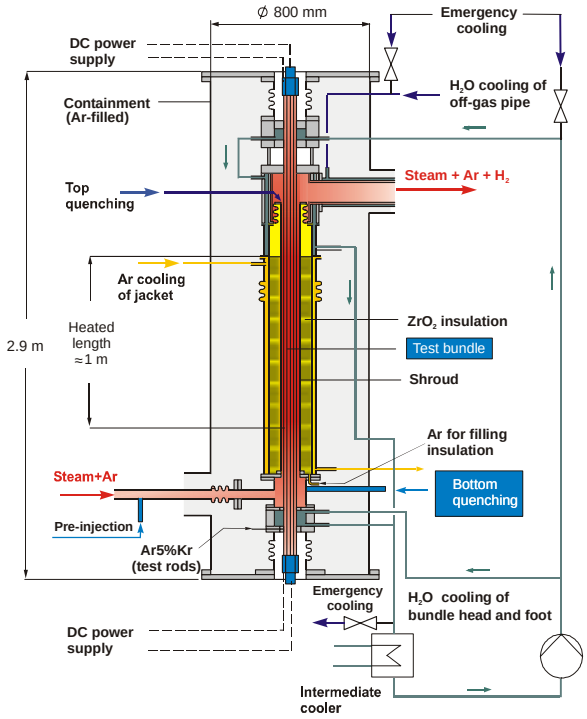

Figure 1: QUENCH Test Section

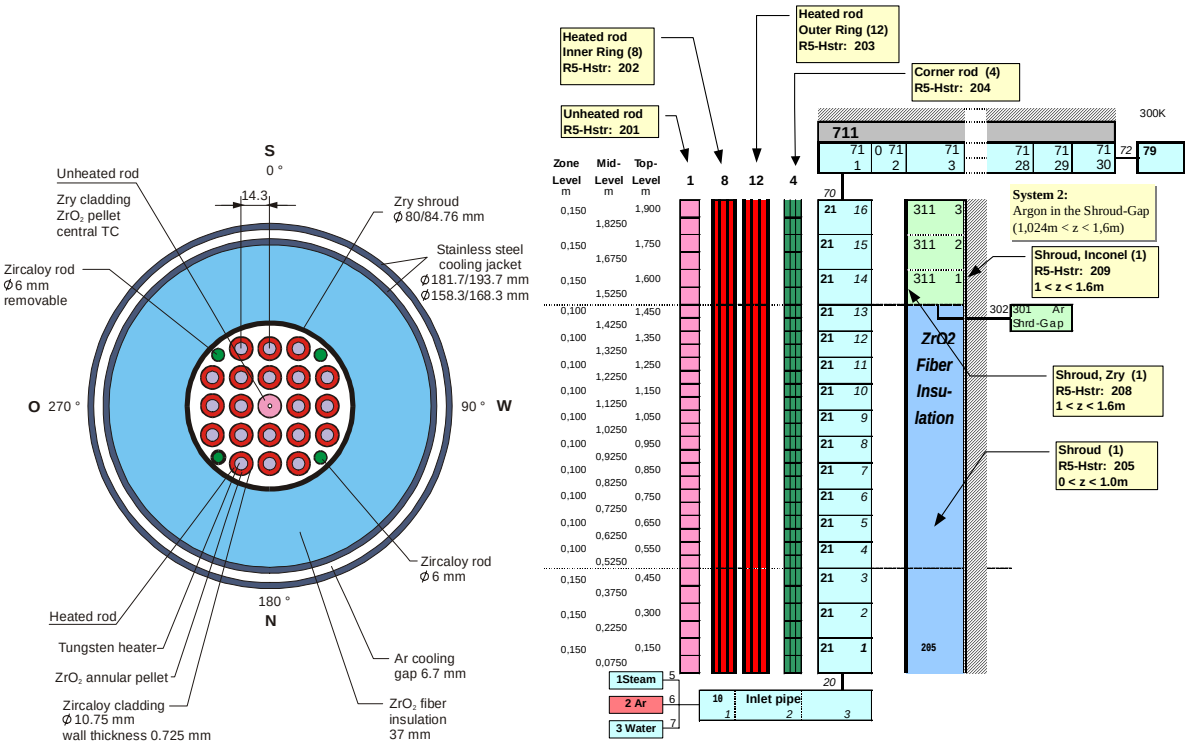

Figure 2: QUENCH-04 Fuel Rod Simulator Bundle (left)
and its RELAP5/MOD 3.2 Representation (right)

In the QUENCH-04 experiment, the bundle was initially heated from room temperature to ca. 900 k, in an atmosphere of flowing argon (3 g/s) and steam (3 g/s). The bundle was stabilized at 900 K for about 2 hours, at an electrical power level of 4.3 kW. At the end of this stabilization period, the electrical power was increased so that the bundle was ramped at 0.31 W/s per rod, giving an average temperature increase of 0.35 K/s between 900 - 1400 K, and 1.0 K/s between 1400- 1750 K, respectively, until the power level reached 16.2 kW. Table 1 presents the complete sequence of events in the QUENCH-04 experiment.

Table 1: Quench-04 Sequence of Events

Time [s]	Event
0	Start of data recording
90	Start of electric power transient
2012	Corner rod B withdrawn from the bundle (T ~ 1780K)
2030	Begin of temperature escalation at the 750 mm level (1560 K) and at the 1050 mm level (1570 K)
2033	Begin of temperature escalation at the shroud (1050 mm, 1350 K)
2040	Begin of significant H2 production, based on the mass spectrometer data
2065	Steam flow of 3 g/s turned off and cool-down steam turned on, cool-down-steam at 42 g/s, strong temperature decrease at –250 mm
2088	16.2 kW of electric bundle power reached, start of electric power reduction from 16.2 kW to 4 kW
2103	Electric power of 4 kW reached
2302	Electric power shut off
2303	Cool-down steam flow turned off
2304	Steam flow at zero
2528	End of data recording

To simulate the QUENCH series of tests with RELAP5/MOD 3.2, the test section has been discretized spatially as depicted in the diagram on the right-side of Fig. 2. The RELAP5/MOD 3.2 simulation of the QUENCH-04 experiment commenced with the initiation of the power transient and was terminated 1000 s (actual time) into the test transient in order to ensure that the physical phenomena during the respective time period did not exceed the code-system's capabilities to simulate them.

3. ASM-REL/TFH: The Coupled Two-Fluid/Heat Structure Adjoint Sensitivity Model

The two-fluid model in RELAP5/MOD 3.2 consists of a system of nine coupled nonlinear partial differential equations describing the conservation of mass, momentum and energy for the liquid and

gaseous phases, including non-condensable materials in the gaseous phase and boron concentration in the liquid field. Corresponding to these nine equations, there are nine state (i.e., dependent) variables, as follows: the gas specific internal energy, U_g, the fluid specific internal energy, U_f, the void fraction, α_g, the pressure, P, the total non-condensable mass fraction, X_n, the non-condensable mass fraction for the i-th non-condensable species, X_{ni}, the boron density, ρ_b, the gas velocity, v_g, and the fluid velocity, v_f. The nine field equations are re-arranged into the so-called "Numerically Convenient Set of Differential Equations", which are then solved numerically by using a staggered spatial mesh and either a semi-implicit or a nearly-implicit integration procedure in time.

Heat structures in RELAP5 permit calculation of the heat transferred across solid boundaries of hydrodynamic volumes. Modeling capabilities of heat structures include fuel pins or plates with nuclear or electrical heating, heat transfer across steam generator tubes, and heat transfer from pipe and vessel walls. In RELAP5, the heat structures are represented by one-dimensional conduction in rectangular, cylindrical, or spherical geometry. Temperature-dependent thermal conductivities and volumetric heat capacities are provided in tabular or functional form, either from built-in or user supplied data. The time-dependence of the heat source can be obtained from reactor point-kinetics, tables of power versus time, or a control variable. Boundary conditions include symmetry or insulated conditions, a correlation package, tables of surface temperature versus time, heat transfer rate versus time, and a heat transfer coefficient versus time or surface temperature. The heat transfer correlation package can be used for heat structure surfaces connected to hydrodynamic volumes, and contains correlations for convective, nucleate and transition boiling, and film boiling heat transfer from the wall to water, and reverse transfer from the water to wall (including condensation). The coefficients that enter in these correlations, as well as the coefficients describing the initial and boundary conditions for the heat conduction equations for the respective structures (and for the two-fluid equations, too) are parameters to be investigated as part of a comprehensive sensitivity analysis.

The heat conduction equations for the heat structures together with the respective initial conditions and boundary conditions (which couple the heat transfer through the structures to the two-fluid model), are discretized by using finite difference methods. For each heat structure Hs, (s = 1,...,NH = total number of heat structures), connected to a hydrodynamic volume L (located between hydrodynamic junctions j and j+1, respectively), the discretization procedure yields the following matrix equation:

$$\underbrace{\begin{bmatrix} hb_1^n & hc_1^n & & & \\ ha_2^n & hb_2^n & hc_2^n & & \\ & \cdots & \cdots & \cdots & \\ & & ha_{M-1}^n & hb_{M-1}^n & hc_{M-1}^n \\ & & & ha_M^n & hb_M^n \end{bmatrix}}_{(AS)_s^n} \begin{bmatrix} T_{s1} \\ T_{s2} \\ \\ T_{sM-1} \\ T_{sM} \end{bmatrix}^{n+1} = \begin{bmatrix} hd_1^n \\ hd_2^n \\ \\ hd_{M-1}^n \\ hd_M^n \end{bmatrix}, \qquad (1)$$

where for each heat structure s, the dependent variables are the surface temperatures $T_{s,i}^n$, at the spatial mesh-point index i = 1,…, Ms (= maximum number of mesh points for structure s), and the time-step index n = 1,…,NF (= final time-step).

The functional dependencies of the components in Eq. (1) are as follows:

(i) for the left boundary:

$$\begin{aligned}
&hb_1^n\left(P_L^n, U_g^n, U_f^n, \alpha_g^n, X_n^n, v_{g,j}^n, v_{g,j+1}^n, v_{f,j}^n, v_{f,j+1}^n, T_{s,1}^n, T_{s,2}^n\right),\\
&hc_1^n\left(P_L^n, T_{s,1}^n, T_{s,2}^n\right),\\
&hd_1^n\left(P_L^n, U_g^n, U_f^n, \alpha_g^n, X_n^n, v_{g,j}^n, v_{g,j+1}^n, v_{f,j}^n, v_{f,j+1}^n, T_{s,1}^n, T_{s,2}^n\right),
\end{aligned} \tag{2}$$

(ii) for each interior mesh-point i=2,M-1:

$$\begin{aligned}
&ha_i^n\left(P_L^n, T_{s,i-1}^n, T_{s,i}^n, T_{s,i+1}^n\right),\\
&hb_i^n\left(P_L^n, U_g^n, U_f^n, \alpha_g^n, X_n^n, v_{g,j}^n, v_{g,j+1}^n, v_{f,j}^n, v_{f,j+1}^n, T_{s,i-1}^n, T_{s,i}^n, T_{s,i+1}^n\right),\\
&hc_i^n\left(P_L^n, T_{s,i-1}^n, T_{s,i}^n, T_{s,i+1}^n\right),\\
&hd_i^n\left(P_L^n, U_g^n, U_f^n, \alpha_g^n, X_n^n, v_{g,j}^n, v_{g,j+1}^n, v_{f,j}^n, v_{f,j+1}^n, T_{s,i-1}^n, T_{s,i}^n, T_{s,i+1}^n\right).
\end{aligned} \tag{3}$$

(iii) for the right boundary:

$$\begin{aligned}
&ha_M^n\left(P_L^n, T_{s,M-1}^n, T_{s,M}^n\right),\\
&hb_M^n\left(P_L^n, U_g^n, U_f^n, \alpha_g^n, X_n^n, v_{g,j}^n, v_{g,j+1}^n, v_{f,j}^n, v_{f,j+1}^n, T_{s,M-1}^n, T_{s,M}^n\right),\\
&hd_M^n\left(P_L^n, U_g^n, U_f^n, \alpha_g^n, X_n^n, v_{g,j}^n, v_{g,j+1}^n, v_{f,j}^n, v_{f,j+1}^n, T_{s,M-1}^n, T_{s,M}^n\right).
\end{aligned} \tag{4}$$

The Adjoint Sensitivity Analysis Procedure (ASAP) is implemented by applying the general procedure described by Cacuci (1981), along the same conceptual lines as was done for the two-fluid model in RELAP5/MOD3.2 (Cacuci and Ionescu-Bujor, 2000). The first step is to G-differentiate Eq. (1) with respect to the dependent variables and parameters, respectively. Then, we relate the resulting equations to the sensitivity DR of the system's response R in such a way as to eliminate the need to calculate the G-derivatives of the dependent variables. Specifically, this procedure involves introducing the adjoint operators to the G-differentiated two-fluid/heat structure equations, and relating the source for the resulting adjoint equations to the sensitivity DR. Although the length of the actual derivations preclude them from being reproduced here, the end-result for the expression of the sensitivity DR of a generic system response R can be represented in scalar-product form as

$$DR = (\Phi A)^T (KA), \tag{5}$$

where: (i) the superscript T denotes "transposition", (ii) the block column vector (KA) contains the (Gateaux-) derivatives of the coupled two-fluid/heat structure equations with respect to all of the parameters that enter in these equations, and (iii) the adjoint function $(\Phi A)^T$ is the solution of the coupled two-fluid/heat structure adjoint system, referred henceforth as the ASM-REL/TFH system. In block-matrix form, the ASM-REL/TFH can be written as

$$(GA)^T (\Phi A) = QA, \tag{6}$$

where the block column vector $(QA) \equiv \begin{bmatrix} (QA)^o \\ \vdots \\ (QA)^{NF} \end{bmatrix}$ has components $(QA)^n \equiv \begin{bmatrix} Q^n \\ QS^n \end{bmatrix}$, and where

Q^n and $(QS)^n$ are the adjoint sources (which depend on the response under consideration) corresponding to the two-fluid and heat structures, respectively.

In component form, Eq. (6) becomes

$$\begin{bmatrix} I_A & \left(HA^{o}\right)^{T} & 0 & \cdots & 0 & 0 \\ 0 & \left(GA^{o}\right)^{T} & \left(HA^{1}\right)^{T} & \cdots & 0 & 0 \\ 0 & 0 & \left(GA^{1}\right)^{T} & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \left(GA^{NF-2}\right)^{T} & \left(HA^{NF-1}\right)^{T} \\ 0 & 0 & 0 & \cdots & 0 & \left(GA^{NF-1}\right)^{T} \end{bmatrix} \begin{bmatrix} \Phi A^{o} \\ \Phi A^{1} \\ \Phi A^{2} \\ \cdots \\ \Phi A^{NF-1} \\ \Phi A^{NF} \end{bmatrix} = \begin{bmatrix} QA^{o} \\ QA^{1} \\ QA^{2} \\ \cdots \\ QA^{NF-1} \\ QA^{NF} \end{bmatrix} \tag{7}$$

where the components are themselves block-matrices of the form

$$HA^{n-1} \equiv \begin{bmatrix} H^{n-1} & OT^{n-1} \\ ES^{n-1} & US^{n-1} \end{bmatrix}; \quad GA^{n-1} \equiv \begin{bmatrix} G^{n-1} & NT^{n-1} \\ 0 & AS^{n-1} \end{bmatrix}; \; n = 1,..., NF \; (\text{time} - \text{step index}) \tag{8}$$

Note that the block-matrices H^{n-1} and G^{n-1} result from taking G-derivatives of the two-fluid equations with respect to the two-fluid dependent variables. Similarly, the block-matrices US^{n-1} and AS^{n-1} result from taking G-derivatives of the heat structures equations with respect to the heat structures dependent variables. Furthermore, the block-matrices OT^{n-1} and NT^{n-1} result from taking G-derivatives of the two-fluid equations with respect to the heat structures dependent variables. Finally, the block-matrix ES^{n-1} results from taking G-derivatives of the heat structures equations with respect to the two-fluid dependent variables.

Performing the block-matrix multiplications in Eq. (7) highlights the ASM-REL/TFH system's time-dependence, namely:

$$\begin{cases} \left[GA^{NF-1}\right]^{T} \left(\Phi A\right)^{NF} = \left(QA\right)^{NF}, \;\; \text{for } n = NF; \\ \left[GA^{n-1}\right]^{T} \left(\Phi A\right)^{n} + \left[HA^{n}\right]^{T} \left(\Phi A\right)^{n+1} = \left(QA\right)^{n+1}, \;\; \text{for } n = NF-1,...,1; \\ \left(\Phi A\right)^{o} + \left[HA^{o}\right]^{T} \left(\Phi A\right)^{1} = \left(QA\right)^{1}, \;\; \text{for } n = 0. \end{cases} \tag{9}$$

As indicated in Eq. (9), the ASM-REL/TFH equations are first solved at the final time-step, n=NF, in the sequence:

$$\begin{cases} \left(G^{NF-1}\right)^{T} \Phi^{NF} = Q^{NF}, \; (\text{two - fluid adjoint equation}), \\ \left(AS^{NF-1}\right)^{T} \Psi^{NF} = QS^{NF} - \left(NT^{NF-1}\right)^{T} \Phi^{NF}, \; (\text{adjoint equation for heat structures,} \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{coupled to the eq. above}). \end{cases} \tag{10}$$

Usually, Q^{NF} and QS^{NF} are zero (due to the definition of the sensitivity DR of the response R), so that Φ^{NF} and Ψ^{NF} are usually zero.

As indicated in Eq. (9), the next set of adjoint equations to be solved backwards in time, for n=NF-1,...,1, are

$$\begin{cases} \left(G^{n-1}\right)^{T} \Phi^{n} = Q^{n} - \left(H^{n}\right)^{T} \Phi^{n+1} - \left(ES^{n}\right)^{T} \Psi^{n+1}, \\ \left(AS^{n-1}\right)^{T} \Psi^{n} = QS^{n} - \left(NT^{n-1}\right)^{T} \Phi^{n} - \left(OT^{n}\right)^{T} \Phi^{n+1} - \left(US^{n}\right)^{T} \Psi^{n+1}. \end{cases} \quad \text{for } n = NF-1,...,1. \tag{11}$$

Note that the above equations fully couple contributions from the two-fluid equations with those from the heat structure equations.

Finally, the calculation of the ASM-REL/TFH is completed by solving the last adjoint equation in Eq. (9), for n=0, namely:

$$\begin{cases} \Phi^{o} = Q^{o} - \left(H^{o}\right)^{T} \Phi^{1} - \left(ES^{o}\right)^{T} \Psi^{1}, \\ \Psi^{o} = QS^{o} - \left(OT^{1}\right)^{T} \Phi^{1} - \left(US^{o}\right)^{T} \Psi^{1}. \end{cases} \quad \text{for } n = 0. \tag{12}$$

4. Adjoint Sensitivity Analysis of the QUENCH-04 Experiment: Illustrative Results

The coupled two-fluid/heat structure adjoint sensitivity model ASM-REL/TFH has been validated by calculating sensitivities of various time-dependent temperatures in the test bundle to variations in various initial conditions for the Quench-04 experiment. The tables below present typical time-dependent sensitivities calculated with ASM-REL/TFH; these sensitivities have been validated by comparisons with exact recalculations for by using 1% variations in the initial conditions for the respective temperatures. Thus, Table 2 presents typical sensitivities of the temperature in the unheated fuel rod.

Table 2: Sensitivities of central temperature in unheated fuel rod

Perturbation	t (s)	No. of time steps	nominal value Tnom (K) at t = tfinal	adjoint method Tpert-Tnom (K)	Exact Recalculation Trec-Tnom (K)
1% of central temperature in 201-001	1	71	509.983	2.24750	2.252
	2	111	509.959	1.17470	1.178
	10	431	510.918	0.43609	0.436
	50	2031	516.452	0.40431	0.405
	100	4031	522.898	0.36920	0.370
	120	4831	525.339	0.35620	0.357
	150	6031	528.868	0.33772	0.338
	200	8031	534.435	0.30942	0.310
	300	12031	544.504	0.26095	0.261

Table 3 presents typical time-dependent sensitivities of the temperature in the heated rod; the exact recalculations were performed by effecting a 1% variation in the initial condition for the central and cladding temperatures, respectively.

Table 3: Sensitivities of temperatures in heated fuel rod

Perturbation	t (s)	time steps	nominal value Tnom (K) at t = tfinal	adjoint method Tpert-Tnom (K)	Exact Recalculation Trec-Tnom (K)
1% of central temperature in 202-006	1	71	740.015	5.45720	5.458
	2	111	740.075	4.10230	4.103
	10	431	742.562	0.92352	0.924
	50	2031	760.786	0.60792	0.608
	120	4831	789.881	0.53774	0.536
	150	6031	801.600	0.51035	0.508
	300	12031	864.215	0.39430	0.390
1% of cladding temperature in 202-006	1	71	739.471	0.16926	0.169
	2	111	740.459	0.11829	0.118
	10	431	744.851	0.07277	0.073
	50	2031	762.938	0.06639	0.066
	300	12031	864.215	0.04309	0.043

Typical time-dependent sensitivities of the temperature in the ZrO_2-insulation to the initial value for this temperature are presented in Table 4, below; the exact recalculations were performed by effecting a 1% variation in the respective initial condition.

Table 4: Sensitivities of temperature in ZrO_2-Insulation

Perturbation	t (s)	time steps	nominal value Tnom (K) at t = tfinal	adjoint method Tpert-Tnom (K)	Exact Recalculation Trec-Tnom (K)
1% of temperature in 205-003	1	71	575.410	0.25792	0.258
	2	111	575.353	0.14989	0.150
	10	431	574.717	0.05672	0.057
	50	2031	571.161	0.04914	0.049
	120	4831	566.360	0.03840	0.039
	300	12031	560.364	0.02024	0.021

Typical time-dependent sensitivities of the temperature in the cooling jacket to a 1% variation in the initial condition of the cladding temperature are presented in Table 5, below.

Table 5. Sensitivities of Temperature in Cooling Jacket (at volume 311-1)

Perturbation	t (s)	time steps	nominal value Tnom (K) at t = tfinal	adjoint method Tpert-Tnom (K)	Exact Recalculation Trec-Tnom (K)
1% of cladding temperature in 209-001	1	71	304.476	0.59733	0.597
	2	111	303.455	0.39149	0.392
	10	431	300.886	0.02786	0.027

CONCLUSIONS

This work has presented illustrative results for sensitivities to initial conditions of various important temperature profiles in the heated and unheated rods, ZrO_2-insulation and cooling jacket for the Quench-04 experiment. These sensitivities indicate that the numerical solution of the coupled two-fluid/heat structure adjoint model, ASM-REL/TFH, is as robust, accurate and stable as the original RELAP5/MOD 3.2 model. Current work un the implementation of the ASAP procedure in the RELAP5 code system focuses on obtaining sensitivities to the many hundreds of parameters in the two-fluid and heat structure equations. The long-range goal of this work is to provide an efficient way to perform comprehensive sensitivity/uncertainty analyses for reactor safety transients.

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