



Porous Debris Behavior Modeling of QUENCH-02, QUENCH-03 and QUENCH-09 Experiments

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ABSTRACT

The heat-up, melting, relocation, hydrogen generation phenomena, relevant for high-temperature stages both in a reactor case and small-scale integral tests like QUENCH, are governed in particular by heat and mass transfer in porous debris and molten pools which are formed in the core region.

Porous debris formation and behavior in QUENCH experiments (QUENCH-02, QUENCH-03, QUENCH-09) plays a considerable role and its adequate modeling is important for thermal analysis. In particular, the analysis of QUENCH experiments shows that the major hydrogen release takes place in debris and melt regions formed in the upper part of the fuel assembly.

The porous debris model was implemented in the Russian best estimate numerical code RATEG/SVECHA/HEFEST developed for modelling thermal hydraulics and severe accident phenomena in a reactor.

The original approach for debris evolution is developed in the model from classical principles using a set of parameters including debris porosity; average particle diameter; temperatures and mass fractions of solid, liquid and gas phases; specific interface areas between different phases; effective thermal conductivity of each phase, including radiative heat conductivity; mass and energy fluxes through the interfaces. The debris model is based on the system of continuity, momentum and energy conservation equations, which consider the dynamics of volume-averaged velocities and temperatures of fluid, solid and gaseous phases of porous debris.

The model is used for calculation of QUENCH experiments. The results obtained by the model are compared to experimental data concerning different aspects of thermal behavior: thermal hydraulics of porous debris, radiative heat transfer in a porous medium, the generalized melting and refreezing behavior of materials, hydrogen production.

1 INTRODUCTION

The heat-up, melting, relocation and hydrogen generation phenomena, relevant for high-temperature stages both in a reactor case and small-scale integral tests like QUENCH [1], are governed in particular by heat and mass transfer in porous debris and molten pools which are

formed in the core region. The rods eventually lose their mechanical holding and collapse into heaps of particles named “porous debris bed”. The accurate modelling of its behavior is very important for adequate description of dynamics.

The analysis of TMI-2 accident [2] and the results of integral out-of-pile (CORA [3], QUENCH [1]) and in-pile experiments (PHEBUS [4], PBF [5]) have shown that before the water succeeds in cooling the fuel pins there will be an enhanced oxidation of the zircaloy cladding that in turn causes a sharp increase in temperature, hydrogen production and fission product release.

The new concepts which are now used in the development of best-estimate computer codes include the detailed self-consistent modelling of wide spectrum of physical phenomena typical of late stage of severe accident. This is why the adequate calculation of porous debris behavior is now a very important part of severe accident analysis using best-estimate computer codes.

Porous debris models will allow more realistic physical modeling of the core degradation, and move the sophistication of the thermal evaluations more parallel to other processes simulations. This is an incremental improvement to a code customized to thermal-hydraulic and severe fuel damage evaluations.

Beside that, porous debris module should ensure:

- sufficient accuracy of the debris heat and mass transfer problem’s solution when the extent of detailed description of core and in-vessel structures is given by external thermal hydraulic code;
- high computational speed and stability of running in the integral code designed for severe accident description;
- some universality which would allow to apply the module to different types of reactors and to different nodalizations within the bounds of one type of reactor.

Unfortunately, the physical processes taking place during the late phase of severe accidents are very complicated and rather far from complete understanding. The main phenomena important for adequate description of debris behavior are as following: debris formation, coolant flow through debris and corresponding heat transfer, mass and energy transfer in debris, phase transitions and chemical reactions, decay and chemical heat generation, convective and radiative heat transfer, solid crust formation and disappearance on region boundaries.

It is assumed that new metallic surfaces are formed by cracking and fragmentation of the oxygen-embrittled cladding tubes as a result of the thermal shock during flooding leading to enhanced oxidation and hydrogen generation.

Cladding melt relocation occurred laterally and axially within the confinement of the scale by which the surface area is diminishing and the thermal contact to the pellets is improving [1]. This contributes to the development of large temperature variations. Together with the embrittlement of bare scale (without contact to metallic cladding but in contact with the steam) this can result in scale cracking and triggering of internal oxidation and outward melt penetration, which will accelerate the steam oxidation. The analysis of QUENCH-02, QUENCH-03 and QUENCH-09 experiments shows that the major hydrogen release took place in debris and melt regions formed in the upper part of the fuel assembly.

The factors which complicate the problem are eutectics formations between interacting materials typical of reactor technology (UO_2 , ZrO_2 , Zr, Fe, Cr, Ni, B_4C) and a lack of thermo-physical data for high temperature region (in the course of an accident, the temperature reaches the value 3100K and higher).

The degradation is non-homogeneous and the core exhibits, at the same time, both damaged and undamaged regions. The important part of porous debris numerical analysis is the modelling of radiative heat transfer in the debris and between debris and non-debris

(initial geometry) meshes. Some approaches are used in the literature to describe the radiative heat transfer in the core [13,14].

Heat and mass transfer in porous media have been investigated intensively during the last two decades due to their extremely wide applications including not only nuclear engineering but also geothermal energy, oil industry, pollutant migration in waters, different types of heat exchangers, thermal isolation in buildings and tubes etc. [6-8]. A detailed review of the subject of flow in porous media has been recently done by Pop and Ingham [9].

The debris models have been implemented into known severe accident codes such as RELAP/SCDAP [10], MELCOR [11] and CATHARE/ICARE [12].

The basic differences between the model used in this paper and existing debris bed models implemented into severe accident numerical codes listed above include the unified approach to the description of flowing objects for different stages of degradation (drop, stream, debris, pool), the possibility for application to the constructive and geometrical features of VVER, and the choice of the mechanisms of debris formation.

This work is aimed to the development of a numerical module which is able to model porous debris thermal hydraulics and heat and mass transfer phenomena, and to application of this module to the modelling of QUENCH experiments.

The porous debris mathematical model is developed for the description of the in-vessel stage of severe accident. The basis of the model is the system of continuity, momentum and energy conservation equations, which consider the dynamics of volume-averaged velocities and temperatures of fluid, solid and gaseous phases of porous debris.

The different mechanisms of debris formation are considered, including degradation of fuel rods according to temperature criteria, taking into consideration some correlations between rod layers thicknesses; degradation of rod layer structure due to thermal expansion of melted materials inside intact rod cladding; debris formation due to sharp temperature drop of previously melted material due to reflood; and transition to debris of material from elements lying above.

The results obtained by the model are compared to experimental data concerning different aspects of core behavior during the late stage of degradation: thermal hydraulics of porous debris, radiative heat transfer, hydrogen production and the generalized melting and refreezing behavior in QUENCH-02, QUENCH-03 and QUENCH-09 experiments.

2 QUENCH EXPERIMENTS

The QUENCH experiments (Fig. 1) are to investigate the hydrogen source term that results from the water injection into an uncovered core of a Light Water Reactor (LWR) [1].

The test bundle (Fig. 2) is made up of 21 fuel rod simulators with a length of approximately 2.5 m. 20 fuel rod simulators are heated over a length of 1024 mm, the one unheated fuel rod simulator is located in the center of the test bundle. Heating is carried out electrically using 6-mm-diameter tungsten heating elements installed in the center of the rods and surrounded by annular ZrO₂ pellets. The rod cladding is identical to that used in LWRs: Zircaloy-4, 10.75 mm outside diameter, 0.725 mm wall thickness. The test bundle is instrumented with thermocouples attached to the cladding and the shroud at 17 different elevations with an axial distance between the thermocouples of 100 mm.

The unheated rod simulator is filled with ZrO₂ pellets (bore size 2.5mm internal diameter) for QUENCH-02 and QUENCH-03 tests. In the test QUENCH-09, the control rod was arranged in the bundle center, consisting of absorber rod (B₄C pellets/stainless steel cladding) and zircaloy guide tube. For the heated rods 6mm diameter tungsten heating elements

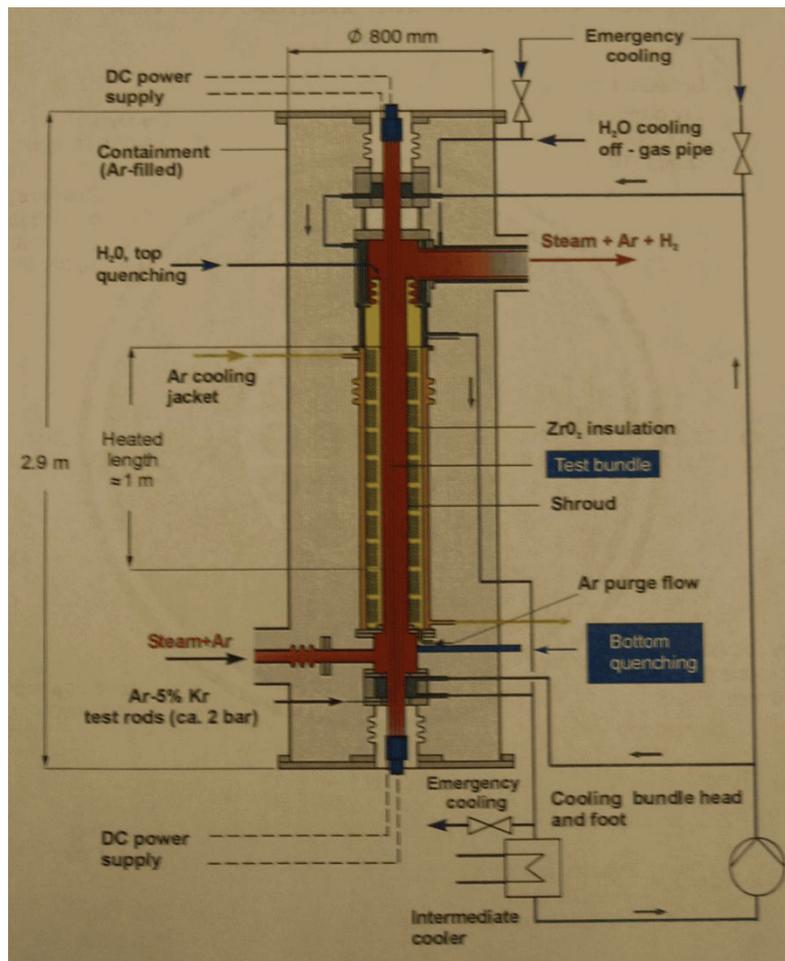


Fig. 1. Schematic representation of QUENCH test section facility

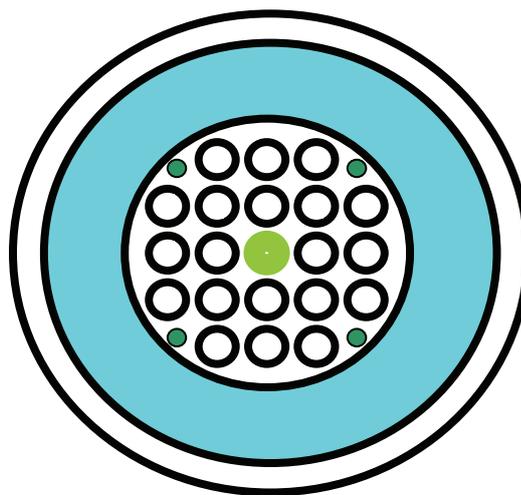


Fig. 2. Cross-section of QUENCH test bundle (20 heated, 1 unheated, 4 corner rods)

are installed in the center of the rods and are surrounded by annular ZrO₂ pellets. The tungsten heaters are connected to electrodes made of molybdenum and copper at each end of the heater.

2.1 QUENCH Facility Modelling

The nodalization scheme of the QUENCH test facility for RATEG/SVECHA/HEFEST thermal hydraulics and severe accident phenomena numerical code is presented in Fig. 3.

The maximum effective heat element radius r_{\max} for square grid relevant to QUENCH fuel assembly is equal to

$$r_{\max} = \frac{d}{\sqrt{\pi}} \quad (1)$$

where d is a pitch. This parameter is important for free volume calculations and the control of mass transfer in intact geometry and debris regions.

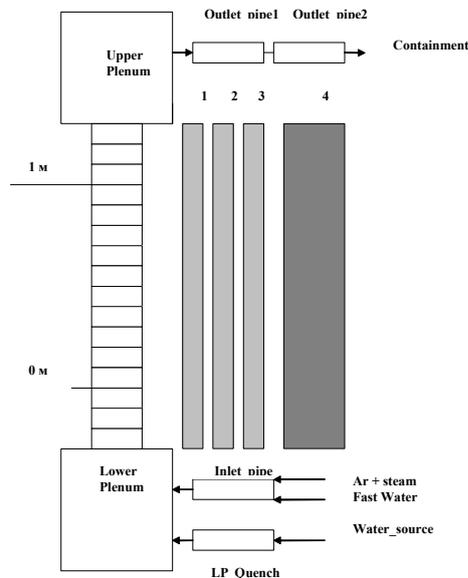


Fig. 3. Nodalization scheme of QUENCH facility

The nodalization scheme used in the debris module for computation of QUENCH experiments had 7 radial and 17 axial meshes. Each axial mesh is 0.1m long.

Let us consider in detail the modelling of the porous debris thermal hydraulics and mass transfer, the processes which are the subject of investigation in this paper.

3 GOVERNING SYSTEM OF EQUATIONS

On the basis of existing experimental data the different mechanisms of porous debris formation from initial rod-like geometry are considered. The criteria for debris formation were derived from the existing physical notions and validated by the computational analysis

of severe accident experiments like QUENCH-03, PHEBUS B9+ (PWR specific) and CORA-W2 which reproduced VVER-type geometry and materials.

3.1 Main Assumptions of Analysis

The main assumptions under which the analysis is done are as following:

- We deal with non-Darcian porous medium in the presence of internal heat generation;
- The viscous dissipation is neglected;
- The fluid is assumed to be viscous and heat-generating;
- The solid is assumed to have a different temperature and is also heat-generating;
- We use conservation equations for mass, momentum and energy for debris dynamics;
- Two-dimensional problem is considered with axial symmetry.

3.2 Basic Equations

Continuity, momentum and energy equations for each phase are used to describe the porous debris dynamics. The approach is based on the phenomenology from the works [15-20] and presented in [21].

For example, a generalized momentum equation for a porous medium is written in the following form:

$$\frac{\rho_f}{\varepsilon s} \frac{\partial \langle \bar{u}_f \rangle}{\partial t} + \frac{\rho_f}{\varepsilon s} \left(\langle \bar{u}_f \rangle \cdot \bar{\nabla} \right) \left(\frac{\langle \bar{u}_f \rangle}{\varepsilon s} \right) = -\bar{\nabla} \langle p \rangle^f + \rho_f \bar{g} + \frac{\mu_f}{\varepsilon s} \Delta \langle \bar{u}_f \rangle - \frac{\mu_f}{K} \langle \bar{u}_f \rangle - \frac{C_E}{K^{1/2}} \rho_f \left| \langle \bar{u}_f \rangle \right| \langle \bar{u}_f \rangle \quad (2)$$

where \bar{u}_f is the velocity vector, ρ_f the fluid density, μ_f the dynamic viscosity, ε the porosity, s the saturation, p the pressure, g the gravity, K the permeability and C_E the Ergun constant [15].

4 NUMERICAL REALIZATION

The system of equations mentioned above was represented in integral form and in two-dimensional geometry for the application of a finite volume (FV) approach. Then, this system was solved using time discretization to find the general independent porous debris parameters (εs , ε , $\langle \bar{u}_{f,ax} \rangle$, $\langle \bar{u}_{f,ra} \rangle$, H_f , H_s and p) for the current time step based on parameters values at the previous time step. Gradient and divergence terms are approximated by ordinary methods typical of FV technics.

The momentum equation in the integral form has the property that the momentum in any control volume (microscopic or macroscopic) is changed only by flow through the surface, forces acting on the surface, and volumetric body forces. This important property is inherited by the discretized equations if the FV approach is used and the surface fluxes for adjacent control volumes are identical. If this is done, then the integral over the entire domain, being the sum of the integrals over the microscopic control volumes, reduces to a sum over the surface of the domain. Overall mass conservation and energy conservation follow in the same way from the continuity and the energy equations, respectively.

The important part of the module (Fig. 4) is the interface sub-module for the heat- and mass transfer between debris and non-debris (initial geometry) meshes. The linkage between

different types of meshes (intact, debris, melt pool) should be done with great accuracy ensuring the total heat- and mass balance in a system.

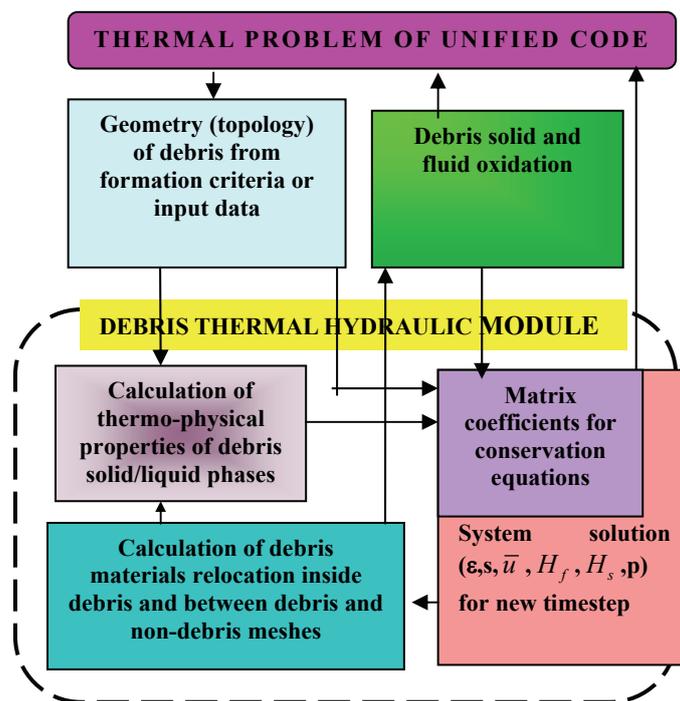


Fig. 4. Block-scheme showing relations between different sub-modules of debris behavior module

5 RESULTS OF QUENCH EXPERIMENTS MODELING

5.1 QUENCH-02/QUENCH-03/QUENCH-09 Test Scenarios

The QUENCH experiments consist of several phases: a first heat-up phase, a thermal equilibrium phase, a second heat-up phase, a pre-oxidation phase (optional), a transient phase, and a quenching phase.

In QUENCH-02 and QUENCH-03 tests, the thermal, mechanical and oxidation behaviour were investigated during the reflood phase for non-pre-oxidized bundle.

The three out-of-pile bundle tests QUENCH-07 to -09 [23], performed at Forschungszentrum Karlsruhe, were dedicated to investigate B₄C control rod behavior and its influence on the fuel rods during a wide range of severe accident conditions under low system pressure in a Western type light water reactor.

Let us consider in more detail the QUENCH-03 and QUENCH-09 tests, for which the wide range of data is well presented in electronic format from the acquisition system, and which, along with QUENCH-02 test, revealed clearly the porous debris behaviour (maximum temperatures achieved are about 2500K). Due to a failure in the data acquisition during the QUENCH-02 experiment only a limited number of data were obtained in this test.

The electric power for QUENCH tests is presented in Fig. 5, and the following scenario is valid (see Table 1) for QUENCH-02, QUENCH-03 and QUENCH-09. There was no pre-oxidation phase in these tests.

During the preliminary heating and heat-up transient phases, superheated steam together with the argon as carrier gas enters the test bundle at the bottom end and leaves the test section at the top together with the hydrogen that is produced in the zirconium-steam reaction.

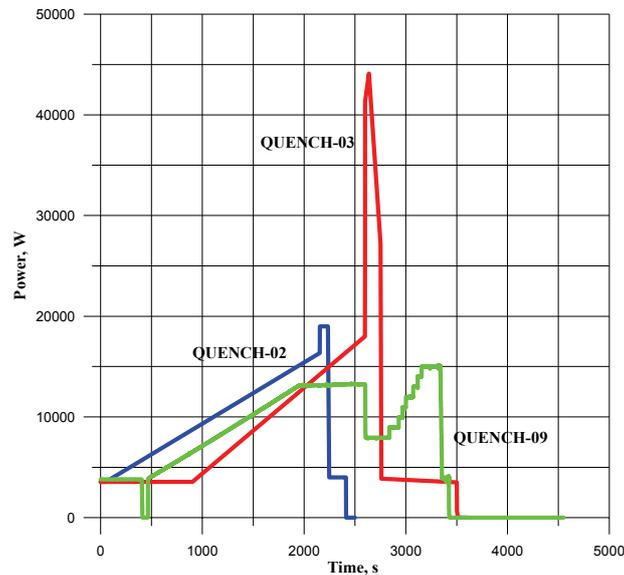


Fig. 5. QUENCH-02/03/09: total electric power history

Table 1: Major Sequence of Events for QUENCH-02, -03, -09

Phase	Rod simulator temperature	Temperature increase	Time
Preliminary heating in argon-steam atmosphere	$\approx 900\text{K}$	$\approx 0\text{K/s}$	$<1000\text{s}$ (QUENCH-03), $<150\text{s}$ (QUENCH-02), $<150\text{s}$ (QUENCH-09)
Heat-up (Ar-H ₂ O)	900-2500K	0.4÷1.6K/s (Q-02), 0.4÷1.0K/s (Q-03), 0.4÷2.0K/s (Q-03)	1000÷2600s (Q-03), 150÷2150s (Q-02) 1000÷3000s (Q-09)
90g/s quench water	$\approx 2500\text{K}$	$\approx 0\text{K/s}$	2600s (QUENCH-03), 2150s (QUENCH-02)
40g/s quench	$\approx 2500\text{K}$	$-(3\div 7)\text{K/s}$	2630s (QUENCH-03), 2175s (QUENCH-02)
50 g/s steam	$\approx 2500\text{K}$	$-(3\div 10)\text{K/s}$	3300s (QUENCH-09)

The quench phase was initiated by turning off the argon and steam flow, filling the lower plenum (Fig. 1) with quench water at a high rate (90 g/s), and injecting argon at the bundle head. About 25÷30s later the test section was reflooded from the bottom at 40÷50 g/s H₂O achieving an injection velocity of 1.6 cm/s (QUENCH-02) and 1.3 cm/s (QUENCH-03). In QUENCH-09 the quench was due turning on the high mass flux (50 g/s) of saturated

steam. As it can be seen from the Fig. 5, during the flooding phase the electrical power was reduced to approximately 4 kW to simulate the decay heat level.

The total amount of hydrogen released during the QUENCH-02, QUENCH-03 and QUENCH-09 experiments was 190g, 123g and 460g, respectively.

The post-test appearance of both test bundles reveals severe oxidation and embrittlement (fragmentation) of the rod claddings and shroud in the upper part as well as melt formation and relocation.

5.2 QUENCH Calculation Results

In Fig. 6 the axial bundle temperature profile for QUENCH-03 is presented for time $t=2250$ s (before the reflood). Fig. 7 and 8 show the temporal dependence of temperature for different axial locations: 850 mm (near the upper part of heated zone) and 650 mm. QUENCH-09 temperature behavior for the level 750 mm is shown in Fig. 9.

The thermal problem is mainly influenced by heat fluxes in a system. The thermal conductivity of the isolation is one of the most pronounced factors. The thermal conductivity data for ZYFB isolation (www.zircarzirconia.com) were used in the modelling.

During the reflood phase strong secondary temperature excursions were observed in the experiment, which is reproduced in computation. This excursion is due to zirconium-steam exothermic reaction.

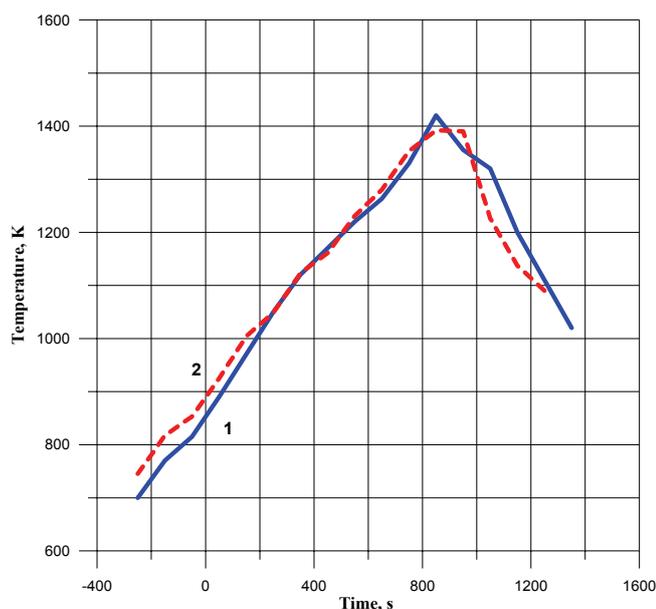


Fig. 6. QUENCH-03: axial temperature profile for $t=2250$ s
1 –experiment, 2 – calculation

Calculated hydrogen integral production for QUENCH-03 is presented in Fig. 10. There were some difficulties in experimental determination of this parameter. Experimental value for H_2 production is estimated as 123 g (18g before the reflood, 105 g after), so this value is in a reasonable consistency with computational results.

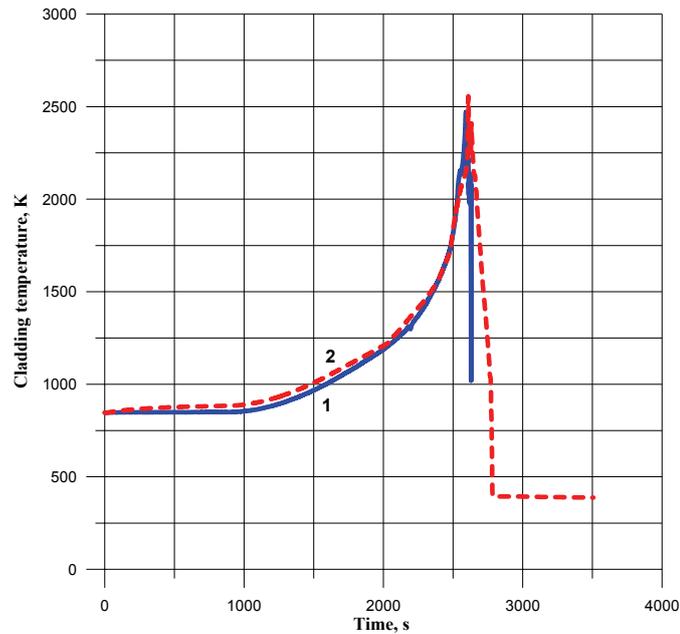


Fig. 7. QUENCH-03: temperature elevation 850 mm:
1 –experiment (TFS3/12), 2 - calculation

Note, that according to calculation results, the oxidation in debris regions contributes a considerable part to integral H_2 production (about 26%), so this circumstance constitutes justification of implemented debris model, of course, only in some extent because the hydrogen production depends on many factors. Calculation results also showed that the major hydrogen release is connected with the reflood phase.

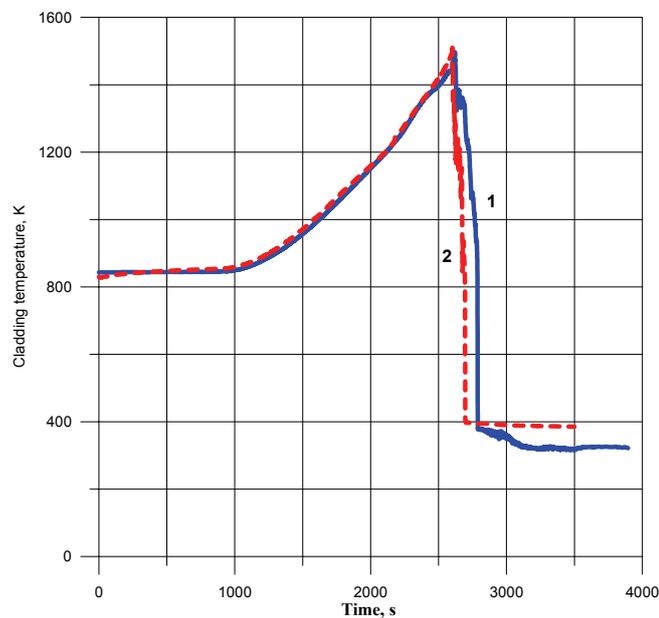


Fig. 8. QUENCH-03: temperature elevation 650 mm:
1 –experiment (TFS3/10), 2 - calculation

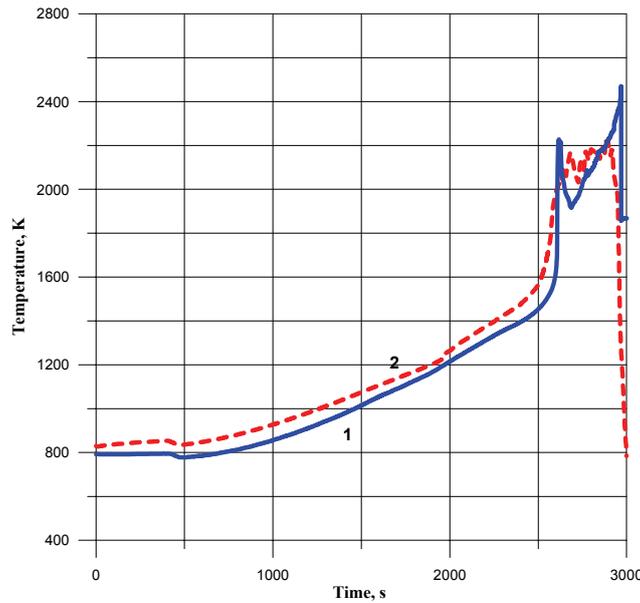


Fig. 9. QUENCH-09: temperature elevation 750 mm:
1 –experiment (TFS4/11), 2 - calculation

As stated in [22], oxidation in molten pool regions has some peculiarities in comparison to oxidation in solid. The oxidation of metallic melts is not described by application of usual kinetic correlations. Melt oxidation together with melt relocation, dispersion and fragmentation is obviously one of the most important quench phenomena.

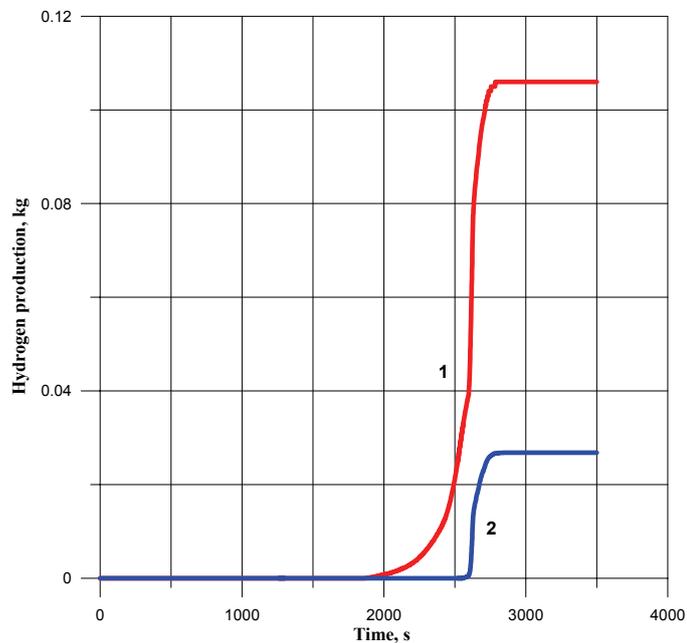


Fig. 10. QUENCH-03 calculated hydrogen production:
1 – total H_2 release, 2 – H_2 release in debris

Fig. 11 shows the net heat balances in a system. The major part of heat to surrounding shroud is due to radiative heat transfer. The heat transferred by steam-argon mixture is the

least part of integral heat balance, which is a characteristic feature of QUENCH-02, QUENCH-03 and QUENCH-09 experiments.

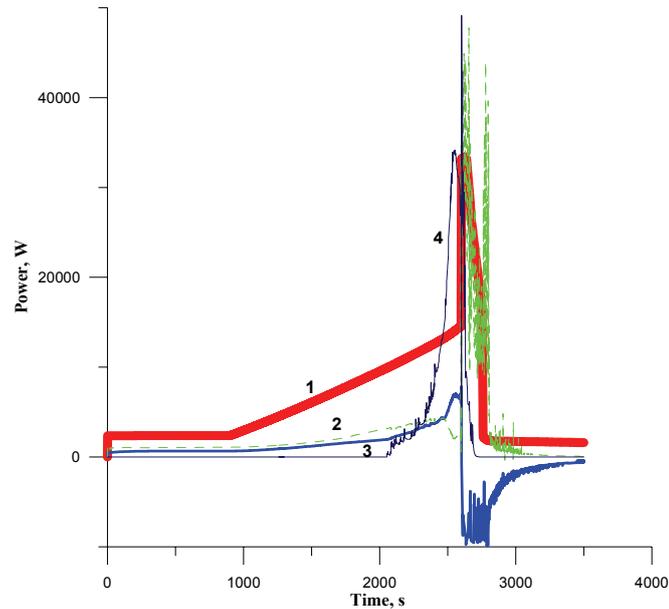


Fig. 11. QUENCH-03 calculation heat balances:

- 1 – total electric power,
- 2 – heat to shroud,
- 3 – heat transferred by gas,
- 4 – chemical power

The debris was formed in calculations at the axial elevations 750 through 850 mm in accordance with experimental results. The fluid part of debris partially flowed down to lower elevation meshes where it was frozen. This qualitative picture is also resembled in post-test observations.

5.3 Mass Relocation in QUENCH Tests

The characteristic value of melt velocity in the experiment is a few mm per second, which is characteristic corium velocity for all QUENCH tests with severe damage (QUENCH-02, QUENCH-03, QUENCH-09 [1,22]). This value is in a good agreement with calculations. The Fig. 12 shows the fluid part of debris velocity module for the second radial group and the elevation of 750 mm for QUENCH-03.

The estimation of melt velocity can be done from the momentum equation (2):

$$\langle \bar{u}_f \rangle \approx \frac{K \rho_f g}{\mu_f} = \frac{Kg}{\nu_f} \quad (3)$$

Let us take the characteristic size for debris particle 3mm. Then, the Kozeny constant K under the conditions of QUENCH tests is about $K \approx 2.75 \cdot 10^{-9}$, so at characteristic kinematic viscosity of melt $\nu_f \approx 1.0 \cdot 10^{-6} m^2/s$ (value characteristic for metal melts with Zr) we could get the following estimation $\langle \bar{u}_f \rangle \approx 2.75 \cdot 10^{-2} m/s$. Taking into account the relative

permeability K_{rf} [16] in the presence of fluid and solid phases of debris, we get finally $\langle \bar{u}_f \rangle \approx 1 \div 5 \text{ mm/s}$.

Fig. 13 shows the temperature dynamics on different levels during QUENCH-09 test. The spikes correspond to the arrival of fluid part of debris. From the analysis of these curves it is possible to support the above-stated estimation for characteristic fluid velocity in the range of several mm per second. The calculated velocity data are in a good agreement with this estimation (Fig. 14).

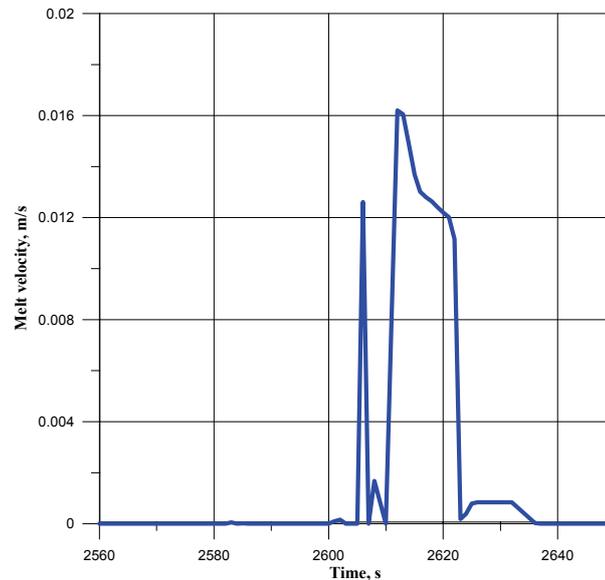


Fig. 12. QUENCH-03 calculated fluid velocity in debris for radial group N=2 and elevation 750 mm

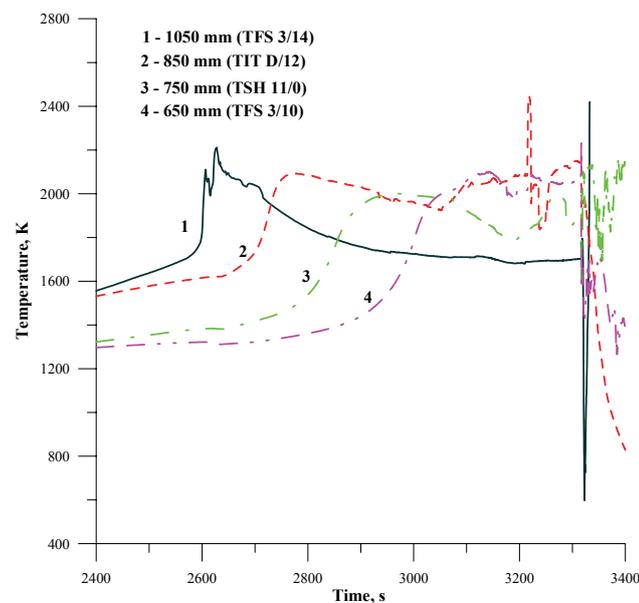


Fig. 13. QUENCH-09 temperature evolution showing mass relocation in debris bed

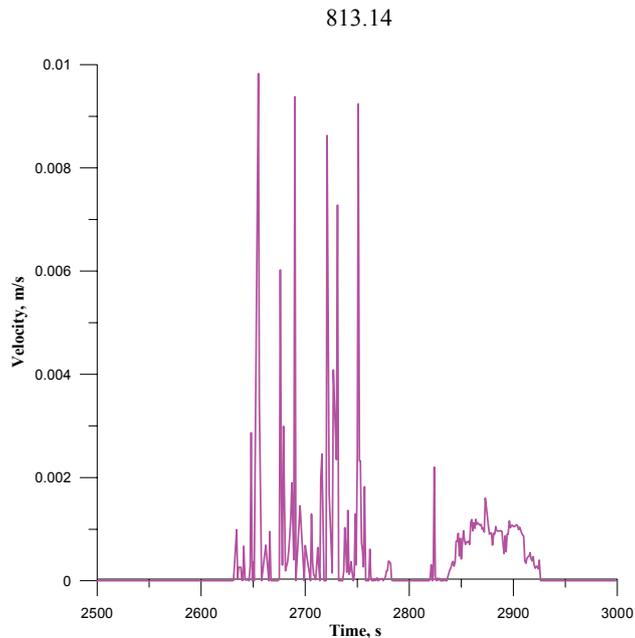


Fig. 14. QUENCH-09 calculated fluid velocity in debris for radial group N=2 and elevation 850 mm

Fig. 15 and 16 demonstrate some interesting debris parameters for second radial zone and elevation of 850 mm: saturation (part of debris pore volume occupied by fluid) and porosity of debris. These figures confirm the complicated dynamics of main porous medium parameters in the course of the experiment.

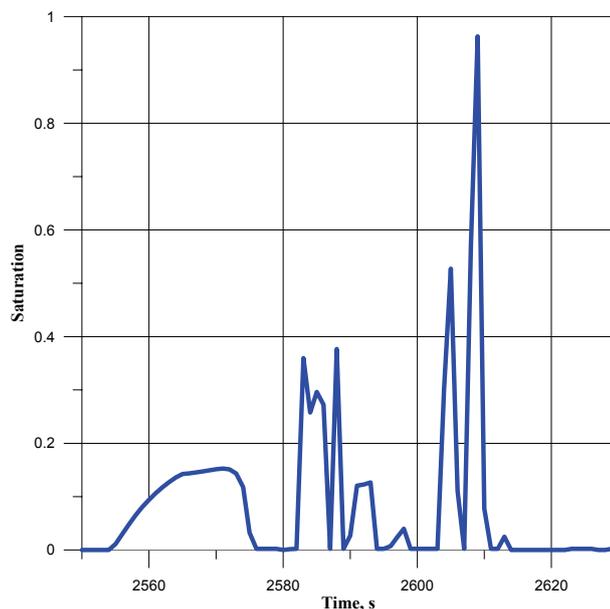


Fig. 15. QUENCH-03 calculated saturation in debris for radial group N=2 and elevation 850 mm

In QUENCH-02 experiment modeling, the similar debris behavior was calculated as in QUENCH-03. Due to different power history in this test, the hydrogen release is more considerable in this case: 40g before the reflood and 133g during the reflood which is in a good consistency with the experimental data.

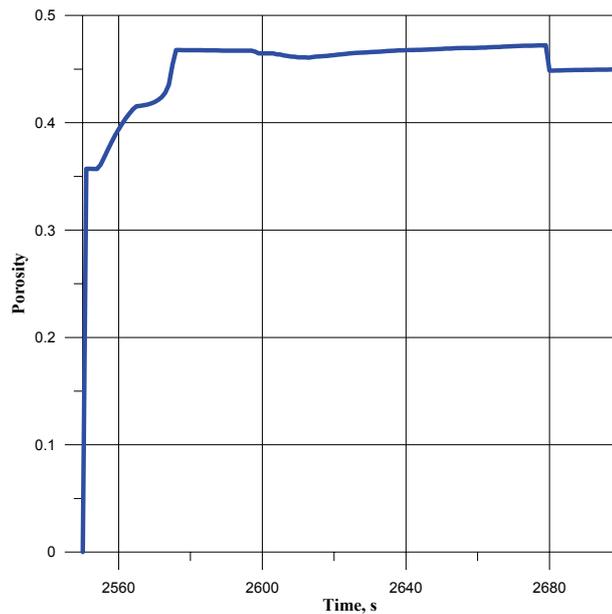


Fig. 16. QUENCH-03 calculated porosity in debris for radial group N=2 and elevation 850 mm

Let us summarize the main results of the investigation. The basic thermal parameters of experiment QUENCH-03 are adequately reproduced by the code. Integral hydrogen production is in a good agreement with the experimental value. Mass transfer in debris is also in a reasonable accordance with observed values, which looks optimistic for justification of implemented debris model.

6 CONCLUSIONS

A module for numerical modelling of core behavior with the formation of porous debris regions during severe accident's late phase is developed. The module is implemented into the Russian best estimate severe accident code, RATEG/SVECHA/HEFEST. This numerical code is able to consider thermal hydraulics, degradation of core and other structures, hydrogen generation, and other phenomena important for realistic description of nuclear reactor severe accidents.

The application of known classical principles and introducing of some special methods allowed to describe the heat and mass transfer self-consistently in the following cases:

- Intact geometry;
- Partially or totally degraded core with debris formation;
- Energy exchange in the cases of considerable zones of degradation including the molten pool regions.

The modelling of QUENCH experiments showed the importance of detailed taking into account of processes in porous debris regions for adequate description of heat and mass transfer as well as hydrogen release.

The QUENCH-02, QUENCH-03 and QUENCH-09 computational results are in a good agreement with experimental data concerning different aspects of thermal behavior: thermal

hydraulics of porous debris, radiative heat transfer in a porous medium, the generalized melting and refreezing behavior of materials.

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