Simulation of Molten Core-Concrete Interaction in Oxide/Metal Stratified Configuration with the TOLBIAC-ICB Code

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ABSTRACT

The frame of this work is the validation of the TOLBIAC-ICB code which is devoted to the simulation of Molten Core-Concrete Interaction (MCCI) for reactor safety analysis. Attention focuses here on the validation of TOLBIAC-ICB in configurations expected to be representative of the long term phase of MCCI i.e. during an interaction between an oxide/metal stratified corium melt and a concrete structure. Up to now the BETA tests performed at the Forschungszentrum Karlsruhe (FzK) are the only tests available to study such kind of interaction. The BETA tests are first described and the operating conditions are reminded. The TOLBIAC-ICB code is then briefly described, with emphasis on the models used for stratified configurations. The results of the simulations are discussed. A sensitivity study is also performed with the power generated in the oxide layer instead of the metal layer as in the test. This last calculation shows that the large axial ablation observed in the tests is probably due to the peculiar configuration of the test with input power in the bottom metal layer. Since in the reactor case the residual power would be mainly concentrated in the upper oxide layer, the conclusions of the BETA tests for the reactor applications, in term of axial ablation, must be derived with caution.

1 INTRODUCTION

In the event of a severe accident in a Pressurized Water Reactor, corium, a mixture of molten materials issued from the fuel, cladding and structural elements, appears in the reactor core. In some scenarios, corium is assumed to melt through the reactor pressure vessel and spread over the concrete basemat of the reactor pit. The main question that has to be addressed is whether and when the corium will make its way through the basemat since it would lead to groundwater contamination.

The development of the TOLBIAC-ICB [1] code was started in 2002 in the frame of an agreement with EDF to provide a numerical tool for safety analysis related to MCCI in reactor situations. The main characteristic of this tool is that it couples thermalhydraulics and

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physicochemistry through a coupling with the GEMINI2 thermodynamic code. Attention focuses here on the validation of TOLBIAC-ICB in configurations expected to be representative of the long term phase of MCCI i.e. during an interaction between an oxide/metal stratified corium melt and a concrete structure.

Up to now the BETA tests [3] performed at the Forschungszentrum Karlsruhe are the only tests available to study such kind of interaction. The BETA experiments are first described and the operating conditions are reminded. This analysis shows that part of the tests are probably not representative of the reactor case principally because of a too high input power. The phenomena occurring in these experiments are presently not modelled in TOLBIAC-ICB since this code is mainly devoted to reactor applications. However, the same analysis indicates that some tests with moderate power input (V2.1, V2.3 and V2.5) might bring into play the phenomena expected in the long term phase of the reactor case. These last experiments were thus selected to validate TOLBIAC-ICB in oxide/metal stratified configuration. The TOLBIAC-ICB code is then briefly described, with emphasis on the models used for stratified configurations. The results of the simulations of BETA test V2.1 are then discussed. They show that the code is able to simulate this stratified configuration with satisfactory agreement. A sensitivity study is also performed with the power generated in the oxide layer instead of the metal layer as in the test. This calculation shows that the large axial ablation observed in the tests is probably due to the peculiar configuration of the test with input power in the bottom metal layer. Since in the reactor case the residual power would be mainly concentrated in the upper oxide layer, the conclusions of the BETA tests for the reactor applications, in term of axial ablation, must be derived with caution.

2 BETA EXPERIMENTS

2.1 General description

The BETA [3] experiments have been performed in the mid 1980-is. The experimental apparatus consists of a concrete crucible (38 cm inner diameter), an induction heating device (maximum power around 2 MW) and a furnace in which the oxide/metallic melt is produced by a thermite reaction. Thermocouples are inserted inside the concrete to follow the ablation of the crucible. The metallic phase is principally composed of a mixture of Fe, Cr and Ni whereas the oxide phase mainly contains Al₂O₃, SiO₂ and CaO. Given the heating technique used in these experiments, the power is injected in the metallic pool and a part is transferred to the oxide phase by convection.

Two series of experiments have been performed. The test matrix of the first series is reported in Table 1. As can be seen here, these experiments are characterised by a high input power except for tests V2.1 to V2.3. Silicate concrete was employed in these experiments except in tests V3.1 to V3.3 to study the effect of concrete. Test V4.1 was performed to analyse the influence of the crucible diameter. The second set of experiments was devoted to the study of the behaviour of non oxidized zirconium and of fission products. Attention focuses in this paper on the experiments of the first series.
Table 1: BETA test matrix [3]

<table>
<thead>
<tr>
<th>Test</th>
<th>Melt</th>
<th>Power kWs</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>V0.1</td>
<td>Iron</td>
<td>0</td>
<td>Test of facility</td>
</tr>
<tr>
<td>V0.2</td>
<td>Iron</td>
<td>400</td>
<td></td>
</tr>
<tr>
<td>V0.3</td>
<td>Iron+Oxide</td>
<td>1700</td>
<td></td>
</tr>
<tr>
<td>V1.1</td>
<td>Iron</td>
<td>Pulsed</td>
<td>Power failed</td>
</tr>
<tr>
<td>V1.2</td>
<td>Iron+Oxide</td>
<td>Pulsed</td>
<td>Lorentz forces excluded</td>
</tr>
<tr>
<td>V1.3</td>
<td>Steel+Oxide</td>
<td>1000</td>
<td>Transient</td>
</tr>
<tr>
<td>V1.4</td>
<td>Steel</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>V1.5</td>
<td>Steel + Oxide</td>
<td>450</td>
<td></td>
</tr>
<tr>
<td>V1.6</td>
<td>Steel + Oxide</td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>V1.7</td>
<td>Steel + Oxide</td>
<td>1700</td>
<td></td>
</tr>
<tr>
<td>V1.8</td>
<td>Steel + Oxide</td>
<td>1900</td>
<td>No dispersion (CaO)</td>
</tr>
<tr>
<td>V1.9</td>
<td>Steel + Oxide</td>
<td>400-200</td>
<td>CaO added</td>
</tr>
<tr>
<td>V2.1</td>
<td>Steel + Oxide</td>
<td>120-150</td>
<td>CaO added</td>
</tr>
<tr>
<td>V2.2</td>
<td>Steel + Oxide</td>
<td>50-90</td>
<td></td>
</tr>
<tr>
<td>V2.3</td>
<td>Steel + Oxide</td>
<td>240</td>
<td></td>
</tr>
<tr>
<td>V3.1</td>
<td>Steel + Oxide</td>
<td>1700-2500</td>
<td>US Limestone/quartzsand heating from 0 to 66 s only</td>
</tr>
<tr>
<td>V3.2</td>
<td>Steel + Oxide</td>
<td>400-1000</td>
<td>US limestone, 30 min heating</td>
</tr>
<tr>
<td>V3.3</td>
<td>Steel + Oxide</td>
<td>600-200</td>
<td>US limestone/quartzsand, 60 min heating</td>
</tr>
<tr>
<td>V4.1</td>
<td>Steel + Oxide</td>
<td>1000-300</td>
<td>600 mm dia. crucible</td>
</tr>
</tbody>
</table>

2.2 Main results

The behavior observed in test V1.8 is representative of the experiments performed with a high input power. That is why it is generally used to describe the results obtained in tests V1. In this test a mixture composed of 350 kg steel with chromium and nickel and 130 kg Al₂O₃ with CaO was poured into the crucible. An inductive heating power of 1900 kW was injected in the metallic phase which corresponds to an internal heating density ten times higher than in the reactor case. Figure 1 shows the evolution of the axial and radial concrete ablation. As can be seen here, the axial ablation is very fast (around 1 mm/s) and far quicker than the radial ablation. This behavior was confirmed by the post-mortem analysis of the crucible which shows that the radius of the cavity do not increase when the depth increases (Figure 1).

![Figure 1: BETA V1.8 – Crucible erosion (left) and final cavity shape (right) [3]](image-url)
Temperature measurements show a rapid cooling of the melt with a decrease of the metallic pool temperature from 2100 K (initial temperature) to 1800 K in less than 200 s. It should be noted that the metallic pool temperature then stabilizes near its liquidus temperature until the end of the experiment (around 500 s).

Results of the BETA V2.1 tests are considered as representative of V2 experiments and are thus used in this paper. In this test a mixture of 300 kg steel with 10 % weight of nickel and 150 kg oxide (70% Al₂O₃, 30% SiO₂) was used. The initial temperature of the melt was around 2200 K and the power injected in the metallic phase was around 130 kW. Figure 2 shows the axial and radial ablation of the crucible as well as the final shape of the cavity. Unlike what has been observed in high power tests (V1), the erosion velocity in the radial direction has the same order of magnitude as in the axial direction. This observation is confirmed by the final shape of the cavity which is more rounded than in the BETA V1.8 experiment. As in test V1.8, a fast decrease of the melt temperature is reported, the metallic pool temperature being close to the solidification temperature.

Figure 2: BETA V2.1 – Crucible erosion (left) and final cavity shape (right) [3]

3 THE TOLBIAC-ICB CODE

The main characteristics of the TOLBIAC-ICB code are summarized hereafter. A more detailed description of the code can be found in [1] and [2].

3.1 The phase segregation model and coupling with GEMINI-2 code

The TOLBIAC-ICB code is based on the phase segregation model [4]. Due to the high liquidus temperature of oxide melts and despite the melting of concrete and the presence of gas issued from concrete decomposition, a solid crust is assumed to form at the concrete wall. The species that encrust are the most refractory species (mainly UO₂ and ZrO₂). A low crust growth, a high liquid diffusivity and a small diffusion boundary layer thickness are also assumed. With this view, the pool is only composed of liquid and consequently has a low viscosity. The interface temperature between the liquid pool and the solid crust is equal to the liquidus temperature corresponding to the current composition of the remaining oxide liquid phase. The interface temperature is the temperature which is used to calculate the heat flux between the pool and the concrete. The crust is assumed to move with the melting front of the concrete and to be permeable to the decomposition products from the concrete. The crust thickness is calculated using a steady state assumption.
Physico-chemistry in TOLBIAC-ICB code is calculated with an intrinsic coupling to the GEMINI2 code, developed by THERMODATA\textsuperscript{2}. The data base that was used by GEMINI2 for the results presented here is NUCLEA03, including carbon. First an equilibrium calculation is performed with GEMINI2 at each time step for the melt. The temperature of the melt and the mass of species in the pool (including gas from concrete ablation) are used as input. The result is the modified melt composition taking into account the chemical reactions. At each time step, a second calculation with GEMINI2 is performed in order to obtain the liquidus temperature and the composition of solid that encrusts: given the species in the pool, several iterative GEMINI2 runs are performed with varying temperature, until the temperature at which the first solid appears (liquidus temperature) is found.

3.2 Physical properties

Physical properties are not of minor interest, since they are used for determination of melt height and heat transfer areas (density), and also for heat transfer coefficients and void fraction model. The physical properties of individual species used in TOLBIAC-ICB are principally those defined in the frame of the ECOSTAR European project [5] for the densities, and also in the CORPRO data base of CEA [6] for specific heat, conductivity and surface tension.

The density of the mixture is obtained by a volume weighting, whereas the heat capacity, conductivity and surface tension are obtained using a mass weighting. The dynamic viscosity of the melt is calculated following the method proposed by Sudreau et al. [7] for mixture with silica above the liquidus temperature: the Urbain model is used depending on the mole concentration of the species in the mixture. The species are divided into former (SiO\textsubscript{2}), modifiers (CaO, FeO, MgO, UO\textsubscript{2}, ZrO\textsubscript{2}) and amphoterics (Al\textsubscript{2}O\textsubscript{3}, Cr\textsubscript{2}O\textsubscript{3}, Fe\textsubscript{2}O\textsubscript{3}, NiO). In case of a metallic layer, the Andrade model is used.

3.3 Heat transfer correlation

Given the remaining uncertainties related to the power split on the pool boundaries [8], the code user may select a correlation on each boundary among several different heat transfer correlations (e.g. [9],[10]). The code user may also simply modify the ratio between the bottom and lateral heat transfers, in the frame of sensitivity studies.

3.4 Top heat transfer model

A crust generally appears at the upper surface of the pool because of radiative heat transfer towards the reactor cavity or water aspersion. A crust thickness and crust surface temperature are calculated, supposing a steady state regime. The heat transfer between melt and crust is governed by the heat transfer coefficient and the interfacial temperature, and does not depend on the external conditions. The crust surface temperature and crust thickness depend on the external conditions, which may be radiation or heat exchange with a water layer.

3.5 Energy and mass balances

The energy balance is solved in terms of temperature, including the wall and top heat transfer, the residual power (defined in the data set as power versus time or volumetric power versus time), the chemical reaction heat (given by GEMINI2), the heat corresponding to

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\textsuperscript{2} THERMODATA, 6 rue du Tour de l’Eau, 38400 SAINT MARTIN D’HERES, FRANCE.
corium that is poured into the reactor pit versus time, and an inertial term. The mass balance is solved for each species that may exist in the melt. Chemical reactions are taken into account (calculated by GEMINI2), as well as crust formation or remelting, and the source term of corium versus time.

### 3.6 Stratified melts

When the thermodynamic equilibrium result by GEMINI2 provides two immiscible liquids in case of a pool containing oxides and metals, a mixing criterion is used to predict the stratification or mixing of these two liquids. Either the BALISE correlation [11] or the Esptein criterion [12] can be used. The first correlation depends explicitly on the density of the liquids and on the gas superficial velocity. The Epstein criterion also depends on the height of the layers but takes the gas superficial velocity into account though the pool void fraction.

Concerning the physico-chemistry of the stratified melt, two options corresponding to two different situations may be chosen [13]. Following the miscibility gap model proposed by Seiler et al. [14], both metallic and oxidic liquids can be assumed to be at thermodynamic equilibrium. In such case, the two layers are globally bounded by one refractory crust and have the same boundary temperature. A single crust composition is considered and calculated with GEMINI2 since no crust exists at the interface between the two layers. On the other hand, one can also assume that both liquids leave thermodynamic equilibrium. In this second case, both liquids may be bounded by a different crust: an oxide refractory crust for the oxide pool and a metallic crust in front of the metallic pool. Since the liquidus temperature of the oxide is higher than the liquidus temperature of the metallic pool, an oxide crust is expected to form at the interface between both layers. Thermodynamic calculations are then performed for both liquids in order to determine the crust composition and the liquidus temperature related to each layer. Moreover in this case the presence of refractory oxidic debris in the metallic layer is considered (Figure 3). Evidence of one scenario or the other are not clear, since MCCI experiments with prototypic materials and oxidic/metallic pool stratification do not exist. However the scenario with no equilibrium between the two layers seems to be more probable [13].

![Figure 3: Stratified pool configuration](image)

### 4 TOLBIAC-ICB RESULTS

#### 4.1 Calculations matrix – Choice of BETA experiments

The analysis of the experimental results (power in the melt, crucible erosion) shows that the heat flux between the metallic pool and the concrete are often far higher than those expected in the mid and long term phase in the reactor case (around 100 to 150 kW/m²). In the BETA V1.8 test for example, the heat flux can be estimated around 6 MW/m² which would correspond to a metallic crust thickness less than 1 mm and a gas superficial velocity higher than 1 m/s. Given these order of magnitude, the formation of a metallic crust at the
interface between the metallic pool and the concrete crucible as assumed in TOLBIAC-ICB (and as expected in the mid and long term phases of the reactor case) is unlikely. The corium concrete interaction cannot certainly be described by the same modelling as those required for the reactor situation. That is why the BETA V1 tests are presently not included in the validation matrix of TOLBIAC-ICB.

The situation is quite different in the BETA V2 tests in which the heating power is far less than in the BETA V1 experiments (ten times less). In BETA V2.1 for example, the erosion velocity is around 0.06 mm/s which corresponds to a heat flux around 350 kW/m². Although this heat flux is higher than those expected in the reactor case, it would lead to a metallic crust thickness of 1.7 cm and a gas superficial velocity around 6 cm/s. The existence and stability of the metallic crust is thus more likely in these cases which are used for the validation of TOLBIAC-ICB in metal/oxide pool configurations.

4.2 Calculation results

4.2.1 Calculation results of BETA V2.1

Attention focuses here on the results obtained in the calculation of BETA V2.1 which are representative of those of low power tests. Table 2 summarizes the initial conditions and melt compositions used in the numerical simulation. The same heat transfer correlation [9] is used on every pool boundaries and at the interface between the two layers.

Table 2: Initial conditions and melt compositions

<table>
<thead>
<tr>
<th>Initial temperature (K)</th>
<th>2173</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metallic melt (kg)</td>
<td>Fe: 270 Ni: 30</td>
</tr>
<tr>
<td>Oxide melt (kg)</td>
<td>Al₂O₃: 105 SiO₂: 45</td>
</tr>
<tr>
<td>Power input t(s) – P (kW)</td>
<td>0 – 120 600 – 120 2100 – 170 5100 – 105 6000 - 105</td>
</tr>
</tbody>
</table>

Calculation results obtained with TOLBIAC-ICB V2.2 are reported on Figure 4 to Figure 6. As indicated by Figure 4 the fast temperature decrease observed in the BETA experiments is found in the calculations. The assumption of a crust formation between the metallic pool and the concrete together with high heat transfer coefficient makes the metallic pool temperature close to its liquidus temperature (or solidification temperature) as mentioned by the experimentalists. This temperature remains nearly constant as observed during the experiments [3].

Concerning the ablation of the cavity, Figure 5 shows a satisfactory agreement between the calculation and the experimental data despite a low underestimation of the axial ablation velocity at the end of the simulation. This agreement is confirmed by the final shape of the cavity reported on Figure 6 in red line. The maximum axial and radial ablation is quite similar in the experiment and in the calculation.
Figure 4: BETA V2.1 – Pool temperature vs time (experimental data not available)

Figure 5: BETA V2.1 – Axial and radial ablation of the cavity

Figure 6: BETA V2.1 – Final shape of the cavity
4.2.2 Calculation with power injected in the oxide phase

A calculation of the BETA V2.1 experiment with the power injected in the oxide phase has been performed in order to highlight the effect of the power injection in the metallic phase on the cavity erosion. The result of this calculation is reported on Figure 7 and shows that the final shape of the cavity is different from the one obtained in the previous calculation. In that case the radial ablation in front of the oxide phase is higher and the final axial ablation is less. The peculiar behaviour observed in the BETA experiments can thus be attributed to the location of power in the pool.

![Figure 7: TOLBIAC-ICB calculation with power injected in the oxide phase](image)

5 CONCLUSION

The main purpose of this paper was to present the TOLBIAC-ICB calculation results obtained in oxide/metal pool configuration. The analysis of the BETA tests show that part of the experiment are probably not representative of the reactor situation because of a too high input power and the location of power injection. Since the TOLBIAC-ICB code was developed for safety analysis of MCCI in reactor scenarios, it is expected that these experiments cannot be simulated with the modelling implemented in the code. However, the same analysis indicates that some tests with moderate power input (e.g. V2.1) might bring into play the phenomena expected in the long term phase of the reactor case. This experiment was thus selected to validate TOLBIAC-ICB in oxide/metal stratified configuration. The comparison between TOLBIAC-ICB results and the experimental data issued from BETA V2.1 shows a satisfactory agreement which indicates that the modelling implemented in TOLBIAC-ICB is relevant for such situations. Additional calculations with power injected in the oxide phase also highlight that the peculiar behaviour observed in the BETA experiments may probably be attributed to the location of power injection in the pool. Further studies on MCCI in stratified configurations with prototypic materials are required to conclude more firmly.
REFERENCES


[6] P. Piluso, CORPRO V1.5 – Base de données propriétés physiques du corium, CEA.


