# Assessment and Development of Molten Corium Concrete Interaction Models for the Integral Code ASTEC

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**Abstract:**
The WEX and MEDICIS codes are currently part of the integral code ASTEC V1 for the simulation of MCCI phenomena that may evolve during a severe core melt accident in PWR nuclear power plants. WEX represents the traditional modelling approach to the MCCI phenomenology and is limited in flexibility for additional models and model options. MEDICIS has recently been developed with the objective of a more generalised, flexible MCCI code, which is capable of a tighter coupling to thermo-chemical data bases. More insights in the capabilities, limitations and differences of the current models used in these codes are obtained by a parallel use of WEX and MEDICIS for some selected experiments, e.g. BETA 5.2, MACE M3b and OECD-MCCI CCI 2. The interface temperature between melt and crust and the effective heat transfer coefficient between melt and concrete are identified here as important model parameters in recalculations of the experiments. The fixing of these model parameters is difficult since indications from experimental results are weak. The conclusion from the test CCI 2 on the homogeneous heat flux distribution remains to be confirmed in further experiments. Parametrical reactor calculations performed with MEDICIS show its capabilities for reactor applications and point out other uncertainties in MCCI modelling influencing the long term MCCI phase: the oxide/metal heat transfer in the case of a stratified pool configuration and the pool configuration evolution models.

## 1 INTRODUCTION

The integral code ASTEC (Accident Source Term Evaluation Code) [1] is being commonly developed by IRSN and GRS with the aim to obtain a fast running code for the simulation of complete severe accidents sequences in LWR, starting from the initiating event up to a possible release of fission products into the environment. Such pathways may eventually be caused by consequences of the interaction of molten core material with the concrete structures (MCCI = Molten Corium-Concrete Interactions) of the containment.

### 1.1 Basic aspects of MCCI for containment safety issues

In case of a hypothetical severe accident large amounts of molten corium may enter the reactor cavity after the reactor pressure vessel has failed. In succession to this serious MCCI situations will establish during which some major hazards for the environment may be encountered:

- Because of the continuous release of decay heat in the corium there is a potential for a melt-through of the concrete foundation of the containment by ablation of the concrete, thus opening a downward pathway for radioactive fission products into the soil and groundwater located underneath.

- Concrete ablation generates gas release – especially the gases $H_2$, $H_2O$, CO and $CO_2$ – into the containment atmosphere. Whereas the production of steam and carbon dioxide contributes to the pressure increase in the containment, the release of hydrogen and carbon monoxide may eventually lead in addition to the formation of explosive gas mixtures in the containment atmosphere. Both effects have impact on the boundary conditions for long-term leakage processes and may even lead directly or indirectly to an overpressurisation failure of the containment. Thus an early radiological source term may be promoted.

The primary objective for an analysis code dedicated to the simulation of MCCI (e.g. WEX and MEDICIS in ASTEC) is to evaluate the time evolution of the major processes described above (in particular the quantities of the axial and radial ablation depths and pool temperature, see also Figure 1) with 'best-estimate-approaches' and sufficient accuracy. Further, the code must be able to quantify the heat and mass transfer processes between the molten pool and containment atmosphere for the purpose of coupled containment thermal-hydraulics calculations.

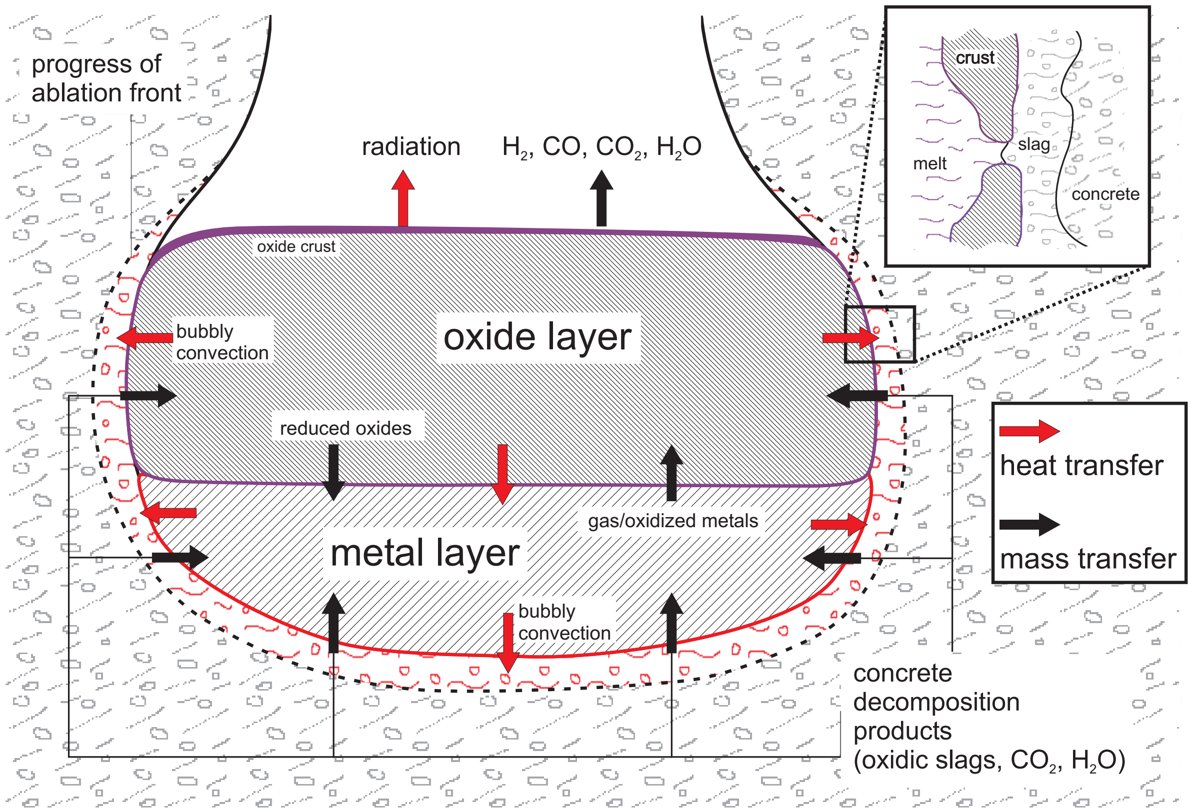


**Figure 1: Basic sketch of a stratified two-layer configuration of the molten pool (metal below oxide) and the relevant heat and mass transfer pathways to be regarded for the simulation of MCCI phenomena**

## 2 SHORT DESCRIPTIONS OF THE MCCI MODELS AVAILABLE IN ASTEC

At the start of the ASTEC development some important model approaches, e.g. WECHSL (developed at FZK in the 1980s [2]), WEX (a GRS-development on the basis of WECHSL [4]) and the US-code CORCON (SNL [3]) already existed. These model approaches were essentially based on experimental data for metallic melts (e.g. from the BETA-experiments at FZK) or from one-dimensional experiments with oxide melt (ACE/MACE test series at ANL, USA) which are extrapolated to reactor scale.

For many years the codes WECHSL and WEX [4] had been used by IRSN, FZK and GRS to simulate MCCI phenomena in post-test analyses of experiments and generic studies for PWR severe accidents. Consequently the most recent WECHSL/WEX version was historically the first choice for the implementation of a MCCI module into ASTEC V0.
However, in the past it has become obvious that despite of the many successful validation results with WEX the applicability of the code for future needs within ASTEC is limited. The requirements which WEX is actually lacking of were identified as [5]:

- Coding modularity (for easy further development and extensions),
- Flexibility (for convenient use and choice of optional models),
- Generalised modelling of pools using a layer averaged description for coupling with thermo-chemistry,
- Numerical robustness.

For these reasons the development of MEDICIS [6] has been initiated by IRSN in cooperation with GRS in 2002, the first version being implemented in ASTEC (version V1.1) middle of 2004. It is planned that MEDICIS should in a near future become in ASTEC the unique MCCI code. The structure of MEDICIS is flexible enough to allow an easy implementation of new models generated by R&D outcomes. MEDICIS uses a robust algorithm for 2D cavity erosion. An extension of this algorithm to 3D is foreseen but not achieved yet. This module is interfaced with the general physico-chemistry package MDB of ASTEC for element speciation in a mixture, thermodynamic data (liquidus temperatures, enthalpies…), and thermo-physical properties (density, viscosity…). Other models (e.g. for melt coolability, evolution of pool configuration…) have been recently added to MEDICIS.
In the current version of ASTEC (V1.2 delivered middle of 2005) WEX and MEDICIS codes are available for the simulation of MCCI phenomena. Their basic features are described below.

### 2.1 WEX

WEX [4] is a lumped parameter code which has been developed by GRS in the frame of COCOSYS project for the analysis of the thermal and chemical interaction of reactor materials with concrete in a two-dimensional as well as in a one-dimensional, axisymmetric concrete cavity. The code performs calculations from the time of initial contact of a hot molten pool with concrete until long-term basemat erosion causing possibly a basemat melt-through.
WEX considers either one oxide layer, which can contain a homogeneously dispersed metallic phase, or a separation of the molten pool into metal and oxide layers. Internal energy release is considered in form of decay heat or by exothermic chemical reactions. Energy is transferred to the melting concrete (ablation heat flux) and to the upper containment (thermal radiation or evaporation of sump water possibly flooding the surface of the melt). Gases generated during concrete decomposition pass through the melt. Water vapour and carbon dioxide are reduced as they pass through the metallic layer. Heat transfer between the molten layers is described. For the heat transfer from the melt to the concrete a film model, a discrete bubble model or a transition boiling model is used, depending on the existing gas flow and on the inclination of the interface. The bulk of each layer of the melt is assumed to be isothermal with boundary layers at the interfaces. During cooling of the melt transient crust formation is modelled. Crusts are assumed to be permeable to gases. Solidus and liquidus temperatures for the oxidic phase are determined from a quasi-binary phase diagram. The relevant chemical reactions are formulated by gross reaction equations. The condensed phase reactions are calculated within each time interval with the equilibrium concentration of the products achieved completely. The reactions are assumed to proceed in the order Zr, Si, Cr, Fe, so that Fe is oxidised only when all available amounts of Zr, Si and Cr have been consumed.

### 2.2 MEDICIS

Like WEX, MEDICIS [5] [6] uses a lumped parameter approach based on a layer averaged description. The description of basic physical and chemical phenomena is similar to that of WEX, excepted for the more simplified treatment of heat transfer at the corium/concrete interface without any film model. This code describes either an axisymmetric concrete cavity or a slab-shaped cavity. It is characterized by a large flexibility permitting an easy addition of new models as well as a convenient use of optional models.

The melt pool may be either homogeneous or stratified and may evolve versus time. In principle the code might treat any number of layers. However, due to the difficulty of defining properly each layer in the general case, only four layer types are possible in the present version: an oxide layer, a mixed oxide/metal layer in the case of a homogeneous pool, a metallic layer and the upper crust built-up at the pool upper interface. For each layer, mass balance equations are written per chemical element and the energy balance equation uses enthalpies of element mixtures, which allow solving mass and energy balance equations independently of the detailed corium chemistry evolution. The cavity erosion algorithm assumes that the cavity boundary is a succession of truncated cones in case of an axisymmetric geometry or a succession of prisms in case of a slab geometry. The 2D-profile of the cavity boundary versus time is determined using the local energy conservation at each boundary node and Stefan's relation to evaluate the ablation velocity. The heat transfer from corium to concrete is described by a simple thermal resistance model including in series the convective heat transfer, the heat conduction across the semi-solid corium zone called 'crust' at a temperature below the freezing temperature and the heat transfer in a slag layer.
Corium quenching models of the CORQUENCH code [7] including the melt eruption model have been introduced in MEDICIS.

Precise thermo-chemical data (liquid fraction versus temperature and composition, solidus and liquidus temperatures) can be generated outside MEDICIS by an interface with the GEMINI2 code [8] using the NUCLEA database [9] for mixtures of a given initial corium with the considered concrete material. MEDICIS determines at any time the thermo-chemical data by interpolation from the interface results; the interpolation parameter is the mass fraction of 'light' oxides arising from the ablated concrete.

## 3 RECENT ASSESSMENT WORKS

### 3.1 Strategy for model assessment

The validation work performed in the past with WEX and MEDICIS showed that a consistent simulation of the broad range of experiments available was not possible. The deviations of post-test calculations with the experiment were found to be approximately a factor 2 in case of the ablation depth and ± 150 K in case of the pool temperature at the end of the experiment. The reasons are the following:

- Empirical parameters in the models (i.e. heat transfer at corium/concrete interface and freezing temperature) are still 'uncertain';
- Knowledge of thermo-chemical data determining the freezing temperature and transport physical properties is still insufficient for some oxide/metal mixtures;
- Evaluation of the 2D heat flux distribution either in an homogeneous pool or a stratified pool configuration is difficult due to the lack of knowledge on 2D heat convection and on oxide/metal heat transfer.

In order to reduce uncertainties on the MCCI knowledge, there are currently many research projects on MCCI in progress, integral experiments using real material (OECD-MCCI at ANL, VULCANO at CEA), high melting temperature simulant experiments (LACOMERA-COMET

at FZK) and analytical simulant experiments (ARTEMIS 1D, 2D and in stratified pool configuration at CEA).
The strategy for the development of MCCI models in ASTEC and their assessment can be summarised as follows:

1. Point out the shortcomings of the existing models found in recalculations of experiments;
2. Elaborate alternative approaches based in particular on detailed analysis of analytical experiments (such as ARTEMIS);
3. Check the applicability of alternative approaches on a wider spectrum of available experiments;
4. Test their predictability by blind calculations of future experiments.

### 3.2 Traditional approaches vs. new formulations including more detailed thermo-chemistry data

There is a common agreement among the experts that the freezing behaviour of the melt influences strongly the MCCI phenomena in the pool. In the more traditional view of the codes WECHSL/WEX and CORCON, this is accounted for by considering an interface condition for the formation of crusts along the melt boundaries (freezing temperature) and relating this freezing temperature to the solidus (and/or) the liquidus temperature of the melt obtained by a quasi-binary phase diagram (see Figure 2 from [10]).

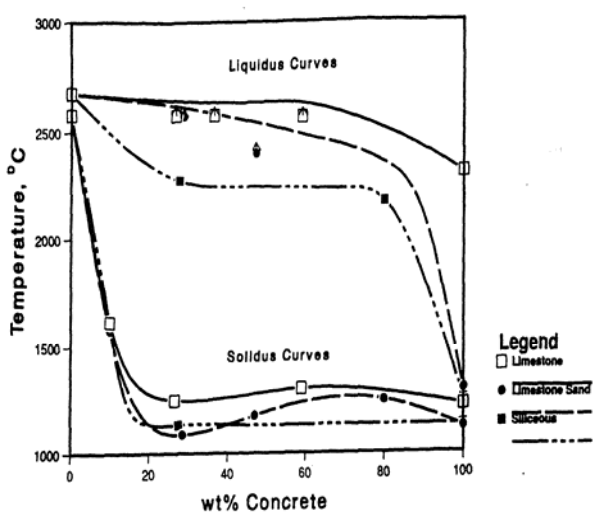


Figure 2: Liquids- and solidus temperatures for quasi-binary core-concrete mixtures

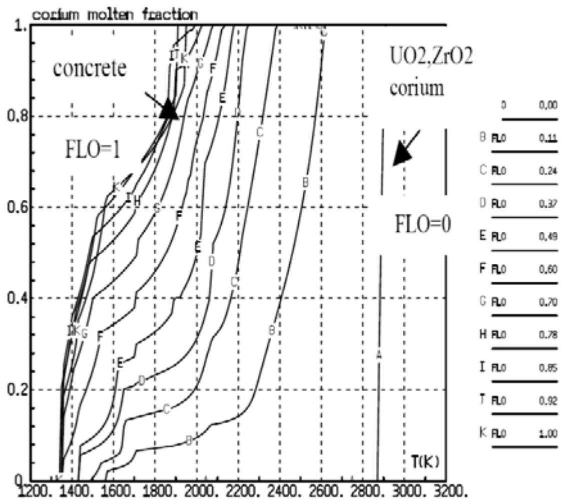


Figure 3: Molten fraction versus temperature T and light oxide fraction (FLO) evaluated by the code GEMINI2 for MEDICIS

In these approaches the freezing temperature for considering the growth of crusts was basically referred to the solidus temperature of the melt, like in steady-state metallurgy. The temperature drop ΔT between the pool and the freezing temperature $T_{solidif}$ is calculated in quasi-steady state from the heat flux density along the crust interface q and the heat transfer coefficient h: ΔT = q/h, which can be large because h is rather low due to the significant corium solid fraction. The success of the validation of these models was limited: only with special adoptions of heat transfer models and correlations for the BETA experiments separately from other experiments consistent results could be obtained.
On the other hand there are indications that lead to a new model approach [11] with stronger links to equilibrium thermo-chemistry: this approach considers that in long-term MCCI situations the interface temperature between melt and crust, the freezing temperature, is near the liquidus temperature of the actual liquid melt (i.e. the initial melt composition minus

the refractory species segregated in the crust plus the concrete slag added to the melt by concrete ablation).
This approach would have strong impact on the dynamics of the pool temperature in MCCI situations. The pool temperature cannot exceed much the equilibrium temperature of the liquid melt at its actual composition because of the high heat transfer coefficient h for the liquid melt. This would imply that a stepwise increase of internal power, like in the experiment MACE-M3b, would not lead a priori to a similar increase in pool temperature, only via the change of melt composition by re-melting of refractory crusts in the first instance.
The deficits of some post-test calculations of experiments with the traditional modelling in predicting the pool temperature is suspected by many authors to be a consequence of selecting the wrong interface temperature condition for the formation of crusts (solidus instead of liquidus as required by the new approaches).
In ASTEC, MEDICIS may either be used in a more traditional way (like WEX) or with a more modern model set-up where detailed thermo-chemical data are pre-calculated (e.g. liquid fraction versus temperature and composition, see Figure 3) by the GEMINI2 code.

### 3.3 WEX and MEDICIS assessment activities

WEX and MEDICIS are used in parallel for the detailed assessment of different available model approaches. Two types of analyses are carried out.

**WEX/MEDICIS benchmarking**

In a first step the calculations with WEX and MEDICIS are performed using the same initial and boundary conditions. Since the models in the codes are not identical the differences in the calculations must then be related to model differences.
In a second step, one of the codes (in general MEDICIS, thanks to its flexibility) is modified in order to get more close to the calculation behaviour of the more traditional code (in general WEX).
The reliability of different possible heat transfer models will be checked in predictions and recalculations of future experiments, e.g. CCI 3 [12], in order to select best-estimate models.

**MEDICIS sensitivity studies**

For all calculations of experiments the standard heat transfer models in MEDICIS are selected, in particular the convective heat transfer coefficient and the slag layer model. The correlation derived from BALI experiments [13] for the convective heat transfer at the corium pool interface has been chosen. A high value of the slag layer heat transfer coefficient is retained, i.e. 1000 $W/m^2/K$, which agrees in order of magnitude with the slag layer model of the CORCON code [3]. Results obtained show a little dependence on this parameter, as long as a crust is present at the corium/concrete interface all along the test, which is verified for all experiments considered here.
Only the value of the $\gamma$ parameter determining the freezing temperature at the boundary between convective corium zone and crust from the relation $T_{solidif} = \gamma\ T_{solidus} + (1 - \gamma)\ T_{liquidus}$, where $T_{solidus}$ and $T_{liquidus}$ are the solidus and liquidus temperatures at the corium composition, is adjusted in each experiment while using adequate thermo-chemistry data. This permits to test the different approaches for modelling the corium freezing at pool interfaces: “traditional one” with a $\gamma$ value equal to 1, thermodynamic equilibrium at zero crust growth with $\gamma$ value equal to 0, or an in-between situation with an intermediate $\gamma$ value assuming some deviation from the two idealistic assumptions.

Table 1 shows the matrix of experiments considered recently with MEDICIS and WEX in ASTEC V1.

**Table 1: Experiments considered in this context for the assessment of MCCI models**

| Experiment | Concrete | Geometry | Melt | Heating |
|---|---|---|---|---|
| ACE L2, L6, L7, L8 | siliceous, LCS, limestone | 1D ablation, cuboid | oxidic corium + Zr | electrical |
| BETA 5.2 | siliceous | 2D ablation, axisymmetric | thermite ($Al_2O_3$ + Fe + Zr) stratified | induction |
| MACE M3b | LCS | 1D ablation, cuboid | oxidic corium + Cr | electrical |
| OECD CCI 2 | LCS | 2D ablation, cuboid | oxidic corium + Cr | electrical |

## 3.4 Assessment results

### *3.4.1 MEDICIS assessment against ACE tests*

The validation of MEDICIS code against some selected experiments (L2, L6, L7 L8) of the well-known program ACE [14] is presented hereafter adjusting the freezing temperature but keeping the standard heat transfer models.
The ACE experiments have been performed at ANL in the frame of an international program in order to determine the concrete ablation rates and the release fractions of low-volatile fission product species during MCCI. The melt is heated initially by tungsten resistance heating and power is then injected by direct electrical heating. The melt temperature and the ablation depth are measured versus time. The experiments differ mainly by the corium and concrete compositions and the injected power; initial features are given for L2 test as an example in Table 2.

**Table 2: Characteristics and geometry of ACE L2 experiment**

| | |
|---|---|
| Initial oxidic corium mass (kg) | $UO_2$: 216, $ZrO_2$: 42.5, CaO: 11.4, $SiO_2$: 21 |
| Initial metal mass (kg) | Zr: 13.4 |
| Pool section, basemat depth | 0.5 m x 0.5 m, 0.3 m |
| Concrete characteristics | siliceous concrete |

It is recalled that precise thermo-chemistry data and in particular solidus and liquidus temperatures have been determined using the interface with GEMINI2 code [7].
A homogeneous configuration is chosen since Zr is oxidised very fast. In order to reduce discrepancies compared to the experiment, experimental data are used to impose the values of some variables, as follows: since a part of released gas escaped downwards, the gas superficial velocity obtained from the experiment is imposed; upwards radiative losses are fitted on experimental data versus time; the pool upper crust built-up is suppressed by user's input in calculations, in agreement with the experimental observations.
The calculation/experiment comparison is performed both on the concrete erosion kinetics and on the pool temperature evolution. As it is not possible to reproduce well enough both ablation kinetics and temperature evolution for a given $\gamma$ parameter value, lower and upper bounds of the $\gamma$ parameter value giving results in broad agreement with the experiment are determined. Detailed results are presented here only for L2.
In a first step, the segregation of refractory material ($UO_2$ et $ZrO_2$) in crusts built-up by freezing along the lateral non-ablatable walls in the melt pool and due to the splashing above the melt pool is ignored. The value of the $\gamma$ parameter giving the best agreement with the measured temperature and erosion kinetics is around 0.28, the average value of temperature

is correctly reproduced but the deviation between calculated and measured temperature evolutions remains rather large.
In a second step, the refractory material segregation in crusts built-up by solidification along melt pool lateral walls and due to splashing as observed in the experiments are taken into account. These effects are maximised: the crusts are supposed to be made of only refractory oxide, and a large mass (up to 70% of the initial inventory) is subtracted from the corium pool inventory from the calculation onset. Two calculations, with minimum and maximum removed masses, are performed. In the maximum case, the removed mass is chosen in order to get a liquidus pool temperature equal to the measured initial temperature. Only results with the maximum segregation case are displayed on Figure 4 and Figure 5.

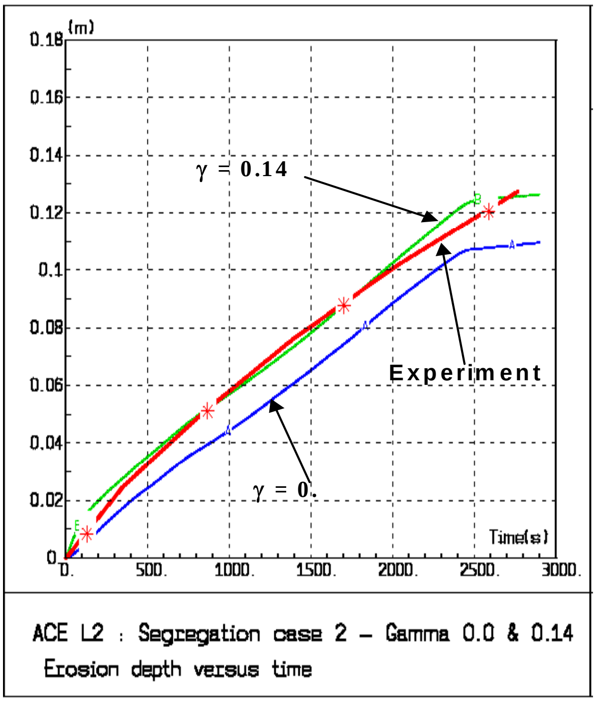


**Figure 4: Concrete ablation kinetics in L2 with refractory material segregation in crusts**

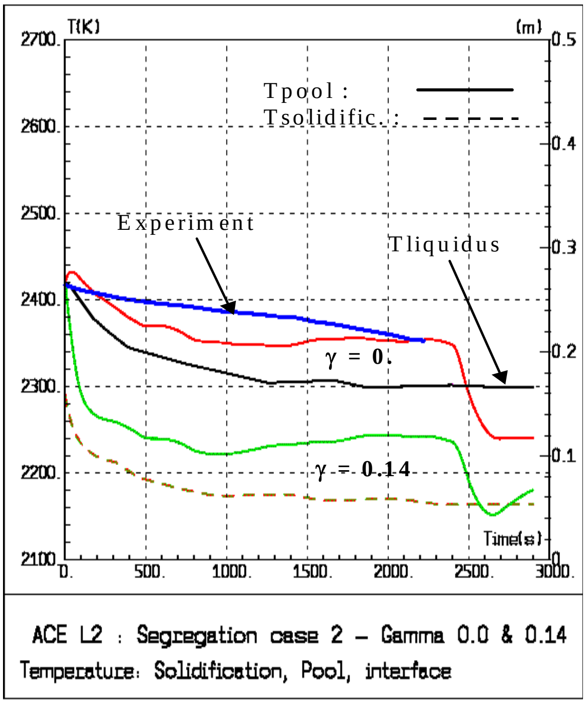


**Figure 5: Temperature evolution in L2 with refractory material segregation in crusts**

The temperature evolution and especially the low decrease rate are rather well reproduced using the segregation assumption (see Figure 5). The reason is clearly the lower liquidus temperature now located below the measured pool temperature even at the experiment onset: indeed, segregation lowers the initial refractory oxide fraction and then the liquidus temperature decreases more slowly with increasing concrete oxide fraction. However the refractory material segregation in crusts needed for decreasing the liquidus temperature below the measured temperature from the beginning is probably unrealistic, because in fact the segregated mass should increase gradually due to the non-instantaneous phenomena of solidification and splashing.
Moreover, even if overestimating the refractory material segregation, the liquidus temperature and then the calculated pool temperature still decrease faster than the measured pool temperature in most experiments, which shows that the measured temperature evolution cannot be explained only by assuming a freezing temperature equal to the liquidus one. Therefore the maximum segregation case has to be considered as a bounding case, giving the permissible minimum $\gamma$ value. The range of $\gamma$ parameter values obtained from the fitting on the L2 experiment stands between 0 and 0.28.
Similar results are obtained for the other ACE tests whatever the concrete type. This analysis shows that in the frame of the present heat transfer modelling, the $\gamma$ parameter value stands in any case between 0 and 0.3, taking into account uncertainties on material segregation in the crusts.

*3.4.2 WEX and MEDICIS assessment against BETA 5.2*

The experiment BETA V5.2 investigates the influence of metallic zircalloy in the melt on the MCCI in a cylindrical crucible made of siliceous concrete. The net heating power (supplied by induction coils) averages to 280 kW in this test. In the BETA V5 experiments the zircalloy additive is dropped into the crucible and heated by induction heating up to 500 K before the melt was poured into the crucible. The melt resulting from the thermite reaction was poured sequentially into the crucible: First the metal and then the oxide.

Calculations are performed here with WEX and MEDICIS using the solidus temperature as freezing temperature, standard models for WEX and a modified heat transfer distribution for MEDICIS.

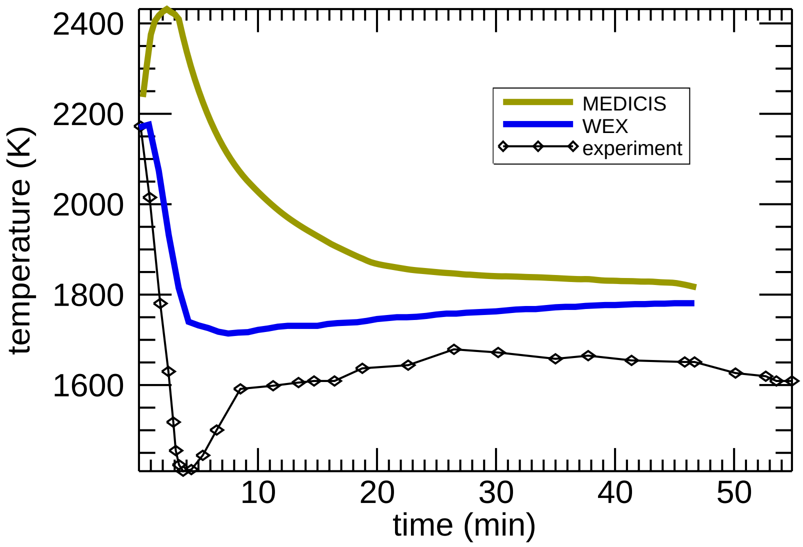


**Figure 6: Melt temperature calculated by WEX and MEDICIS for BETA V5.2**

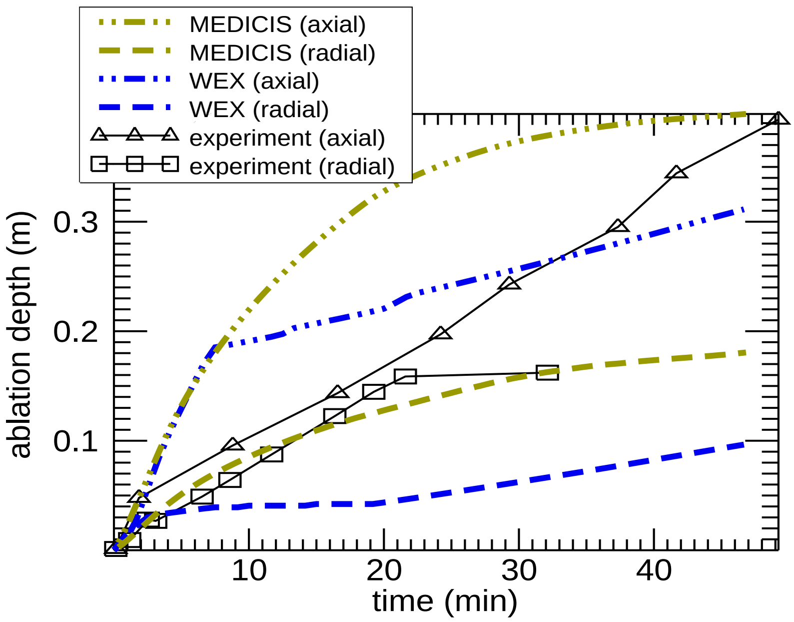


**Figure 7: Ablation depths calculated by WEX and MEDICIS for BETA 5.2**

In order to match the initial temperature at the beginning of the MCCI, the initial temperature of the melt and of the zircalloy is set to the corresponding value (2170 K). The sequential pouring of the melt is treated by WEX input, but ignoring the precise kinetics of the pouring. In WEX, solidus and liquidus temperatures of the melt as function of concrete content are calculated internally by the Schröder - van - Laar equation. The same method is used in other original inputs of FZK for the BETA experiments. Solidus and liquidus temperatures of the oxide melt as function of concrete weight fractions required by MEDICIS are deduced from those calculated in WEX (given as function of mole fractions, by the use of the Schröder-van-Laar equation), approximating the required weight fraction data with the mole fraction data calculated by WEX.

In WEX the splashing model is invoked as recommended by FZK for the post-calculations of the BETA tests to account for the impact of melt material splashing on the melt cooling (see below). In MEDICIS such a splashing model is not available.

The tendency of the metal melt temperature is well predicted by the codes (Figure 6). As a major feature of all BETA experiments the melt temperature decreases fast from the initial temperature to a temperature in between 1600 K and 1700 K. This temperature is believed to be close to the freezing temperature of the metallic melt (predominantly Fe, including some amounts of Zr, Si, B, Cr and Ni). The metal temperature in the calculations is finally slightly above the measurement. This could both be due to differences in the data basis for the freezing temperature of the metal (around 1800 K) and to the initial escalation of the temperature due to the calculated oxidation of the Zr inventory of the melt. The experimenters at FZK explained the rapid initial cooling of the melt in the BETA experiments by the splashing phenomenon (melt material splashing out of the pool onto the upper, sloped side walls of the test cylinder). Only by means of an appropriate model, which had been implemented into WEX, the transient cooling of the melt within the first 200 s could be reproduced by the code WEX despite the internal power release due to the Zr-oxidation reaction.

An anisotropic ablation as found in BETA 5.2 can be recalculated with MEDICIS only by assuming an anisotropic distribution of heat transfer coefficients (e.g. of the slag: 3 $kW/m^2$ K in axial and 1 $kW/m^2$ K in radial direction). But then the axial ablation kinetics is overestimated. Later on, due to crust growth, the calculated heat fluxes and consequently the ablation velocity are reduced in the MEDICIS calculation and the final axial ablation depth is met. This is the same behaviour as in the case of the code WEX, which initially overestimates the axial ablation in BETA 5.2 but switches to a less efficient heat transfer mode because of metal crust growth and is finally in good agreement with the final axial ablation depth (Figure 7).

Since there are still experimental uncertainties concerning the energy balance in the BETA experiments and on the real impact of the splashing phenomenon, an implementation of the splashing model into MEDICIS seems to be premature.

#### *3.4.3 WEX and MEDICIS assessment against MACE M3b*

The MACE-experiments performed at ANL investigated the phenomena of melt coolability after top flooding of the melt with water and are characterised by the following main boundary conditions: pool depth of approx. 25 cm (collapsed melt), realistic corium compositions for PWR- and BWR-plants, realistic initial conditions for MCCI and realistic decay power levels.

In the MACE experiments the melt was generated by a thermite reaction (in the contrast to the ACE test series) and then the melt is directly heated by an electric current.

The one-dimensional experiment MACE-M3b is characterised by a large-scale cavity (1.2 m × 1.2 m square base area) on top of a limestone/common sand concrete basemat. The initial corium mass amounted to approximately 1800 kg of fully oxidised corium including 6 wt.-% of chromium. The experiment lasted around 7.5 h. At 52 min after onset of concrete ablation the melt was flooded with water from the top, leading to sharp peaks in the transient heat fluxes at the top surface. The ablation depth at the end of the experiment was approx. 28 cm.

The initial temperature of the melt in the codes was approximated by averaging the experimental temperature recordings which gave a value of 2100 K at the start of ablation.

Calculations are performed here with WEX and MEDICIS using the solidus temperature as freezing temperature and standard models of each code.

The pool temperatures of the oxide test MACE M3b is underestimated in the long term by MEDICIS and WEX (Figure 8), although the propagation of ablation front is in good agreement with the experimental results (Figure 9).

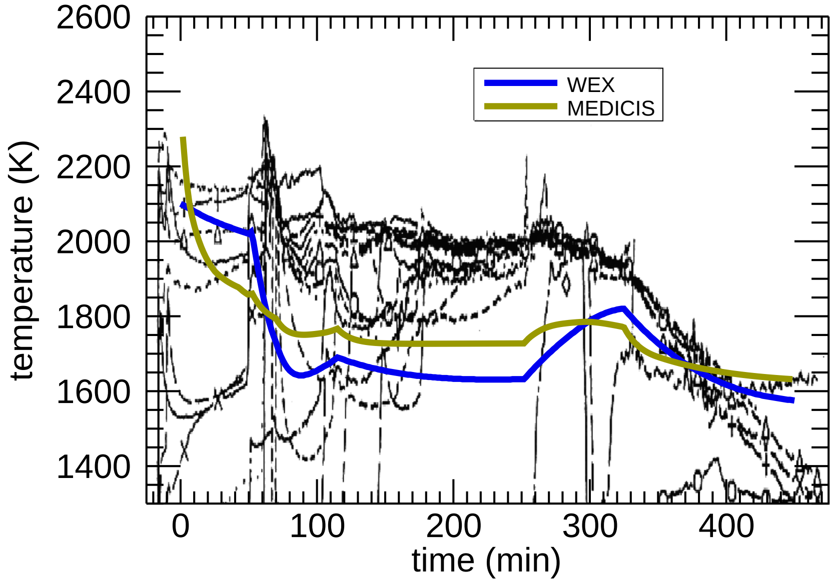


**Figure 8: Melt temperature calculated by WEX and MEDICIS for MACE-M3b.**

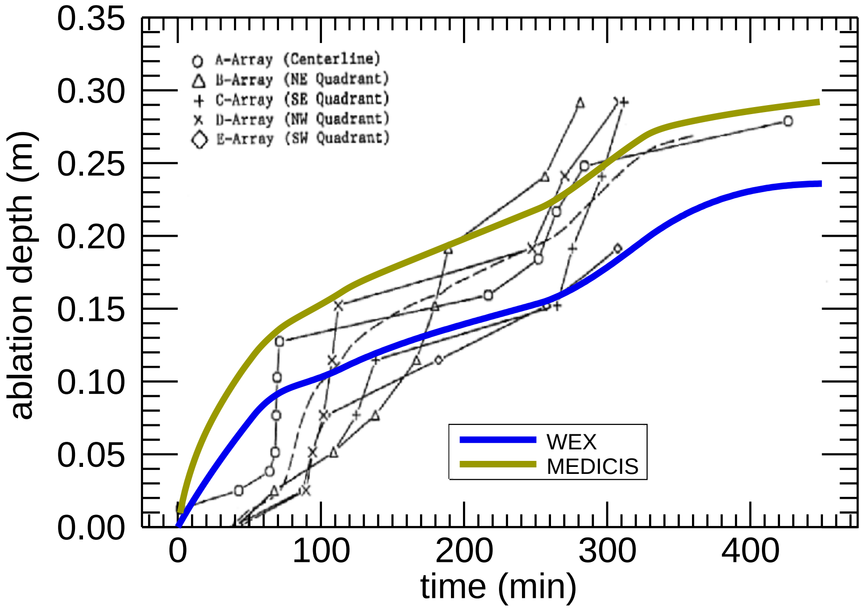


**Figure 9: Ablation depths calculated by WEX and MEDICIS for MACE-M3b.**

Because of that the heat flux distribution seems to be calculated well, but the selection of solidus as freezing temperature in combination with the available heat transfer models leads to an underestimation of the pool temperature in comparison with the experimental data. Either the freezing temperature in MEDICIS could be increased or the overall effective heat transfer coefficient between melt and concrete could be reduced to obtain a better agreement with the experiment with MEDICIS. Thus, the freezing temperature and the total heat transfer coefficient between melt and concrete are identified here as important model parameters in MCCI codes.

The pool temperature was underestimated by WEX. A possible reason may be the extra heat loss term, which was imposed at the top surface of the melt in absence of any coolability models in WEX. For this heat loss term an analytical expression was used to approximate the experimental data for the heat exchange between melt and water. This analytical expression was used to replace the original model in WEX for flooded conditions of the pool, which seemed to underestimate the experimental heat flux data. Although a similar proceeding lead to very good results for MACE-M4 the deviation in the WEX calculation obtained in this case for MACE-M3b might be explained by the fact that the calculated upwards heat loss during the flooding period is not totally consistent with the experimental data of M3b.

### *3.4.4 WEX and MEDICIS assessment against OECD CCI 2*

This experiment of the OECD-MCCI program [15][16] is at present the only 2D MCCI experiment available showing both extended lateral and axial ablation depths. The objectives of CCI 2 is to address remaining uncertainties related to long-term two-dimensional molten core-concrete interactions under both wet and dry cavity conditions.
This experiment has been performed at ANL in the frame of an international OECD program in order to determine the behaviour of a homogeneous corium melt during a 2D ablation process. This experiment has been subject to an international analytical benchmark action conducted in the OECD framework.
Main features of the CCI 2 test are displayed in Table 3. The initial pool cross section is of square shape with 2 non-ablatable walls distant from each other by 0.5 m. In these tests an oxide corium melt is generated by a thermite reaction and the ablation takes place at two opposing side walls and at the basement. Electrode rods made of tungsten are attached to the other two sidewalls for the purpose of direct electrical heating of the melt. The melt temperature is measured versus time and the profile of cavity boundaries is tracked by a dense network of thermocouples within the basemat.

**Table 3: Characteristics and geometry of the CCI 2 experiment.**

| | |
|---|---|
| Initial corium mass (kg) | 100% oxidised PWR with 8wt% concrete<br>$UO_2$: 242, $ZrO_2$: 100, CaO: 12.5, $SiO_2$: 13.6, $Cr_2O_3$: 37.5, MgO: 4.6, $Al_2O_3$:1.6 |
| Pool section | 0.5 m x 0.5 m |
| Radial and axial ablation limits | 0.35 m, 0.35 m |
| Concrete characteristics composition :LCS: (wt-%) | $SiO_2$: 28.8, CaO: 29.8,<br>MgO: 9.8, $Al_2O_3$: 3.6, $H_2O$: 6.2, $CO_2$: 21.8 |

#### 3.4.4.1 Code results with solidus as freezing temperature and standard models

These are the calculations performed in the blind OECD-benchmark. Whereas WEX met the ablation depth as well as the pool temperature for CCI 2 the code MEDICIS – with its model set up defined as close as possible to the WEX calculation – failed to predict the pool temperature but was in good agreement with the ablation depth (Figure 10, Figure 11). This different behaviour is due the different heat transfer modelling at the interface between melt and concrete. Whereas in both calculations the low contact temperature is given primarily by the decomposition temperature of the concrete given as an input, the bulk temperature in the melt is determined by an effective heat transfer coefficient which describes the efficiency of the energy transport from the hot melt to the cold boundaries. The heat transfer coefficient obtained by MEDICIS for the melt/concrete interface is larger than compared to WEX. This explains the difference between pool temperature and concrete decomposition isotherm predicted by MEDICIS in order to obtain the same ablation rate as in WEX.

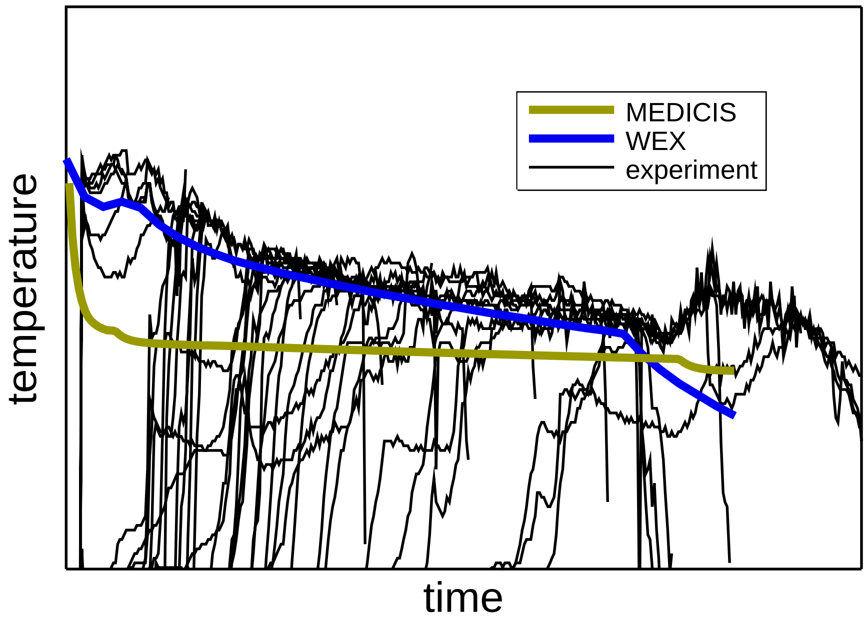


**Figure 10: Melt temperature calculated by WEX and MEDICIS for CCI 2 in a blind calculation**

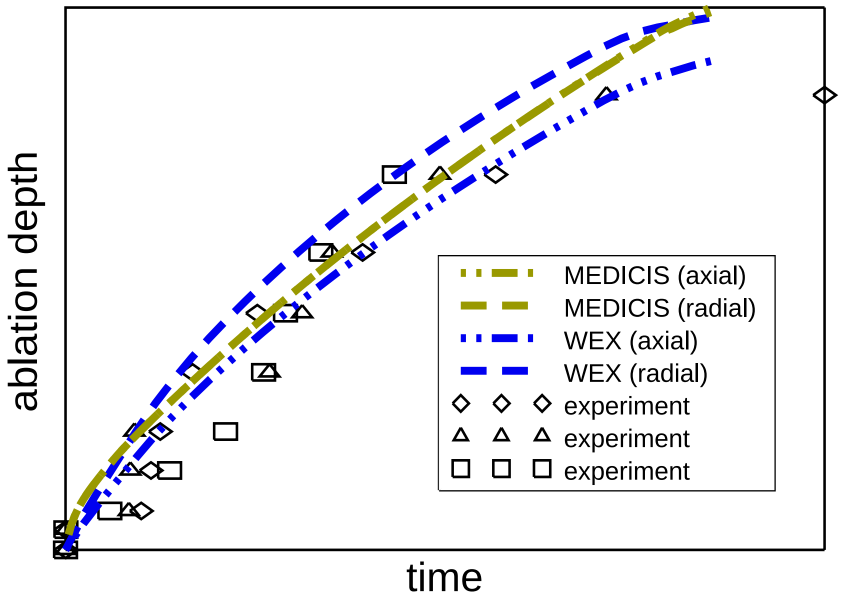


**Figure 11: Ablation depths calculated by WEX and MEDICIS for CCI 2 in a blind calculation**

3.4.4.2 Code results with solidus as freezing temperature and model adaption in MEDICIS

Here a reduced heat transfer coefficient for bubbly melt convection in MEDICIS (by approximately a factor of 0.45) is used so that the effective heat transfer at the interface (resulting from convection, conduction through the crust – if present – and transport through the slag layer) is in the same order as calculated by WEX (around 300 $W/(m^2K)$). Figure 12 shows that the pool temperature in MEDICIS is in better agreement compared with the experiment. Only in the initial phase during which the transient cooling of the melt down to a quasi-steady-state temperature takes place MEDICIS overestimates the cooling of the melt.

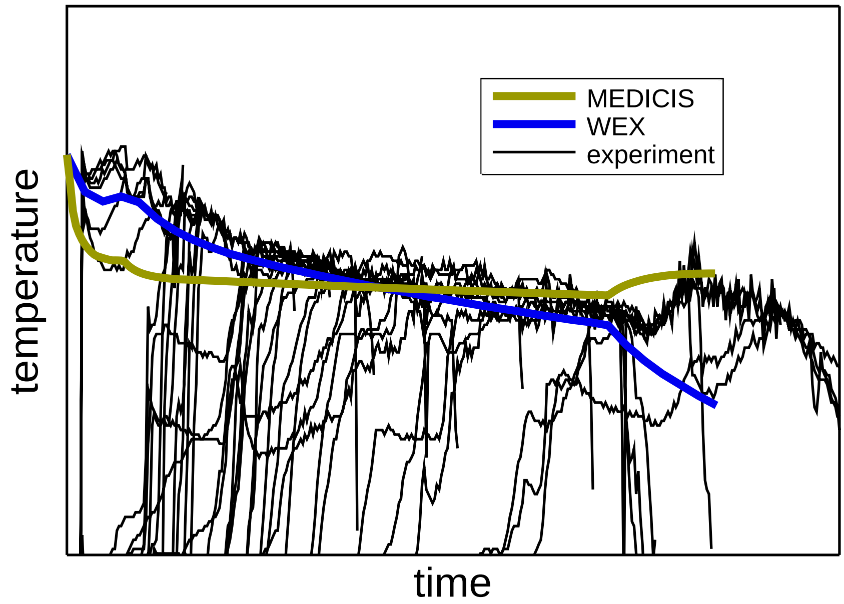


**Figure 12: Melt temperature calculated by WEX and MEDICIS for CCI 2 after adapting heat transfer correlations in MEDICIS**

3.4.4.3 Code results with MEDICIS using an adjusted freezing temperature

As for ACE tests the detailed composition of initial corium and concrete including the species with a minor fraction are taken into account here for the evaluation of thermo-chemistry data. In particular the presence of species MgO and $Cr_2O_3$ (obtained after the fast oxidation of Cr) decrease significantly the liquidus temperature in spite of their low mass fraction.
A splashing phenomenon causing an ejection of a mass of 88 kg, deduced from PTE results [17], is described in a simple way by an initial reduction of the corium inventory. A partial dissolution of UO2 pellets (43 kg) and also a partial dissolution of MgO from non-ablatable walls (33 kg) might be suspected from the final mass balance analysis [17] and are taken into account in present calculations by means of constant mass sources into the corium pool.
The water injection triggered five hours after the beginning of MCCI is described by MEDICIS, but the impact on the erosion kinetics is small since the power decreases fast after onset of water injection and is not analyzed below.
Again here, only the value of the $\gamma$ parameter defining the freezing temperature is adjusted. The heat transfer models are the same as used for the ACE tests. In particular, the convective heat transfer coefficient from bulk pool towards pool interfaces chosen is always that obtained from the BALI correlation [13] and is not depending on the interface orientation, giving a heat flux uniform distribution as long a crust is present at the pool interfaces, which is the case because of the high freezing temperature. The temperature of upper walls receiving the power radiated from the corium pool is assumed to be equal to the concrete ablation temperature. The influence of a contribution of power radiated upwards to the ablation of the upper cavity vault is taken into account.

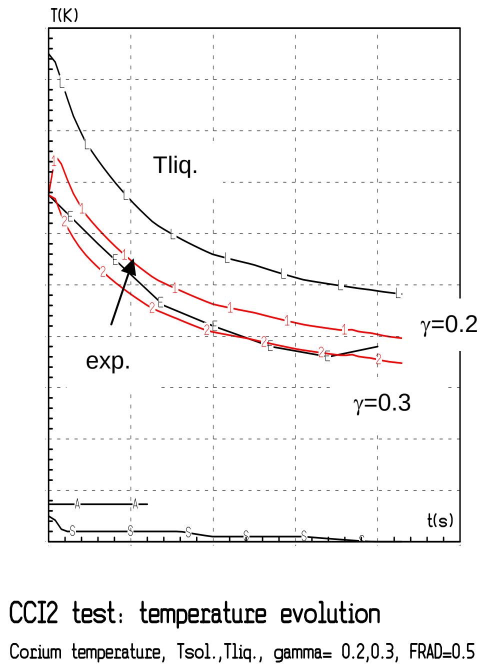


**Figure 13: Evolution of corium temperature in CCI 2**

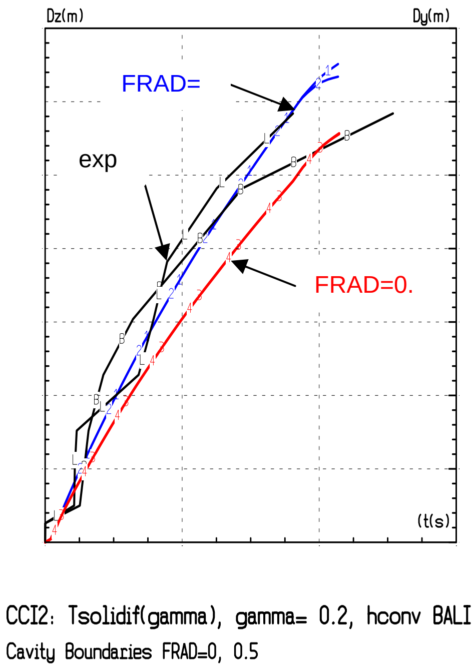


**Figure 14: Concrete ablation kinetics in CCI 2**

Results obtained are shown for the temperature evolution and the erosion kinetics in Figure 13 and Figure 14. A good agreement is obtained for the temperature evolution, using values of the $\gamma$ parameter between 0.2 and 0.3. This best-estimate value of the $\gamma$ parameter will be slightly reduced if additional segregation of refractory material in lateral crusts was deduced from PTE.

The erosion kinetics is not very sensitive on the $\gamma$ parameter value, but depends more strongly of the fraction of power radiated upwards devoted to the ablation of upper concrete walls, FRAD, which is taken to be equal here either to zero or to 0.5. The calculated lateral and axial eroded depths are in reasonable agreement with the experiment (see Figure 14). A better agreement on the erosion kinetics is obtained assuming no contribution of radiation to concrete ablation (see Figure 14, case with FRAD = 0).

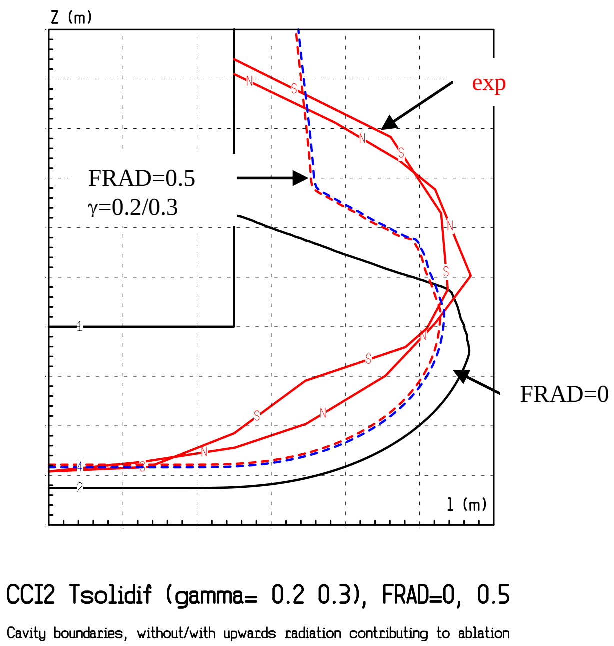


**Figure 15: Final cavity boundaries in CCI 2**

However the shape of the final cavity boundaries is better reproduced, assuming a contribution of half of radiated power to the ablation of the upper concrete vault (see on Figure 15 case with FRAD = 0.5).

The comparison of calculated and measured erosion kinetics (Figure 14 and Figure 15) shows clearly that the ablation depth is rather homogeneous along the cavity boundary and, thus, that the assumption of a homogeneous heat flux distribution is at least approximately verified in this experiment.

The conclusion on the best choice of freezing temperature derived from CCI 2 ($0.2< \gamma < 0.3$) is consistent with the previous validation work on ACE tests. The best agreement between calculation and experiment for both types of experiments is obtained for a value of freezing temperature near $T_{liquidus}$, but slightly below, while keeping the same assumptions for the convective heat transfer and slag layer heat transfer model.

## 4 APPLICATION TO REACTOR CASES WITH MEDICIS CODE

Parametrical calculations in the reactor case are presented here to point out the impact of main model uncertainties on results of reactor safety studies.

### 4.1 Calculations conditions

The considered reactor type is a typical 900 $MW_e$ commercial reactor. Data for the reactor geometry and material compositions are displayed on Table 4.

**Table 4: Reactor data for MCCI calculations**

| | |
|---|---|
| Initial oxidic corium inventory (t) | $UO_2$ mass: 82, $ZrO_2$ mass: 19.5 |
| Initial metallic corium inventory (t) | Zr: 4.8, Fe: 35, Ni: 4, Cr: 6 |
| Reactor pit radius | 3 m |
| Basemat thickness | 3 m to 4 m |
| Concrete characteristics | siliceous concrete with 6% Fe |

Main assumptions, values of key physical parameters and choice of boundary conditions are listed in Table 5. The heat transfer models are the same as in ACE and CCI 2 calculations. The heat transfer coefficient at the pool outer interface is not depending on the interface orientation. Due to large uncertainties remaining on the evaluation of the freezing temperature, the complete range of oxide freezing temperatures between solidus and liquidus temperatures is investigated.
The reactor pit wall temperature is set to a constant value near the steel melting point; in fact the temperature of concrete walls above the corium pool should stay below the ablation temperature; this assumption used for the wall temperature boundary condition is then conservative since it will underestimate the power radiated by the corium pool towards the reactor pit walls. No corium quenching is taken into account in the present calculations.

**Table 5: Choices of assumptions and values of key parameters for reactor calculations**

| | |
|---|---|
| Pool configuration | homogeneous, stratified, with configuration evolution |
| Heat convective coefficients | BALI's correlation at the outer layer |
| | $h_{slag} = 1000$ W/m$^2$/K |
| | Greene's correlation [18] along the oxide/metal layer interface |
| Freezing temperature | from $T_{solidus}$ to $T_{liquidus}$ ($\gamma$ between 1 to 0) |
| Concrete type | reinforced siliceous concrete with 6 % Fe 'standard concrete' |
| Time after scram, decay power (W/(kg U)) | 1 h: 283, 3 h: 227, 7 h: 190, 15 h: 157, 20 h: 145, 50 h: 108, 9 d: 63 |
| Initial corium temperature | 2673 K (the oxide phase is solid) |
| Pit wall temperature | 1700 K |

### 4.2 Reactor calculations results

Due to the large uncertainties still existing on the pool configuration and its possible evolution, we will consider 3 very different scenarios concerning the pool configuration.

First, let us analyze results obtained assuming an homogeneous configuration maintained during the whole MCCI phase (see Figure 16).

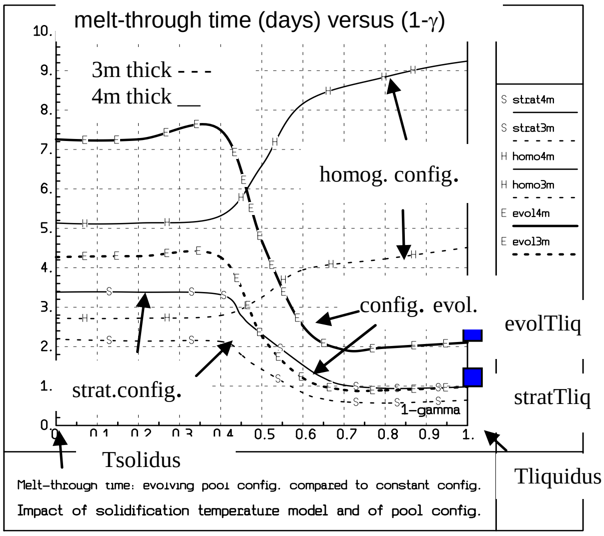


**Figure 16: Melt-through time versus freezing temperature and configuration evolution**

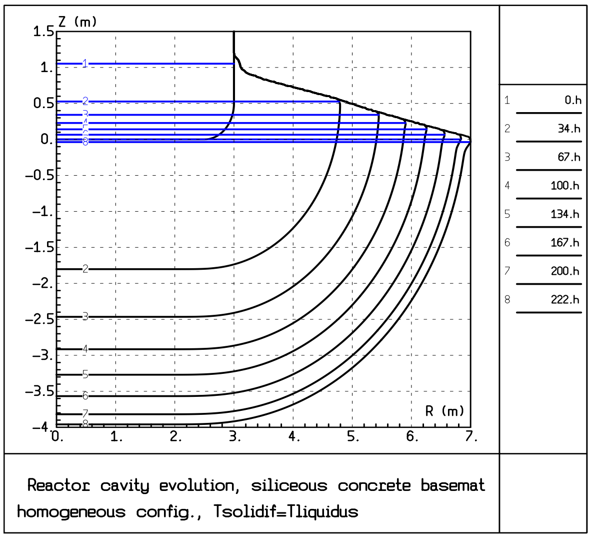


**Figure 17: Cavity erosion with homogeneous configuration; melt-through at 222 h (hgTliq)**

The assumption of an homogeneous configuration (quoted ‘H’ on Figure 16) leads to a slow concrete erosion with melt-through times ranging between 2.8 and 9 days, depending on the choice of freezing temperature and on the basemat thickness (3 m or 4 m). The reason for the slow erosion in case of a ‘H’ pool configuration is the uniform heat transfer coefficient distribution along all pool interfaces, leading to spatially uniform ablation depths. This limits the axial erosion because of the large ablated concrete volume, as it appears on Figure 17 for the reactor case ‘hgTliq’.

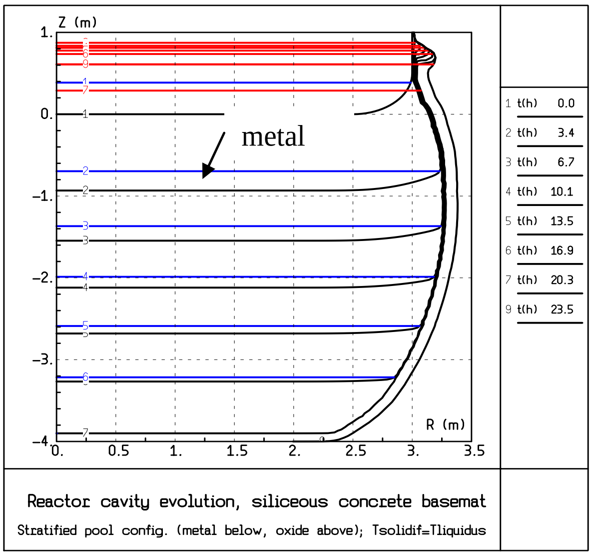


**Figure 18: Erosion of reactor cavity with stratified configuration; melt-through at 23.5 h (stratTliq)**

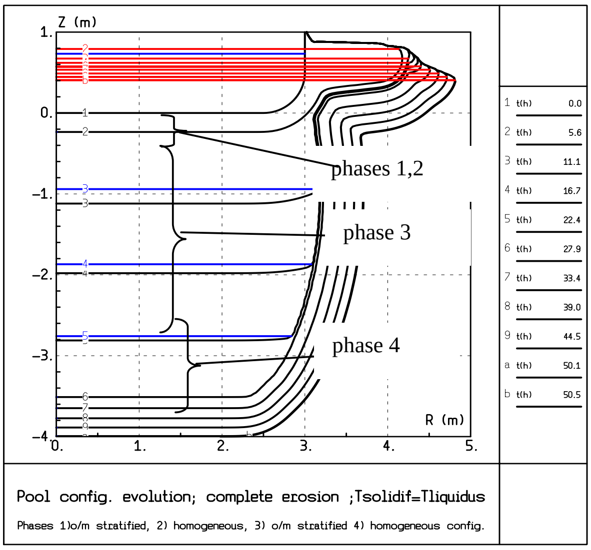


**Figure 19: Case with pool configuration evolution in 4 phases until basemat melt-through at 50.5 h**

In case of a ‘H’ configuration, the melt-through time is reduced with decreasing freezing temperature from $T_{liquidus}$ to $T_{solidus}$ (see Figure 16): indeed the pool temperature decreases with the freezing temperature, the energy needed for the ablation and heating of concrete also decreases and the concrete ablation is therefore faster.

Second, let us look now at results obtained assuming a stratified configuration (quoted ‘S’) maintained during the whole MCCI phase (see Figure 18). The assumption of a ‘S’ configuration gives a faster concrete erosion with melt-through times ranging between only 14 hours and 3.4 days, depending on the choice of freezing temperature and on the basemat thickness.
The reason of the faster erosion in case of a ‘S’ configuration is the high heat transfer coefficient at the oxide/metal layer interface compared to that along the oxide layer/concrete interface (see Table 5). This leads to a focusing of the heat towards the bottom pool interface and consequently an axial erosion faster than the lateral one for the reactor case ‘stratTliq’ on Figure 16. In case of a ‘S’ configuration, the axial erosion kinetics is also depending strongly on the oxide freezing temperature: when decreasing the freezing temperature, the lateral crust built-up along the oxide/concrete interface becomes thinner, which reduces the focusing of heat towards the pool bottom and delays the basemat melt-through (see Figure 16).
Finally, let us look at results obtained taking into account the evolution of pool configuration (see Figure 19), which might be more realistic. In this last scenario, the initial pool configuration is stratified with the oxide layer below the metal layer because of the higher initial oxide density. The subsequent evolution of the pool configuration is evaluated using pool configuration switch criteria roughly consistent with BALISE experiments [19]. The consequence of taking into account the pool configuration evolution, involving 4 phases, 2 of which with a stable homogeneous pool, is the significant delay of the predicted melt-through time by more than 24 hours compared to that obtained in the case of a steady stratified metal/oxide configuration (see Figure 18 and Figure 19).

### 4.3 Discussion

Reactor calculations assuming either a steady metal/oxide pool configuration or a homogeneous configuration give generally respectively lower and upper bounding estimates of the basemat melt-through time. Taking into account the pool configuration evolution leads to intermediate results in most cases. In the case of the corium inventory and reactor pit geometry chosen above, an early melt through time (in less than one day) seems to be unlikely for a 4 m thick basemat but appears to be possible for an only 3 m thick basemat, at least if the freezing temperature stays near the liquidus one.
The convective heat transfer coefficient within a pool layer is assumed here to be independent of the interface orientation. If this assumption is not used, the convective heat transfer coefficient distribution will particularly also influence the basemat melt-through time in the case of a homogeneous pool configuration.
These results are rather conservative because pessimistic boundary conditions are chosen, a very high heat transfer coefficient between oxide and metal layers is used and corium quenching is ignored. It is thought however that the trends obtained on the influence of the freezing temperature and pool configuration assumptions, are valid whatever the boundary conditions may be.

## 5 CONCLUSIONS

The codes WEX and MEDICIS are currently available in the integral code ASTEC V1.2 for the simulation of MCCI during a severe core melt accident in PWR nuclear power plants.
WEX has a long history and represents a more traditional modelling approach to the MCCI phenomenology. The range of available models in WEX and also their options are limited. A WEX feature is a simplified model of thermo-chemical behaviour of the melt. In the past validation work at GRS the free model parameters in WEX have been adapted to important experiments which are representative of the recent technical state-of-art (BETA, MACE).
MEDICIS is being developed by IRSN in collaboration with GRS, with the objective of a more generalised, flexible MCCI code. It is planned to model the most relevant phenomena identified by updated knowledge from recent or future research programs. The MEDICIS current version already permits a stronger coupling to thermo-chemical databases, a capability that was recommended by recent theoretical work on MCCI [11]. MEDICIS can also be applied with the same model settings as in WEX, except for the heat transfer model at the melt/concrete interface.
For experiments with real corium homogeneous melts, e.g. ACE, MACE and OECD-CCI, the ablation velocities are well reproduced by both codes. This is referred to a correct partition of energy fluxes from the heated pool (radiation/ablation). Two different approaches for the description of the interface behaviour have been investigated. In the first approach, the corium/crust is set to the solidus temperature and a specific heat transfer model giving a lower effective heat transfer coefficient is used. A reasonable prediction of the temperature evolution in these experiments is obtained by WEX and also in MEDICIS, if the effective heat transfer coefficients are adapted from that calculated in WEX. In the second approach (only possible with MEDICIS) the corium/crust is set near the liquidus temperature, but possibly a little lower. Here, a satisfactory prediction of the temperature evolution in the ACE tests and OECD-CCI 2 is also obtained for the same choice of freezing temperature using standard heat transfer models as found in literature, provided that a certain loss of refractory material from the melt pool due to crust segregation or splashing is taken into account.
For experiments with stratified thermite melts based on alumina (e.g. BETA, with oxide on top of the heated metal layer) WEX is successful in predicting the faster axial ablation compared to the radial ablation. In MEDICIS such behaviour can be simulated by defining the heat transfer coefficients as function of inclination of the interface. With this input settings both codes tend to overestimate the initial axial ablation compared to the experiment. The need for an improved model of lateral heat transfer in MEDICIS for situation similar to those of BETA will be investigated in the future.

The validation work presented here has permitted to identify the freezing temperature and the effective heat transfer coefficient between melt and concrete as important model parameters in MCCI codes, for which there is a substantial lack of knowledge. Therefore a further assessment of alternative approaches for modelling the interface behaviour is still needed.

Another interesting result of the CCI 2 test and of recalculations is that the convective heat flux distribution appears to be homogeneous. However the question on the profile of effective heat transfer coefficient and the variation of the crust stability along pool interfaces is still to be investigated in detail. This question will be addressed in further 2D MCCI experiments with real material (CCI 3, VULCANO, MCCI-OECD follow-on program) and simulants (ARTEMIS 2D).

Parametrical reactor calculations show the capabilities of the MEDICIS code for the description of long term MCCI and point out the significant impact on reactor predictions of the freezing temperature, of the oxide/metal heat transfer coefficient in the case of a stratified pool and of the models determining the pool configuration evolution.

Within the next months, the two above assessment approaches will be applied to the OECD-CCI 3 test, first in a blind configuration and then in an open one. Later, first results of interpretation of VULCANO and ARTEMIS tests will be available. This whole work will allow the IRSN and GRS specialists to develop best-estimate models for the melt-concrete interface behaviour and the 2D heat flux distribution within a corium pool, including WEX capabilities that have been identified as necessary in the assessment work. They will be implemented in MEDICIS – thanks to its flexibility and its capabilities – so that MEDICIS will be in the near future the unique MCCI code in ASTEC.

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