Simulation of Melt Spreading in Consideration of Phase Transitions

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Abstract: The analysis of melt spreading and relocation phenomena in the containment of LWR power plants in case of hypothetical severe accidents leading to core melting is an important issue for reactor safety investigations. For the simulation of melt spreading the code \textit{LAVA} has been developed on the basis of a method from the related subject of volcanology by adding more detailed models for heat transfer phenomena and flow rheology. The development is supported by basic analysis of the spreading of gravity currents as well as experimental investigations of the rheology of solidifying melts. These exhibit strong non-Newtonian effects in case of a high content of solids in the freezing melt. The basic model assumption in \textit{LAVA} is the ideal Bingham plastic approach to the non-Newtonian, shear-thinning characteristic of solidifying melts. For the recalculation of melt spreading experiments, the temperature-dependent material properties for solidifying melt mixtures have been calculated using correlations from the literature. With the parameters and correlations for the rheological material properties approached by results from literature, it was possible to recalculate successfully recent spreading experiments with simulant materials and prototypic reactor core materials. An application to the behaviour of core melt in the reactor cavity assumed a borderline case for the issue of spreading. This limit is represented by melt conditions (large solid fraction, low volume flux), under which the melt is hardly spreadable. Due to the persistent volume flux the reactor cavity is completely, but inhomogeneously filled with melt. The degree of inhomogeneity is rather small, so it is concluded, that for the long-term coolability of a melt pool in narrow cavities the spreading of melt will probably have only negligible influence.

1 INTRODUCTION

In order to limit potential consequences of a hypothetical severe accident in existing nuclear power plants, a special knowledge of the molten core materials with focus on melt behaviour within the containment and its long-term coolability is of substantial importance. In the past years an intensive discussion took place about the characteristic behaviour of core melt in the containment and the possibility of an extensive erosion of the basemat. A decisive factor for the actual course of a severe accident after the release of molten core material from the reactor vessel is whether a long-term cooling of the core melt in the area of the reactor cavity is possible. An extensive erosion of the basemat has to be prevented, but also the chemical reactions of long-term molten core – concrete interactions (MCCI) leading to the formation of combustible gas-mixtures, which may endanger the integrity of the containment, have to be accounted for.

Coolability would be improved considerably if the melt, which is released into a cavity after the melt-through of the reactor pressure vessel, could spread over a wide area. The cooling of the mixture of molten materials has a major influence on its spreading and relocation.

The present paper gives an overview of the current status (theory and application) of the code \textit{LAVA} developed for the simulation of melt spreading and relocation in the containment.\textsuperscript{1} Based on the knowledge that solidifying melts show a non-Newtonian material behaviour, the hypothesis is put up that Bingham's rheology has to be included in the modelling of the spreading process to cover the influence of material cooling on the retarding forces during the spreading of the melt. The development of \textit{LAVA} is completed and it has already been integrated into the containment code \textit{COCOSYS} [1].

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2 MODELLING OF MELT SPREADING

2.1 Basic characteristics of melt spreading driven by gravity

A one-dimensional melt dome spreading in a channel is considered as shown by Fig. 1. The average melt height (thickness) is given by \( \zeta_0 \), the extent of the spread melt is represented by \( L \) and the velocity in \( x \)-direction of the front is denoted by \( u_0 \), which is of the order \( L/t \). As long as the force of gravity is the only one acting on the mass of the melt, the melt will be accelerated (increase of \( u_0 \), decrease of \( \zeta_0 \)) and the potential energy \( E_{pot} = \frac{1}{2} m g \zeta_0 \) will be minimised. If the area, on which the melt spreads, is infinitely large, and the cooling effects on the melt can be neglected, the spreading is limited at last by the surface tension \( \sigma \) of the melt. This is the case, when the hydrostatic pressure at the average melt thickness \( \zeta_0 \) of the shallow melt layer equals the corresponding capillary pressure. This condition is defined by

\[
\zeta_0 = 2 \sqrt{\frac{\sigma}{\rho g}}.
\]  

(1)

2.1.1 Hydrodynamic boundary conditions

In case of sufficiently small fluid velocities (\( \frac{1}{2} \rho u^2 < p_0, p_h \) representing the ambient pressure) the pressure gradient can be expressed as a function of fluid height \( \zeta \), generally known as the hydrostatic pressure distribution.

Since the gravity tends to deform the melt volume quickly into a shallow layer, for not too small times the horizontal extent \( L \) of the melt dome can be expected to be much bigger than the vertical one (\( \zeta \)). Because of the very low aspect ratio (\( \zeta/L \ll 1 \)) the velocities and their derivatives along the \( z \)-direction can be neglected with regard to the overall result of the spreading and a low-dimensional formulation represents a justified simplification for a modelling approach.

2.1.2 Influence of cooling

The extent \( L \) of a spread melt could be easily evaluated from Eq. (1) using the expression \( V = L \zeta_0 d \) for the volume of the melt. Assuming \( \sigma \approx 0.5 \text{ N/m} \) and \( \rho = 4600 \ldots 8000 \text{ kg/m}^3 \) (depending on composition) for a prototypic corium melt, \( \zeta_0 \) can be expected to be approx. 5\ldots7 mm. However, in real spreading processes other retarding forces occur prior to the surface tension and are able to balance the driving force of gravity:

- Inertial forces, tending to maintain the uniform motion,
- viscous forces, depending on temperature (and freezing) of the material,
- non-Newtonian forces, due to interactions of the solid particles whilst being sheared.

The results of important spreading experiments with prototypic corium melts (COMAS at Siempelkamp Krefeld [2, 3], and KATS at Forschungszentrum Karlsruhe [4], indicate average melt thicknesses of about 2\ldots4 cm. Even if a high level of porosity (50 %) is assumed, the experimental melt thicknesses exceed clearly the equilibrium thickness \( \zeta_0 \) given by Eq. (1). This indicates that there is a strong influence of cooling on real spreading processes, which has to be covered precisely by a numerical model.
2.1.2.1 Effective viscosity: In modelling approaches for melt spreading the viscous effects are usually accounted for by a correlation for the effective viscosity $\eta$ of a partly frozen material. There are several parameters with influence on the dynamic viscosity of a melt. For a general discussion see [5, 6]. For the simulation of corium melts and simulant materials these main parameters with influence on the effective viscosity have been identified:

- Temperature: The viscosity increases with decreasing temperature. For the viscosity of liquids Arrhenius’ law is generally valid:

$$\eta(T) = \eta_0 \exp \left( \frac{C}{kT} \right).$$

- Phase composition: The viscosity of the liquid phase can be determined by Urbain’s general viscosity model for oxidic slags depending on composition [7]. According to the thermodynamics of phase equilibria in multi-component systems the composition of liquid and solid phases changes during solidification. The Urbain model involves target calculations for the composition of the residual liquid for each temperature level by the means of thermochemistry tools [8] (e.g. CHEMSAGE, GEMINI) with an appropriate data base.

- Phase transitions: The effect of phase transitions is accounted for by correlations for the effective viscosity in liquid - solid suspensions. These expressions relate the effective viscosity of a suspension with the volume fraction of dispersed solids ($\phi_s$), see Fig. 2, and are fitted to experimental results. The correlations include one or more parameters which refer to the very special rheology of the investigated systems. These are the correlations which are commonly in use for the description of corium spreading:
  
  - Chong/Stedman [9, 10]:

$$\eta(T) = \eta_0 \left( 1 + \frac{0.75 \frac{\phi_s}{\phi_{s,\text{max}}}}{1 - \frac{\phi_s}{\phi_{s,\text{max}}}} \right)^2.$$

  - Extended Arrhenius [11]:

$$\eta(T) = \eta_0 \exp \left( 2.5 C_\eta \phi_s(T) \right).$$

![Figure 2: Model approaches for the effective viscosity $\eta$ of solidifying melts.](image)

2.1.2.2 Bingham yield stress: The non-Newtonian rheology of solidifying melts is commonly accepted [12, 13, 14, 15, 5, 16, 17, 18]. A simple approximation to the rheology of solidifying melts is the two-parameter approach of the ideal Bingham plastic, characterised by yield stress and plastic viscosity (Fig. 3). This has been particularly
Figure 3: The ideal Bingham plastic.

shown for a corium-concrete mixture with 27.5 wt.-% SiO$_2$ by Epstein’s analysis [19] of Roche’s viscosity data [20]. Temperature dependent yield stress data of arbitrary suspensions are not sufficiently known as they do not only depend on temperature but also on many other parameters, which cannot be investigated properly.

In 1961 D. G. Thomas derived a power law correlation for the yield stress of aqueous ThO$_2$ suspensions with low concentrations of thorium oxide:

$$\tau_0 = C \varphi_s^3.$$  \hspace{1cm} (5)

For higher concentrations of solids the yield stress tends to have a steeper increase, similarly to the case of the effective viscosity. For solid volume fractions above a critical value ($\varphi_c \approx 50\%$) the correlation

$$\tau_0 \propto \left( \frac{\varphi_s}{1 - \varphi_s} \right)^{5.15}$$  \hspace{1cm} (6)

may be an approach. This correlation was derived from experiments with glass beads dispersed within a clay suspension [21].

2.1.3 Spreading regimes

Recent research work on the spreading of gravity currents under isothermal conditions [22] has shown, that the influence of retarding forces (e.g. viscous forces $F_{\text{viscous}}$) increase together with the melt covered area ($= Ld$ in Fig. 1), and that there is a sharp transition from an initial spreading regime controlled by a balance of inertial forces ($F_{\text{inertial}}$) and gravity ($F_{\text{gravity}}$) towards a spreading regime controlled by a balance of viscous forces and gravity. Both these isothermal regimes can be modelled by the appropriate force balance equations:

$$F_{\text{inertial}} = F_{\text{gravity}}$$

$$0 = F_{\text{gravity}} + F_{\text{viscous}}$$

for $F_{\text{inertial}} \gg F_{\text{viscous}}$, \hspace{1cm} (7)

for $F_{\text{inertial}} \ll F_{\text{viscous}}$. \hspace{1cm} (8)

A similar balance equation can also be set up for a spreading regime controlled by gravity and Bingham forces.
2.2 Modelling of melt spreading in \textit{LAVA}

The assessment of the statements of section 2.1 leads to the following specifications for a reasonable modelling strategy:

- A precise description of the terminating flow regime (balance of gravity and retarding forces) has priority.
- A low-dimensional formulation (e.g. shallow water approximation / lubrication theory) seems to be appropriate.
- Non-Newtonian forces have to be taken into account.
- The cooling and freezing behaviour of the material must be described carefully.

The code \textit{LAVA} has been developed according to these specifications for the simulation of core melt spreading phenomena with special regard to the cooling of the material and the phase transitions affecting the rheological parameters of the melt. The basic idea followed here is the analogy of core melt spreading to volcanic lava flows. In the field of volcanological research an efficient algorithm for the realistic simulation of lava flows based on Dragoni’s downslope flow model of a Bingham liquid current [23] was proposed [24]. This flow model is based on a balance of Bingham stresses and gravity and its basic idea is the assumption of “plug”-regions in the flow domain at locations, where the shear-stress $\tau$ is smaller than the yield-stress $\tau_0$. This algorithm is the basis for further development [25, 26, 27, 28], whereby models for

- phase transitions,
- crust formation,
- rheological behaviour,
- cellular automaton method for simulation of 2d spreading [29],
- heat transfer in the substratum,
- Newtonian velocity profiles for pure Newtonian melts and
- volumetric heating

have been added to the code.

2.2.1 Newtonian velocity profiles for pure Newtonian materials

As long as there is no influence of Bingham stresses, the Newtonian flow model is used for the calculation of the volume flux $\dot{v}$ per mesh width, since there is only evidence for the investigated corium mixtures and simulant melts to exhibit non-Newtonian behaviour at increasing solid volume fraction. Thus, without the assumption of any plug regions in the flow interior, the integration of $w_x$ (from the lubrication theory) across the melt’s thickness yields

$$\dot{v} = \int_0^\zeta w_x(z) \, dz = \frac{\rho g}{3\eta} \zeta^3 \left( \sin \alpha - \frac{dc}{dx} \cos \alpha \right).$$

Velocity profiles in a Newtonian liquid and an ideal Bingham plastic are schematically sketched in Fig. 4.

2.2.2 Automaton method for simulation of 2d spreading

An improved algorithm for the reduction of the grid dependencies is introduced by Miyamoto and Sasaki in [29]. The modifications are based on an analysis, which – with focus on a central cell – relates the area fraction of neighbouring cells along the diagonals to the area fraction of adjoining cells along the main axes. Taking this relation into account the volume flux to meshes in direction of the main axes is more strongly weighted than volume flux in direction of the diagonals. This weighting is achieved by a stochastic selection of a mesh’s neighbours to which the volume flux is being calculated. The method leads to calculation results that show isotropic spreading of the melt on an isotropic surface and no longer a strong bias towards the main axes of the system which was observed using the original algorithm of Ishihara (Fig. 5).
2.2.3 Modelling of heat losses and solidification

Three basic heat transfer mechanisms are modelled by LAVA:

- heat transfer by mass transfer,
- by radiation from the free surface and
- by conduction into the substratum.

The calculation of radiation and conduction is done separately from the hydrodynamical problem and is based on empirical heat transfer correlations. The bulk of the fluid at a location \((x, y)\) on the spreading plane is assumed to be nearly isothermal within the corresponding LAVA control volume and so a mean temperature is calculated. The flow properties \((\eta, \tau_0)\) are then constant within the fluid column at a location \((x, y)\).

2.2.3.1 Radiation: Heat losses at the free surface are given by

\[
\dot{q}_{\text{rad}} = \varepsilon \sigma_0 (T^4 - T_a^4).
\] (10)

\(\varepsilon\) represents the emissivity of the solid material which is initially formed at the free surface and \(T_a\) denotes the ambient temperature.
The surface temperature $T''$ can be much smaller than the maximum temperature $T_{\text{max}}$ in the bulk of the fluid and a crust might be formed at the free surface. The temperature difference is expected to be of the magnitude $\approx 300 \text{ K}$ and this phenomenon requires a precise model for crust formation at the free surface which has been added to LAVA.

### 2.2.3.2 Crust growth:
Crust growth is possible, if the surface temperature of the fluid $T''$ falls below the crust formation temperature $T'$ between the liquid (or mushy) melt and the solid crust. In this model $T'$ is defined by the "softening temperature" of the system. The softening temperature is the temperature below which convection is weak or non-existent [30]. Hence, for temperatures below the softening temperature the viscosity increases enormously due to solidification effects and only heat conduction is effective. When a crust begins to grow, a curved temperature profile within the crust is formed because of transient heat conduction. The one-dimensional temperature profile is approximated by

$$T(\xi, t) = T' + (T'' - T') \left[ \chi \left( 1 - \frac{\xi}{s} \right) + (1 - \chi) \left( 1 - \frac{\xi}{s} \right)^2 \right]$$

(11)

with $T(0, t) = T''$ and $T(s, t) = T'$. The symbol $\xi$ represents the $z$-coordinate of the crust regime and $s$ stands for the crust thickness ($0 \leq \xi \leq s$). $\chi$ is a time dependent coefficient describing the shape of the profile. Applying the Heat Balance Integral technique (HBI, [31]) and considering the Stefan boundary condition at the interface between liquid and solid the functions $T(\xi, t)$ and the crust thickness $s(t)$ are determined numerically. It is assumed that the local crust thickness does not vary due to convective melt transport.

### 2.2.3.3 Liquid - solid dispersion:
If the melt bulk temperature is lower than $T_{\text{liq}}$ (but higher than $T'$) solid phases are formed according to the temperature dependent relation for solid volume fraction $\varphi_s(T)$. The code then calculates phase transitions considering the release of latent heat as a volume source in each LAVA mesh, in which the bulk temperature falls below $T_{\text{liq}}$. In this approach the specific latent heat $h_s$ is assumed to be equally distributed along the mushy temperature interval.

### 2.2.3.4 Heat transfer between melt bulk and interfaces:
The convective heat transfer from the bulk of the liquid melt to the interfaces is expressed by standard correlations for convective heat transfer from a liquid to a horizontal surface [32]:

$$P_r = \frac{n \cdot c_p}{\lambda}$$

(12)

$$Gr = \frac{g \cdot \zeta_0^3 \cdot \beta \cdot \Delta T}{\nu^2}$$

(13)

$$Nu \propto \left( Gr \cdot Pr \right)^{1/4} \ldots \left( Gr \cdot Pr \right)^{1/3}$$

(14)

The reference length $\zeta_0$ represents the height of the fluid.

### 2.2.3.5 Heat transfer into the substratum:
Heat conduction in the substratum is modelled by an explicit solver for one-dimensional, transient heat conduction below each LAVA surface mesh.

An additional resistance for heat transfer $R$ at the interface between melt and substratum surface, considering non-ideal contact between melt and substratum surface (gap, crust formation), is assumed by the model. From comparisons between numerical and experimental temperature profiles in the substratum a realistic value

$$R = 2000 \ \text{m}^2 \text{K} \ \text{W}^{-1}$$

(15)

was found.

Because the exact processes at the interface between fluid and substratum are unknown to a substantial degree it is alternatively suggested to use an approximative constant value $\alpha_{\text{bot}}$ for the overall heat transfer from the melt to the substratum representing a time and space average. Experimental results of COMAS-5a and COMAS EU-2b yield values $\alpha_{\text{bot}} = 300 \ldots 400 \ \text{W} \ \text{m}^{-2} \text{K}^{-1}$ with good agreement to the analytical approximation using Equations (14) and (15). A value of $\alpha_{\text{bot}} = 400 \ \text{W} \ \text{m}^{-2} \text{K}^{-1}$ was used for the validation calculations with LAVA.
3 RESULTS

3.1 Validation

3.1.1 KATS-14

This spreading experiment was performed at Forschungszentrum Karlsruhe with thermite melt as corium simulation. An oxidic mass of 176 kg and 154 kg of iron melt was spread in separate channels on cordierite plates. The composition of the liquid oxide mixture is given in Tab. 1.

Table 1: Composition of the oxidic mixture used in the KATS experiments.

<table>
<thead>
<tr>
<th>component</th>
<th>wt.-%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₂O₃</td>
<td>85</td>
</tr>
<tr>
<td>SiO₂</td>
<td>10</td>
</tr>
<tr>
<td>FeO</td>
<td>5</td>
</tr>
</tbody>
</table>

Boundary conditions and material properties are taken from [33]. The experiment KATS-14 is characterised by a nearly constant, low volume flux during the inflow time of Δt = 37.6 s. The low initial superheat in comparison to $T_{\text{liq}}$ results in a spreading controlled by retarding forces (friction, yield stress, crustal stress) [34].

The results of the LAVA-calculation (Fig. 6) approximate the experimental result for the maximum spreading length ($L = 6.5 \ldots 7$ m) very well. In Tab. 2 the calculated melt temperatures are compared with the measured temperatures corresponding to the maximum voltage of the used W/Re thermocouples. At the locations $x = 1$ m and $x = 3$ m the measured temperatures are overestimated in the calculation by 77 °C and 65 °C, respectively. Regarding the experimental data an uncertainty of approx. ±50 °C has to be considered. Calculated and measured temperatures at the third location are in very good agreement.

![Figure 6: KATS-14: Calculated leading edge propagation in comparison to the experiment.](image-url)
Table 2: KATS-14: Comparison between calculated ($C_a = 2$) and experimental temperatures of the melt.

<table>
<thead>
<tr>
<th>time (s)</th>
<th>x (m)</th>
<th>$T$ (exp.) (°C)</th>
<th>$T$ (calc.) (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16.0</td>
<td>1.0</td>
<td>1870</td>
<td>1947</td>
</tr>
<tr>
<td>23.0</td>
<td>3.0</td>
<td>1830</td>
<td>1895</td>
</tr>
<tr>
<td>44.0</td>
<td>5.0</td>
<td>1840</td>
<td>1859</td>
</tr>
</tbody>
</table>

3.1.2 COMAS EU-2b

In the spreading experiment COMAS EU-2b an oxidic melt mixture with addition of silica (COMAS reference type “Corium R”) was spread in one-dimensional channels of different substratum materials (concrete, ceramics and cast iron). Table 3 shows the actual composition of the spread melt [3]. The three channels were filled with a total mass of 630 kg during a time interval of 6 s. Boundary conditions, material properties and calculation parameters are taken from [35, 3]. The maximum temperature at the beginning of the inflow process was +150 K above the calculated liquidus temperature of the oxidic melt mixture. In spite of this superheat the motion of the leading edge stopped immediately after end of pouring. This characteristic is reproduced very well by the LAVA calculation in agreement with the experiment (Fig. 7). The experimentally observed progression of the melt front is bounded upwards by the calculated line using a transient volume flux and downwards by the calculation using a constant average volume.

![Figure 7: COMAS EU-2b: Calculated melt front propagation on cast iron measured from the visible edge of the channels in comparison to experimental data.](image)

Table 3: COMAS EU-2b: Composition of the melt.

<table>
<thead>
<tr>
<th>component</th>
<th>wt.-%</th>
</tr>
</thead>
<tbody>
<tr>
<td>UO$_2$</td>
<td>31.1</td>
</tr>
<tr>
<td>ZrO$_2$</td>
<td>23.8</td>
</tr>
<tr>
<td>FeO</td>
<td>18.8</td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>15.1</td>
</tr>
<tr>
<td>Cr$_2$O$_3$</td>
<td>5.7</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>4.6</td>
</tr>
<tr>
<td>CaO</td>
<td>0.9</td>
</tr>
</tbody>
</table>
flux. A slight overestimation of the leading edge propagation is observed. This is due to the transient characteristic of the large volume fluxes in the COMAS experiments: At larger volume fluxes the spreading of gravity currents is controlled rather by inertial forces than by viscous forces. The calculated melt front propagation controlled by a balance of viscous forces with gravity is steeper as the corresponding solution obtained by a balance between inertial forces and gravity (see analytical lines in Fig. 7). Hence, the code LAVA, which is based on the equations for viscous spreading, tends to overestimate slightly an initial melt spreading domain controlled by inertial forces.

Figure 8: COMAS EU-2b: Comparison of calculated and measured substratum temperatures (cast iron).

Fig. 8 shows a good approximation of the measured substratum temperatures by the calculation results, using the model assumptions of section 2.2.3.5.

3.1.3 VULCANO VE-U7

The experiment VULCANO VE-U7, which was performed at CEA Cadarache, is characterised by a prototypic, oxidic corium melt spread into a two-dimensional sector geometry at a low temperature level, which is close to the limit of immobilisation. These limiting conditions for a further progression of the melt front can generally be expected at elevated values of the solid volume fraction close to 50...60%, assuming rheological correlations for viscosity and yield stress as outlined in section 2.1.2. The oxidic melt in VE-U7 was mainly composed of UO$_2$ and ZrO$_2$ and included only small amounts (< 10 wt-%) of FeO and SiO$_2$. The trapezoidal spreading area was bisected by a wall along the central axis of symmetry and each half of the substratum was made of a different material (zirconia and siliceous concrete, respectively). The melt was simultaneously poured into the two sections with a low volume flux. On the basis of the experimental data set [36], which confirms a rather high initial content of solid fraction in the melt, a preliminary analysis of the spreading on the substratum made of ceramics was performed with LAVA. The good agreement between experimental and calculated results (Fig. 9)$^2$ demonstrates LAVA's capability to simulate such a spreading process with conditions representative of a melt close to its immobilisation. The calculated substratum temperatures are in agreement with the measured ones (Fig. 10). The small deviations can be explained by uncertainties of the material properties (e.g. thermal conductivity) and of the measurement (positions of thermocouples). Fig. 11 shows the integration of heat losses from the total melt volume by radiation and conduction into the substratum as calculated by LAVA. They are of the same order, but much more heat is transferred to the substratum than radiated at the free surface. In previous work it was already shown, that the actual amount of heat transferred to the substratum surface is nearly independent of the substratum material properties [28].

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$^2$ Because of unresolved proprietary rights of the experimental data, the ordinate axes in Figures 9 and 10 are given in relative values.
Figure 9: VULCANO VE-U7: Calculated leading edge propagation in comparison to the experiment.

Figure 10: VULCANO VE-U7: Comparison of calculated and measured substratum temperatures at two different z-coordinates.
3.2 Real plant application

A typical German PWR of the “Konvoi”-type has been selected for the following analysis of a hypothetical severe core melt-down accident with an early failure of the reactor pressure vessel (RPV).

3.2.1 Initial and boundary conditions

The boundary conditions for the melt release into the cavity are given by a MELCOR calculation for the PWR chosen [37]. This calculation assumed a 50 cm\(^2\) leak in the reactor coolant system as initiating event for the accident. At the time of RPV failure (\(t_{\text{fail}} = 3.24\) h) under low pressure conditions the MELCOR calculation predicts a melt mass of approx. 180 \(\cdot 10^3\) kg comprising the components given in Tab. 4. A value of 150 W/kg is estimated for the internal heat source corresponding to the decay power at \(t_{\text{fail}}\).

Table 4: Composition of the melt (oxides, Zr and steel) released into the reactor cavity of a German PWR, calculated by MELCOR for the assumed scenario.

<table>
<thead>
<tr>
<th>component</th>
<th>wt.-%</th>
</tr>
</thead>
<tbody>
<tr>
<td>UO(_2)</td>
<td>67</td>
</tr>
<tr>
<td>ZrO(_2)</td>
<td>8</td>
</tr>
<tr>
<td>Zr</td>
<td>9</td>
</tr>
<tr>
<td>Fe</td>
<td>12</td>
</tr>
<tr>
<td>Cr</td>
<td>3</td>
</tr>
<tr>
<td>Ni</td>
<td>1</td>
</tr>
</tbody>
</table>
3.2.1.1 Borderline cases for melt spreading in the cavity: There are two limiting cases for the issue of core melt spreading in the reactor cavity:

- A large mass of melt with large superheat released into a narrow reactor cavity with a high mass flux. In this case the melt will quickly fill-up the cavity, forming a homogeneous pool.
- A small mass of melt, which is already partly frozen and close to immobilisation conditions, is released with a low mass flux into the reactor cavity. A priori it is not known, whether the melt release from the RPV into the reactor cavity will lead to a homogeneous distribution of the melt.

The second case is of more interest, since it decides, whether the spreading in the cavity has to be taken into account before the long-term cooling of the melt could be investigated. This “lower” limit to the issue of spreading is more realistic, if the leak in the RPV is small and not located in the bottom center of the lower head, but at a small latitude (0...20°). The equator of the bottom head is 0° latitude and the center of the lower head is 90° latitude (see Fig. 12). Assuming such a lateral location of the leak, the melt is expected to impinge on the outer periphery of the reactor cavity at \( r \approx 2.2 \ldots 2.5 \text{ m} \). In order to focus on a borderline case it is furthermore assumed that the lateral hole is of the size \( 0.2 \text{ m} \times 0.2 \text{ m} = 0.04 \text{ m}^2 \) and the amount of mass released from the opening into the cavity is only 10 wt.-\% (\( \approx 18 \times 10^3 \text{ kg} \)) of the melt pool in-vessel. The in-vessel pool will be separated into a bottom oxidic layer of higher density with a metallic layer on top. Thus, it can be assumed, that the melt released will contain more metals than oxides. In order to define limiting conditions it is supposed that the melt is well mixed according to its overall composition given in Tab. 4. Earlier investigations have shown, that the spreading of mixed phases can be simulated by assuming mixture material properties for density, thermal conductivity etc. with the exception of rheological properties (e. g. viscosity and yield stress). The latter are characterised in the model approach by the oxide phase only.

As it was shown in the post-test calculation of the VULCANO VE-U7 experiment, a partly solidified oxide melt with approx. 50 vol.-\% of solids spreads but is already close to immobilisation. Corresponding to these melt conditions, a steep evolution of solid fraction \( \varphi_s \) with decreasing temperature is assumed here (Fig. 13). The initial conditions correspond to \( \varphi_s = 0.5 \).

3.2.1.2 Boundary conditions for the LAVA calculation: The boundary conditions for the LAVA calculation are based on the assumptions of the last section. They represent a limiting case to the issue of melt spreading in the reactor cavity. The volume flux into the reactor cavity is approached by Torricelli's theorem, yielding a linearly decreasing volume flux. For the set-up of the computational grid, a mesh size of \( 0.1 \text{ m} \times 0.1 \text{ m} = 0.01 \text{ m}^2 \) was assumed (see Fig. 14). For completeness, the material properties of the oxide phase are approximated by the RASPLAV data for corium C-22 [38]. The mixed material properties in Tab. 5 are calculated on the basis of appropriate mixture assumptions.
3.2.2 Results:

The calculated results show a slow motion of the melt in the reactor cavity (Fig. 16). The inner, horizontal circular area with radius $R = 1.7$ m is completely covered after a time of 30 s, but the melt distribution is not homogeneous. At that time, nearly 2/3 of the total amount of melt have already entered the cavity. Due to the decreasing mass flux within the following 45 s, the average depth of the melt pool increases. At the end of the melt release phase into the cavity, the melt immobilises fast. Meanwhile the inhomogeneous melt distribution is sustained and differences in local melt thicknesses are of the order of 5 cm in the final melt distribution (Fig. 15).
Table 5: Material properties and boundary conditions.

<table>
<thead>
<tr>
<th>quantity</th>
<th>value</th>
<th>mixture model</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ [kg/m$^3$]</td>
<td>8000000</td>
<td>$(\frac{\xi_{\text{ox}}}{\rho_{\text{ox}}} + \frac{\xi_{\text{met}}}{\rho_{\text{met}}})^{-1}$</td>
</tr>
<tr>
<td>$c_p$ [J/kg K]</td>
<td>617950</td>
<td>$(\xi_{\text{ox}} c_{p,\text{ox}} + \xi_{\text{met}} c_{p,\text{met}})$ metal dispersed in oxide [39, 40]</td>
</tr>
<tr>
<td>$\lambda$ [W/m K]</td>
<td>14129</td>
<td>$h_{s,\text{ox}} \xi_{\text{ox}}$</td>
</tr>
<tr>
<td>$h_s$ [10$^3$ J/kg]</td>
<td>220100</td>
<td>$T_{\text{liq,ox}}$</td>
</tr>
<tr>
<td>$T_{\text{liq}}$ [K]</td>
<td>2673000</td>
<td>$T_{\text{sol,ox}}$</td>
</tr>
<tr>
<td>$T_{\text{sol}}$ [K]</td>
<td>2173000</td>
<td>$\eta_0,\xi_{\text{ox}}$</td>
</tr>
<tr>
<td>$\eta(T_0)$ [Pa s]</td>
<td>0.006</td>
<td>$h_{s,\text{ox}}$</td>
</tr>
<tr>
<td>$V_0$ [l/s]</td>
<td>60000</td>
<td></td>
</tr>
<tr>
<td>$\Delta t$ [s]</td>
<td>75000</td>
<td></td>
</tr>
<tr>
<td>$T_0$ [K]</td>
<td>2606000</td>
<td></td>
</tr>
<tr>
<td>$b$ [m]</td>
<td>0.100</td>
<td></td>
</tr>
<tr>
<td>$C_n$ in Eq. (4) [1]</td>
<td>5500</td>
<td></td>
</tr>
<tr>
<td>$C_{r_0}$ in Eq. (5) [Pa]</td>
<td>500000</td>
<td></td>
</tr>
</tbody>
</table>

Figure 15: Cross sections through the immobilised melt in the reactor cavity at different $y$-locations (including topographic elevations at the periphery) as calculated by LAVA.
Figure 16: Calculated spreading of the melt in the reactor cavity of a German PWR.
Motivated by a closer look into the phenomenology of melt spreading driven by gravity, the code *LAVA* for the simulation of spreading phenomena has been developed on the basis of a well-established method from volcanology. In *LAVA* the process of melt immobilisation due to cooling effects is described using non-Newtonian material characteristics in terms of a plastic viscosity and a Bingham yield stress. Both are dependent on the content of solids in a freezing melt. For the calculation of the rheological material properties viscosity and yield stress correlations are taken from literature and the relevant model parameters were estimated. Detailed heat transfer models have been added to *LAVA* accounting for solidification in form of a liquid - solid suspension as well as for the growth of a crust at the free surface, in case of local temperatures below the crust formation temperature.

*LAVA* has been validated against numerous European spreading experiments (particularly the German COMAS- and KATS-test series). The presented post-test calculations of spreading experiments range from KATS-14, an experiment with a well known simulant material and boundary conditions rather matching the basic modelling assumptions, to experiments with prototypic oxidic corium melts: COMAS EU-2b, initially controlled by inertial forces, and VULCANO VE-U7, controlled by viscous forces from the very beginning. The post-test calculation of the experiment VULCANO VE-U7 shows, that the spreading of oxidic corium melts with a rather high content of solids is adequately described by *LAVA*. This experiment is representative for melt conditions, which are close to immobilisation of the melt.

At last an application to real plant conditions (spreading in the reactor cavity of a PWR) has been performed, assuming similar melt conditions as in the VULCANO VE-U7 test and rather adverse melt release conditions with regard to the dynamics of melt distribution in the reactor cavity (small volume flux). For larger times the simulation results show a very inhomogeneous spreading of the melt with final differences in melt thickness of about 5 cm. These rather small deviations in local melt thickness are expected to have only a minor influence on the long-term cooling of the melt. The suggested scenario represents only a borderline case for the issue of spreading in the reactor cavity. Based on these findings it is concluded that nearly in all cases with a direct melt release from the RPV into the reactor cavity the spreading will lead to a sufficiently homogeneous melt distribution in the cavity. This conclusion is no more valid if a melt relocation from the reactor cavity to adjacent rooms in the containment has to be considered in case of a melt-through of a partition wall. Such relocation phenomena after the onset of MCCI will be the major subject for the application of *LAVA* for severe accident investigations focussed on containment integrity.
References


