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Report on the implementation of the DEM model in the CATHARE code

Work Package 3.1

“Multiscale and Multiphysics Simulation of LOCA

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Summary

This deliverable deals with the new development of the DEM model focused on thermodynamic non-equilibrium conditions, which prevail in the flashing flow process near the critical section. This model, developed at the University of Louvain (UCL), is the 1-D Delayed Equilibrium Model (DEM) for choked or critical flow rate in steady state or quasi-steady state conditions. The DEM are assessed against experimental data such as Super Moby-Dick and BETHSY experiments done in CEA during the eighties. The DEM model has been recently implemented in the WAHA code, which is based on a two fluid 1D six equations model. The methodology can be applied to other system code (CATHARE, RELAP, etc.).

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1 INTRODUCTION

This document deals with the new development of the DEM model focused on thermodynamic non-equilibrium conditions, which prevail in the flashing flow process near the critical section. This model, developed at the University of Louvain (UCL), is the 1-D Delayed Equilibrium Model (DEM) for choked or critical flow rate in steady state or quasi-steady state conditions. The DEM are assessed against experimental data such as Super Moby-Dick and BETHSY experiments done in CEA during the eighties. The DEM model has been implemented in the WAHA code, which is based on a two fluid 1D six equations model. The methodology has been applied to the CATHARE code (CATHARE, RELAP, etc.). This work is still in progress.

2 DELAYED EQUILIBRIUM MODEL: BRIEF SUMMARY

2.1 General Assumption

The local instantaneous equations of the flow can be averaged statistically and spatially in a cross-section of the flow. The equations have then a more appropriate form with respect of their use in this section: only average values of the parameters in a channel cross-section are considered in this paper. Moreover, for the sake of simplicity, we introduce some approximations related to the following assumptions:

H0.- The flow is steady-state.
H1.- The channel is fixed, not vibrating, not elastic, not porous: it can have a non-uniform cross-section profile \( A(z) \): its axis is rectilinear.
H2.- The surface and statistical correlation factors, which are the ratios between the averages of the products of the variables and the products of the averages of these variables, are all equal to unity. This implies that all transverse profiles are sufficiently flat in every cross-section, and do not vary too much statistically.
H3.- The pressure is uniform in any cross-section.
H4.- The transverse components of the velocity are neglected.
H5.- The averaging process over the cross-section is extended to the thermodynamic relationships, and in particular to the equation of state, taking H2 into account.
H6.- The effects of thermal dissipation and turbulence are not taken into account.
H7.- The wetted and heated perimeter are equal \( P_w = P_h = P \).

2.2 Delayed Equilibrium Model (DEM) : Basic Equations

In addition to assumptions H1 to H7 made in the previous section, some additional assumptions support the Delayed Equilibrium Model (DEM). The most specific assumptions is:

H8.- Mechanical equilibrium: \( W_\alpha \equiv W_i \triangleq \dot{v} \)

Let us consider the adiabatic expansion of a liquid in a tube (Fig. 1). Assume that the state of the liquid at the inlet of the pipe is \((p_{in}, T_{in})\) with \( p_{in} > p_{sat}(T_{in}) \). Due to the friction, the pressure decreases along the pipe, and reaches saturation at section “s”. Between section “s” and the onset of flashing, the liquid is metastable. The onset of flashing occurs at section “o”, where the pressure \( p_o \) is typically (Lackmé [12]):

\[
p_o = (0.95 \ldots 0.98) p_{sat}(T_{in})
\]

For turbulent liquid flows, the slope of the straight pressure line between the inlet and the onset of flashing, i.e. the pressure gradient is proportional to the square of the mass velocity. The distance between point “o” and the tube outlet depends on the inlet subcooling and on the mass velocity. Here we will assume that the inlet subcooling and the mass velocity are such that the onset of flashing is located inside the pipe. Between point “o” and the pipe outlet, a two-phase bubbly flow develops rapidly, and the pressure gradient increases. If the pressure at the outlet is low enough, the flow is choked, and the outlet pressure is the critical pressure \( p_c \). One can expect that the over-heating (or metastability) of the liquid phase does not vanish
instantaneously at point “o”, but persists in the two-phase part of the flow, depending on one hand on the intensity of the heat transfer from the bulk of liquid to the interface and on the other hand on the rate of pressure decrease.

For large subcoolings, the onset of flashing is close to the pipe outlet, and the critical mass velocity can be approximately deduced from the single-phase pressure gradient, considering that it is constant over the whole pipe length (Lackmé [12]). For small subcoolings, accurate predictions of the critical mass velocity cannot be obtained without the complete modeling of the flow. For all cases, the accuracy on the prediction of the critical pressure is a relevant indicator of the validity of the two-phase critical flow modeling.

![Fig. 1 A typical pressure profile along a pipe with a critical section at its end.](image)

\[
\text{The Delayed Equilibrium Model (Lackmé [12], Féburie et al. [10], Attou et al. [2,3], Bartosiewicz et al. [5], L. Bolle et al. [7]) assumes that, at a given cross-section, only a mass fraction } \gamma \text{ of the fluid is transformed into a saturated mixture, the remaining } (1 - \gamma) \text{ fraction being the bulk metastable liquid. This fraction undergoes a near-isentropic evolution since the heat of vaporization is exchanged between the saturated liquid and saturated vapor. The mass fraction of vapor in the saturated part of the mixture is denoted by } \psi, \text{ and, consequently, the specific volume and the mixture enthalpy of this kind of “three-phase mixture” are given by:}
\]

\[
v_m = \frac{\Delta(1 - \gamma)v_{fM} + xyv_{q,sat} + (y - x)v_{f,sat}}{\Delta h_{fM} + xyh_{q,sat} + (y - x)h_{f,sat}}
\]

\[
\frac{dy}{dz} = 0.02 \frac{P_w}{A} (1 - \gamma) \left[ \frac{p_s(T_m) - p}{p_{cr} - p_s(T_m)} \right]^{0.25}
\]

This relaxation law expresses that the decrease of the mass fraction of superheated liquid \(d(1 - \gamma)\) over an element of length \(dz\) is proportional to the remaining quantity of superheated liquid, and to the power 0.25 of the metastability expressed in a non dimensional way by means of the difference between the critical pressure of the fluid and the saturation pressure of the mixture. The factor \(P_w/A\) takes into account the relative importance of the wall surface, on which nucleation is supposed to be triggered, with respect to the volume of the fluid in the pipe. It has been introduced to make Equ. 12 applicable for small as well as large diameter pipes. All results of the DEM presented in this paper have been obtained with a fixed coefficient 0.02 and a constant exponent 0.25.

This relaxation law has been generalized and recently improved to take into account not only the nucleation at the wall (constant \(C_1\)) but also in the bulk of the flow (constant \(C_2\)). These constants have been determined experimentally from an extensive series of experiments considering experiments performed in
small nozzles and in very large nozzles as well (Attou et al. [3], Féburie et al. [10], Rousseau [14], Sozzi et al. [16–17], Marviken experiments, etc.) and the relaxation law is now written as:

\[
\frac{dy}{dz} = \left( C_1 \frac{P_w}{A} + C_2 \right) (1 - y) \left[ \frac{pS(T_{FM}) - p}{p_{crit} - pS(T_{FM})} \right]^{0.25}
\]  

(12)

with \( C_1 = 0.008, C_2 = 0.56 \) and where \( p_{crit} \) is the critical pressure of the fluid (221 bars for water).

By analogy to the equation system obtained for the HEM model and by choosing the quality \( X \), the pressure \( p \), the velocity \( W_m \) and the mass fraction \( y \) as dependent variables, the equations system in the framework of the DEM can be written:

\[
\begin{bmatrix}
    v_g - v_{f, sat} & v_{f, sat} - v_{fM} & +(y - x)v'_f & -\frac{v_m}{w_m} \\
    0 & 0 & 1 & \frac{w_m}{v_m} \\
    h_g - h_{f, sat} & h_{f, sat} - h_{fM} & +(y - x)h'_f & w_m \\
    0 & 1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
    \frac{dx}{dz} \\
    \frac{dy}{dz} \\
    \frac{dp}{dz} \\
    \frac{dw_m}{dz}
\end{bmatrix}
= \begin{bmatrix}
    \frac{v_m}{A} \frac{dA}{dz} \\
    -\frac{P}{A} r_w - \frac{1}{v_m} g \cos \theta \\
    -g \cos \theta + \frac{v_m}{w_m} \frac{P}{A} q_w \\
    f(p, y, T_{FM})
\end{bmatrix}
\]  

(13)

with the following definitions of the derivatives of quantities related to the saturated mixture and to the metastable liquid:

\[
v'_k = \left( \frac{\partial v_k}{\partial p} \right)_{sat} \quad \text{and} \quad h'_k = \left( \frac{\partial h_k}{\partial p} \right)_{sat}
\]

\[
v'_{fM} = \left( \frac{\partial v_{fM}}{\partial p} \right)_{S} \quad \text{and} \quad h'_{fM} = \left( \frac{\partial h_{fM}}{\partial p} \right)_{S}
\]  

(14)

where the properties of the metastable liquid and their derivatives depend only on the pressure if an isentropic evolution is assumed for this phase.

In particular, the derivatives of the enthalpy of the metastable liquid can be easily deduced from the following relation:

\[
dh_{fM} - v_M dp = T dS = 0
\]

which means that \( v'_{fM} = 0 \) and \( \left( \frac{\partial h_{fM}}{\partial p} \right)_S = v_M \).

The critical condition of the model is the vanishing condition of the determinant of the system and after some manipulations it appears to be the classical definition of the speed of sound:

\[
w_c = \sqrt{\left( \frac{\partial p}{\partial m'} \right)_{S_{w,y}}}
\]  

(15)

Similar approach about the existence of a superheated liquid in a metastable state during the flashing process in two-phase flow has been developed in the Homogeneous Relaxation Model, called HRM (Z. Bilicki et al. [6], D. Downar-Zapolski et al. [9]). This model has been successfully used in the WAHA code developed in the frame of the 5th European Program for simulating Water Hammer (Tiselj et al. [18,19], Barna et al. [4]).
2.3 Consistency of the DEM Model – Existence of a frozen metastable phase

The DEM model assumes that the metastable liquid phase is somewhere frozen since the onset of flashing (cross-section $z_0$ of fig.1) till the critical section (cross-section $z_c$ of fig.1).

In the following, the expansion of the metastable flashing liquid is almost a frozen process, as it will be shown now.

Considering the very high velocity during the flashing, the transit time between these two cross-sections is very short, i.e. a few millisecond depending on the subcooling of the liquid at the entrance of the nozzle.

Let consider the conduction heat transfer in transient condition through the metastable liquid phase during this very short time delay.

Suppose that at time $t = 0$, the metastable liquid at a temperature $T_{f,M}$ is suddenly in contact with the saturated liquid at a temperature $T_{f,sat}$ assuming to be maintained constant during the transient. In fact, these saturated temperature of the mixture is decreased very rapidly during the flashing due to the very steep pressure drop.

The analytic solution for a semi-infinite transient heat conduction problem is given in figure 2.

Fig. 2 shows the temperature profile in the metastable liquid for different time delay (3 ms, 6 ms and 9 ms). The temperature front only penetrates on a few tens microns. Most of the metastable liquid remains at the same initial thermodynamic state, which exist at the onset of flashing.

![Temperature profiles in the metastable liquid at different time](image)

That means that the metastable liquid must be surrounded by a thin layer of saturated liquid in contact with the vapour, due to the much smaller time scale for the mass transfer from the saturated liquid to the vapor phase.

The increase of the amount of the saturated liquid is thus mainly due to the increase of the interfacial area density, because of a very fast change of the flashing flow patterns from bubbly flow at the onset of flashing to droplets flow at the critical section.

The DEM model considering 3 phases (frozen metastable liquid, saturated liquid and saturated vapor) seems to properly model the physics of the flashing process.
2.4 Recent assessment of the DEM model against the Super Moby-Dick and the BETHSY tests

The DEM model has already been assessed against 500 data of experiments performed on different nozzles, different fluids and different subcooling or saturated conditions at the entrance (Attou et al. [2], Attou et al. [3], Bolle et al. [7], Rousseau [14], Sozzi and Sutherland [16-17], Véneau [21])

In the context of nuclear reactor safety, a pipe break in the primary circuit is the earliest mechanism for initiating a LOCA. The pipe involved could be a main coolant pipe, in which case it leads to a large break LOCA, or a pipe connected to the main coolant loop (e.g. an ECC line) which could lead to an intermediate or small break LOCA.

In a large break LOCA, the critical section can be located at the breach or at some restricted cross section in the surge line or the pump. No specific separate effects test relating to either of these last two possibilities has been found. The pressurizer surge line should in principle be covered by the database for critical flow in pipes.

As it has already been said, when a break occurs in a separating wall structure between a high and low pressure system the flow through the break will depend on conditions upstream of the break and on the break area and shape. Critical flow through a break is similar to critical flow through a nozzle, but the geometry of the break can encompass any shape, location and size from a small crack to a complete 200 percent guillotine break in a flow pipe.

The Nuclear Energy Agency has selected different experiments as reference tests for critical flows occurring during a LOCA. Recently, we have chosen two series of tests in the context of the NURESAFE project for reassessing the DEM model.

The Super Moby-Dick and BETHSY experiments performed by the CEA-Grenoble during the eighties (Rousseau [14,15]) consist in two-phase critical flashing flow experiments.

Steady state critical flow conditions were measured in a long nozzle and in a short nozzle for the Super Moby-Dick test. The long nozzle has an elliptic convergent section at the entrance followed by a straight pipe of about 0.380 m long and of 20 mm inner diameter and ended by a 7° divergent section. The short nozzle has almost the same geometry without the divergent section.

The BETHSY test was also performed at high pressure with different temperatures at the entrance on a short nozzle of 2" long and 5 mm diameter.

Fig. 3 shows the DEM results of critical mass fluxes against the measured data of Super Moby-Dick and BETHSY experiments. The agreement is quite satisfactory, the discrepancy is less than 5%.
The DEM model has recently been further assessed against the Super Moby-Dick experiments as far as the pressure and void fraction profiles along the nozzle are concerned. Twelve reference tests have been chosen for each nozzle for four different pressures at the inlet: 20, 40, 80 and 120 bars. For each pressure, three different temperatures have been tested. The water is subcooled or quasi-saturated at the inlet of the nozzles. For each experiments, a systematic comparison has been done between the experimental profiles and the profiles calculated by the DEM model.

Fig. 4 and 5 give a comparison of the profiles along the long and the short nozzle of the Super Moby-Dick tests. The agreement is also satisfactory.

3 IMPLEMENTATION OF THE DEM IN THE WAHA CODE

The WAHA code has been developed during the WAHALoad project in the frame of the 5th EURATOM programme.
The WAHA code is based on a 6 two-fluid balance equations written for the gas and fluid phases. The six variables are:

\[ p, w_f, w_g, \alpha, u_f, u_g \]

where \( p \) is the local pressure, \( w_f \) and \( w_g \) are both velocities of the phases, \( \alpha \) is the void fraction, \( u_f \) and \( u_g \) are the internal energy of the phases.

In order to impose the mechanical equilibrium in the WAHA code \( (w_f = w_g) \), the interfacial momentum transfer coefficient has been taken to a very high value.

Moreover, the enthalpies of the mixture in the DEM model and in the WAHA code must be equal, which links the vaporization index \( y \) of the DEM model to the variables of the WAHA code. We find the following relation:

\[ (1 - y) = \frac{(1 - X)(h_{fM} - h_{f,sat})}{(h_{fM_{DEM}} - h_{f,sat})} \]  

(16)

On the other hand, the third equation of the DEM model (eq. 14) allows to determine the increase of the quality of the vapor along the nozzle \( (z) \) and leads to the following relation:

\[
\frac{dX}{dz} = - \frac{C(1 - X)(h_{fM} - h_{f,sat})}{(h_{g,sat} - h_{f,sat})} \left[ \frac{X \frac{dh_{g,sat}}{dp} + (1 - X) \frac{dh_{f,sat}}{dp} + (1 - y) \nu_{mDEM}}{h_{g,sat} - h_{f,sat}} \right] \frac{dp}{dz} \] 

\[ - \frac{w_m}{h_{g,sat} - h_{f,sat}} \frac{dw_m}{dz} \] 

\[ - \frac{g \cos \theta}{h_{g,sat} - h_{f,sat}} \]  

(17)

with

\[ C = \left( C_1 \frac{P_w}{A} + C_2 \right) \left[ \frac{p_{sat}(T_{fM}) - p}{p_{crit} - p_{sat}(T_{fM})} \right]^{0.25} \]

Finally, the source term of the interface mass transfer of vapor can be deduced from eq. 18 and implemented in the WAHA code. We obtain:

\[ \Gamma_{DEM} = \rho_m \frac{dX}{dt} = \rho_m \frac{dX}{dz} = \rho_m w_m \frac{dX}{dz} \]  

(18)

The figure 6 shows an example of comparison of the pressure and the void fraction profiles for both codes (WAHA and DEM-UCL code). The agreement is quite good.
Figure 7 gives the comparison of the mass flux between the WAHA code and the DEM model against the data of the Super Moby-Dick tests for the long nozzle.

Figure 7 gives the comparison of the mass flux between the WAHA code and the DEM model against the data of the Super Moby-Dick tests for the long nozzle.

4 CONCLUSION

This deliverable revisited the modelling techniques for the computation of critical two-phase flows relevant to nuclear safety in GENII, GENIII power plants. In addition, several possible benchmarks have been reviewed and proposed for validation purposes in system codes. One of the objectives of the NURESAFE project is to implement such non-equilibrium models in the next generation of the system code CATHARE-3. The results presented in this paper demonstrated that the DEM model could be implemented in the WAHA code, which is quite similar of thermo-hydraulic codes (CATHARE, RELAP, etc.) as far as the basic equations used in these codes are concerned. The DEM model is a good candidate to be implemented in system codes since it
performs well and is physically consistent. The current research track is to implement the DEM model in CATHARE and to relate turbulent pressure fluctuations to trigger the nucleation to justify or modify these empirical parameters. This work is still in progress.

5 REFERENCES


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6 ANNEXES
### 6.1 Annex 1: Document approval by beneficiaries’ internal Quality Assurance

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