MODELLING OF FUEL-COOLANT INTERACTION WITH THE MULTIPHASE FLOW CODE MC3D.

Meignen Renaud[a], Picchi Stephane[b], Lamome Julien[c]

[a] *Institut de Radioprotection et Sûreté Nucléaire (IRSN), DSR/SAGR,*
BP 17 - 92262 Fontenay-aux-Roses Cedex, France,
renaud.meignen@irsn.fr
[b] *CS-SI, Email: stephane.picchi@c-s.fr*
[c] *CS-SI, Email: julien.lamome@c-s.fr*

ABSTRACT

MC3D is a multi-component thermal-hydraulic 3D software developed by IRSN with collaboration of CEA. It is based on an Eulerian description of the mass, momentum and energy balances of multiphase compressible flows. The major application of MC3D has been the development of two models for Fuel-Coolant Interaction (FCI), one for each step of the interaction, namely premixing and explosion. We firstly present the general architecture of the code (solver), then some numerical specificities of the code. Then we describe some major challenges in FCI physical modeling, and conclude with foreseen improvements of both code general structure and physical modeling.

1. INTRODUCTION

MC3D is a software devoted to multiphase thermal-hydraulic flow studies and evaluations in the field of nuclear safety. Developed since about twenty years, its field of applications has evolved several times to become one of the reference tools for the evaluation of (molten) Fuel Coolant Interaction (FCI) in power and experimental reactors. Let us recall that, for power reactors, FCI might occur in the course of a severe accident during some phase of relocation of the molten core (called hereafter melt or fuel) in water. The mixing which occurs during the relocation might evolve as a detonation-like explosion with potential loads that may induce the failure of the containment integrity.

FCI is a complex multiphase flow problem involving very transient situations with several scales regarding dimensions and time, considering the mixing of molten fluid mixtures at about 3000 K (in nuclear reactor situation) in cold water and pressures going from ambient to far beyond the critical point. One major problem for the modeling of FCI is the low number of quantitative experimental data. Due to the particular and extreme conditions, measurement possibilities are limited and most of the data concerns integral properties as the pressure, water level, post-test debris analysis; see [1][2] for premixing experiments and [3] for explosion experiments.

It can be easily understood that modeling FCI is a particularly complex task for different reasons. First, the theoretical physical problem of FCI is not fully solved and there are still some uncertainties and discussions among experts in some crucial parts as the pressurization process itself, fragmentation, melt solidification and chemical interactions. Second, it is a multiphase flow problem with different fluid materials: vapor, non condensable gases, water,

melt composed of a mixture of different oxides and metals. The melt dispersal process occurring during the premixing is particularly complex, involving numerous phase changes. Thus, some particularly crucial choices and simplifications have to be made in the way to handle the problem so that it can be computed in reasonable times.

Two models describing the premixing and the explosion stages were introduced in MC3D which can be in fact understood as a framework for the development of models related to multiphase flow. This was done thanks to a concept of "application" which will be described in the next section.

2. GENERAL ARCHITECTURE AND MAIN NUMERICAL FEATURES

2.1 General architecture

The MC3D software architecture is organized with the concept of "application". An application is defined by a set of material components that can be grouped in volume mixtures (same volume, e.g. gases), momentum mixtures (same velocity) and energy mixtures (same temperature or enthalpy) supplemented with a set of models for interactions among various components (frictions, energy transfer, phase transfer, chemistry). The resolution core is common to all application. Specific models for specific numerical fields can be added. This is summarized in Fig. 1 with an example of two generic applications. The resolution is common to all applications and thus the developer does not have to worry about that. This architecture allows the fast development of applications, provided the physical models are available.

2.2 General numerical aspects

We use the classical Eulerian "two-phase" method (e.g. [4]) where each phase is described by a mass, momentum and energy equation. To limit the computational cost, the phases can be grouped in mixtures as already explained. The balance equations of mass, momentum and energy are solved with a semi-implicit method. The main variables for resolution are:

- the volume fractions α for each volume mixture, supplemented by mass fractions X of each individual constituent in each volume mixture;
- the pressure P (one single pressure as default);
- the velocities $\vec{V}$ of each momentum mixture;
- the temperature T (or enthalpy h) for each energy mixture.

A staggered grid is used (cartesian or cylindrical) where velocities are expressed at the faces and other variables at the centre of meshes (Fig. 2). The phase densities and specific energies are expressed as functions of the pressure and mixture temperature, i.e. $\rho = \rho(P,T)$ and $e = e(P,T)$. The volume mixtures have mixture densities computed as $\rho_v = \sum_{nc} X_c \rho_c$ where nc is the number of components in the considered volume mixture and subscript c stands for the components. The momentum mixture is defined with a volume fraction $\alpha_m = \sum_{nv} \alpha_v$ where nv is the number of volume mixtures in the momentum mixture, and with a mixture density

$\rho_m = \frac{1}{\alpha_m}\sum_{nm}\alpha_v\rho_v$ .The energy mixtures are characterized with $\alpha_e = \sum_{nm}\alpha_m$, $\rho_e = \frac{1}{\alpha_e}\sum_{nm}\alpha_m\rho_m$ and $e_e = \frac{1}{\alpha_e\rho_e}\sum_{nm}\alpha_m\rho_m e_m$ where *nm* is the number of momentum mixtures in the considered energy mixture. The numerical resolution method consists in rearranging the balance equations in order to obtain a matrix containing only the pressure. This matrix is solved and other variables are obtained. To do so, the momentum equations are treated separately from the mass and energy balances in order to express the velocities as functions of local surrounding pressures. Then, these expressions for the velocities are introduced in mass and energy equations so that these ones are only functions of the pressure, volume fractions and temperatures. These balances are solved with an iterative Newton-Raphson procedure.

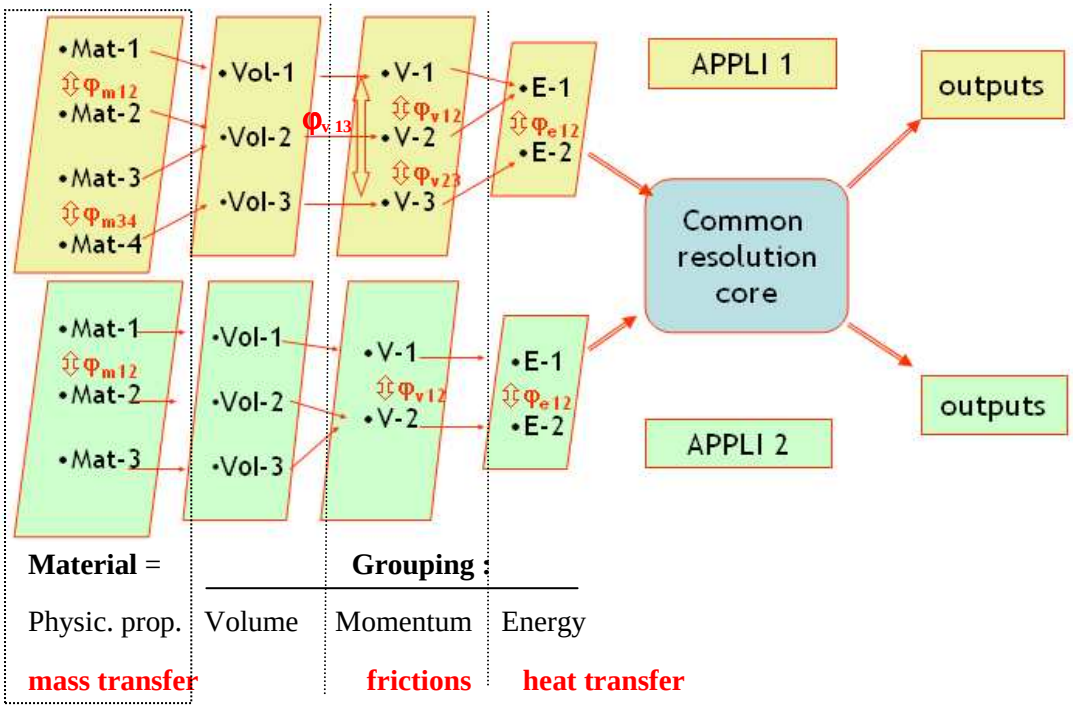

Figure 1. Example of application organisation in MC3D for two generic applications. The φ's are representing exchanges (in red) among components and mixtures

The process starts by considering the momentum equation which is written with the finite difference method. For a momentum mixture, the balance is written in non conservative and mostly implicit form regarding the velocities:

$$\alpha_m^n\rho_m^n\left(\frac{(V_m^{n+1}-\vec{V}_m^{\,n}}{\Delta t}+\vec{V}_m^{\,n}div(\vec{V}_m^{\,n})\right)=-\alpha_m^n\overrightarrow{grad}(P)^{n+1}+\alpha_m^n\rho_m^n\vec{g}+\sum_{l=1,l\neq m}^{nmel}K_{lm}(\vec{V}_l^{\,n+1}-\vec{V}_m^{\,n+1})$$
$$-Kp^n\vec{V}_m^{\,n+1}+\sum_{c=1,c\in l}^{ncons}\left[\sum_{c'=1,c'\in m}^{ncons}\Gamma_{cc'}^{n+1/n}(\vec{V}_l^{\,n+1}-\vec{V}_m^{\,n+1})\right]+T_{add} \quad (1)$$

Subscript *m* refers to the considered momentum mixture, *nmel* and *ncons* are the numbers of momentum mixtures and components, *l* stands for the other momentum mixtures ($l \neq m$), and *c* and *c'* stand for components respectively within momentum mixtures *l* and *m*. The upper

indication n or n+1 indicates the implicitness of the equation. The K_{lm}'s are the interfacial friction coefficients between momentum mixtures l and m and Kp is a friction coefficient on fixed structures. $\Gamma_{cc'}^{n+1/n}$ represents mass transfers between components. The superscript n+1/n expresses the fact that heat transfers are computed in a mixed explicit/implicit way. T_{add} represents additional terms that won't be detailed here. These are the added mass, lift, turbulent dispersion and additional momentum due to fragmentation processes. The set of momentum equations can be formally solved to obtain expressions for each component U, V, W of the velocities as function of nearby pressures. The U, V and W expressions are then introduced in the mass and energy equations which are expressed with finite volume method as:

$$\frac{\left(\alpha_v^{n+1}\rho_v^{n+1}-\alpha_v^n\rho_v^n\right)}{dt}+\sum_{faces}\tilde{\alpha}_v^n\tilde{\rho}_v^n.\frac{S_f}{\Omega}.V_m^{n+1}=\sum_{c,c'}^{ncons}\Gamma_{cc'}^{n+1/n} \tag{2}$$

$$\frac{\left(\alpha_e^{n+1}\rho_e^{n+1}e_e^{n+1}-\alpha_e^n\rho_e^n e_e^n\right)}{dt}+\sum_{faces}\tilde{\alpha}_e^n\tilde{\rho}_e^n\tilde{e}_e^n.\frac{S_f}{\Omega}.V_m^{n+1}+P^{n+1}\left[\frac{\left(\alpha_e^{n+1}-\alpha_e^n\right)}{dt}+\sum_{faces}\tilde{\alpha}_e^n.\frac{S_f}{\Omega}.V_m^{n+1}\right]= \tag{3}$$
$$\sum\Phi^{n+1/n}+\sum_{c,c'}^{nc}\Gamma_{cc'}^{n+1/n}H_c+T_{add}$$

In these equations, v and e are the considered volume and energy mixtures, the tilde (e.g. $\tilde{\alpha}$) stands for "convected" quantities at the faces (e.g. quantity in upwind cell for O(1) convection scheme), Γ represents the mass transfers, Φ the heat fluxes and H the enthalpy of donor phase. S_f is the area of the faces and Ω is the volume of the cell. Heat fluxes are under the general form (except for radiation), $\Phi = h^n A^{n+1}\Delta T^{n+1}$, with h the heat transfer coefficient, written explicitly, A the interfacial area between two fluids and ΔT the temperature difference, both expressed implicitly. In the energy equation, T_{add} stands for various additional terms that cannot be detailed here as conduction, chemical energy, volumetric power sources. The kinetic energy is neglected.

2.3 Some numerical features

For the modeling of FCI, since the energy is transported by the melt (~3000 K), it is essential to be able to describe accurately the melt convection and characteristic scale. For this, several additional numerical models where developed.

2.3.1 Interfacial area transport equations

In MC3D, the choice was made to use a fully Eulerian modeling even for the melt description. The choice is firstly dictated by simplicity. All fields are treated the same way which allows an automatic treatment. A Lagrangian approach might yield several advantages since the follow-up of particles allows some specific treatments as computation of temperature profiles in the drops in an straightforward way whereas Eulerian method needs some specific transport equations (see [6] for a model of transport of crust and temperature profile). However, the complexity of mixing Eulerian and Lagrangian is a severe trick and leads to important limitations in functionality. We are then led to use interfacial area transport equations. This is currently done for the melt drops with the use the classical Ishii's formulation:

$$\frac{\partial A}{\partial t} + \nabla . A\vec{V}_d = \Gamma_{A,\rho} + \Gamma_{frag} \qquad (4)$$

A is the interfacial area and $\Gamma_{A,\rho}$ is a source term to account for the compressibility of the fuel with the temperature (particularly during phase changes) and pressure. Γ_{frag} represents the various source terms due to fragmentation. These will be discussed later. The development for the coolant interfacial area (drops, bubbles) is under way.

2.3.2 Convection scheme

In multiphase flows, the use of a simple upwind scheme leads to severe difficulties. This can be easily understood since, at vanishing amount of material, the affected velocity can have no real physical meaning. Due to the specific resolution scheme, classical high order models can be hardly introduced and we thus developed a specific second order scheme written in a conservative finite volume way. Our purpose here is to evaluate more precisely the velocities at faces. For a given face, the velocity is calculated with a finite volume mass balance over the two adjacent cells. In a 1-D formulation, this leads to (Fig.2):

$$\frac{\alpha\rho\delta U_i}{\delta t} + \frac{\langle \alpha\rho U \rangle_{j+1} \Delta U_i^+ + \langle \alpha\rho U \rangle_{j-1} \Delta U_i^-}{\Delta X_i} = 0 \text{ , with } \Delta U_i^+ = U_{i+1} - U_i \text{ , } \Delta U_i^- = U_i - U_{i-1} \qquad (5)$$

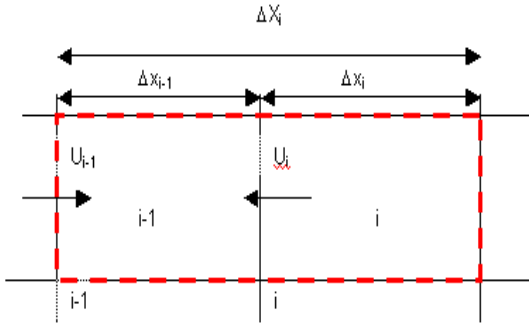

Figure 2 : 1-D representation of the grid for the second order convection scheme.

The brackets indicate flux quantities at faces. Although volume fractions and densities in the fluxes are evaluated in an upwind way, the scheme is essentially centered and it is well known that instabilities are to be expected. These ones are avoided thanks to a detection of unstable situations (analogue to the CFL condition) and smoothly switching to the standard upstream scheme when necessary. For a better result, this scheme can be coupled with a Van Leer type scheme for the evaluation of the convected volume fractions (the α's in the bracket of (5)).

2.3.3 VOF-PLIC method

One important particularity of MC3D is the possibility to represent a continuous medium with an interface tracking VOF-PLIC method. The method is currently implemented only in 2D. This is due to the fact that most of the calculations done with MC3D are made with the use of cylindrical geometry and with preferential directions (vertical – radial directions in general). To limit the dispersion in the azimuthal direction for 3D evaluations, the second order scheme must be used.

In this method, the continuous field is supposed to be bounded by a linear interface in each cell (Fig. 3). The two parameters to be determined for each cell are the normal vector $\vec{n}$, and height of the interface (B_Z). The normal vector is obtained by inspection of the surrounding cells and assuming the functional form: $\alpha_c = ax + by + c$ where α_c is the continuous fuel volume fraction. $a = \frac{\partial \alpha_c}{\partial x}$ and $b = \frac{\partial \alpha_c}{\partial y}$ are the coordinates of the normal vector, and are calculated by a least square method considering the 8 surrounding cells and the considered one. Among the different tested methods, this one gave the best representation with distorted cells (i.e. one side far larger than the other). In this model, the convection of the fluid is calculated simply according the effective common area of the fluid with the cell boundary (Fig. 4). In contrast with common VOF models found in the literature, the global 2-phase flow (e.g. a jet in gas) is modeled with two different fields. This yields some additional difficulties that need some particular numerical adjustments and high precision for various couplings (frictions) between fluids.

With increasing CPU capabilities and solver improvements, it becomes easier to make 3D calculations and thus a 3D extension of the model is foreseen in near future. The difficulty is for the cylindrical geometry as the interface cannot be plane anymore.

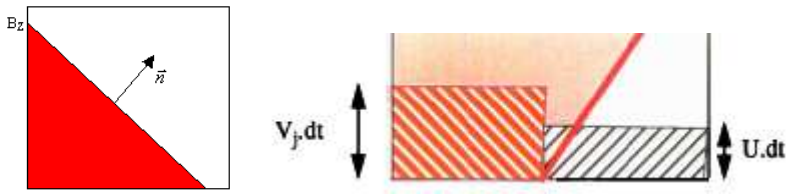

Figure 3: VOF-PLIC principals: left geometric representation of continuous tracked field; right: convected volumes during time step *dt* (dashed). The tracked fluid is red.

3. ILLUSTRATION OF THE PREMIXING AND EXPLOSION APPLICATIONS

We are now at a point where we can illustrate the potential of the code with a short presentation of the two major applications of MC3D. The PREMIXING application was built to be able to evaluate the mixing of melt jets in a volatile coolant (water or sodium). At the moment, the application contains 2 fields to describe the melt, one for continuous melt field (called “jet”), and one for discontinuous field of drops. Drops are generated from the jet through a fragmentation model (discussed in next section). They can also re-agglomerate into the jet. The jet field makes use of the VOF method described above. The coolant is modeled with two fields, one for the liquid, and one for the vapor. As many as necessary non-condensable gases can be used.

Steam explosion is very sensible to the actual initial conditions namely the fuel characteristics (dispersion, interfacial area) and the amount of gas (void) in the (pre)mixture. A high void acts as a mitigating factor of the explosion strength and it is very important to describe it accurately. Also, of high importance in the frame of nuclear FCI is the solidification of the melt. For most of the cases, the melt is supposed to have a rather low superheat (temperature increment above liquidus state) and a quite low latent heat. Then, due to high heat transfers in film boiling, solidification occurs rapidly and has then also an important mitigating effect of steam explosion strength. Indeed, first FCI models were used with guessed conservative initial conditions. These yielded very pessimistic potential explosion strengths and it was concluded that realistic explosion strengths evaluation could be obtained only with a realistic

initial conditions computation. Fig.4 gives an example of visualization of calculation of a premixing flow consecutive to a reactor vessel failure[1]. Other examples of simulations with MC3D can be found e.g. in [4] and [6].

Due to the multiphase aspects, the computational cost is high, compared to standard CFD codes. The premixing application computes at least four mass balances, 12 momentum balances and four energy balance. However, a large part of computational time is spent in evaluating the various interactions among the materials and the vapor and water properties. Nonetheless, what most limits the computation is not the code itself but the robustness of the models. Indeed, the difficulty in the modeling of FCI lays almost in the necessity to have highly coherent models. Inadequate approximations lead inevitably to a crash of the calculation. The modeling involves high evaporation rates from the melt in the water and high condensation rate from the bubbles. Thus meshes are necessarily rather rough. A typical calculation involves about 1000 cells for some days of computation of a flow lasting physically some tens of seconds (Fig.4 gives an example of mesh). Recent improvements of numerical resolution and partial parallelization yielded an improvement in computational cost but the most that can be gained is finally from a high attention to the modeling of physical laws and particularly heat and mass transfers. A particular attention must be paid regarding the situation involving evanescent phases other way strong numerical problems can be expected.

The explosion stage of FCI is computed with a second application, called EXPLOSION. This application is quite similar to the premixing but is supposed to describe different phenomena with a far smaller time scale (some milliseconds) and conditions (often in supercritical conditions). Then the application focuses on the modeling of drop fine fragmentation, heat transfer to the coolant and phase changes of the coolant. The major challenges are, on the numerical point of view, to compute the very high detonation-like pressurization, and on the physical point of view, to compute the physical mechanisms yielding the pressurization, i.e. coolant phase changes. Some highlights are given in the next section regarding the latter challenge. A typical steam explosion involves a pressurization of some tens of MPa in a time scale of some micro-seconds. An example of computation is given in Fig. 5 with the simulation of a KROTOS experiment [3] using an alumina melt (some kg, 2600 K) dropped into cold water. In this case, the premixing is not computed but guessed due to the particular situation obtained with alumina melts. Indeed, due to low melt density (2.5 compared to about 9 for corium melts) the melt is fragmented in rather large drops (about 5 mm) which yield a low amount of void in mixture and low solidification. Thus, in such cases, we are in presence of a “perfect” premixing which allows checking roughly the code behavior. Similar experiments with corium melts cannot be computed with the explosion stage alone due to a fragmentation in smaller particles (about 1 mm) leading to an important solidification and quite high void, yielding far smaller strength s in general [3].

A complete calculation starts from the evaluation of the premixing and, at a time decided by the user (with the help of some criterion), the calculation is stopped and restarted with the explosion application. However, the jet field is no more used in the application and replaced by large drops. In contrast, a fragment field is added where fragments are supposed to be very fine particles (or the order of 100 µm) coming from the fine fragmentation of the drops.

[1] It can be recalled that, in the course of an hypothetical severe accident, the core might melt and form a liquid called corium, that can firstly relocate on the bottom of the reactor vessel. If the melt cannot be cooled, the vessel might in turn fail and the melt relocates in the reactor pit.

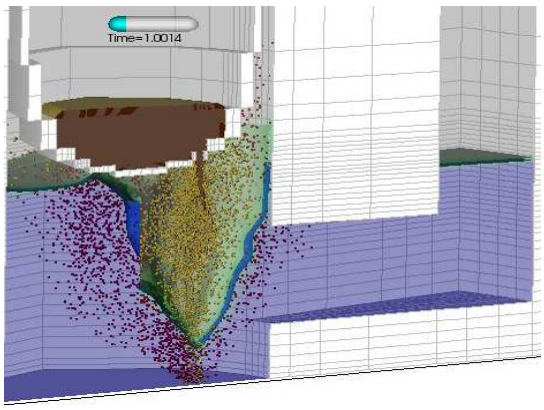

Figure 4: Example of 3D simulation of a melt stream flowing into water in the reactor pit after the failure of the vessel. The jet is visible as brown continuous field; drops are represented by orange and brown points. Background blue represents the water.

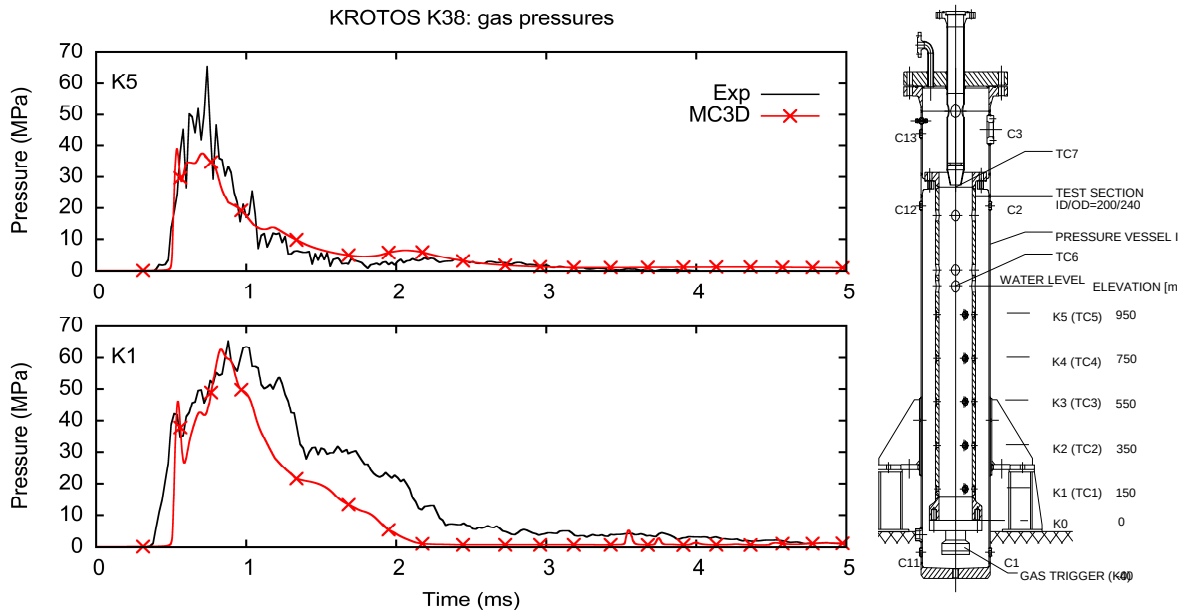

Figure 5: Example of pressure loads computed for a simulation of the KROTOS K38 experiment [3] at two levels in the water: comparison of experimental and computed loads (on the right: sketch of the KROTOS installation).

4. SOME MAJOR CHALLENGES IN MODELLING FCI

For the premixing, it is recognized that the most challenging areas of work are the melt fragmentation, its solidification and the void prediction. We will here focus on the two most specific problems which are the melt jet fragmentation and its solidification. Regarding explosion, the most important uncertainty and challenge for modeling is related to the pressurization process itself. We will now rapidly describe the essence of these models in MC3D but also look towards potential improvements to be implemented in near future.

4.1. Melt jet fragmentation

The melt fragmentation process is of utmost importance since it leads to an increase of interfacial area and then drives all the subsequent events since it drives the heat transfer to the coolant. Fragmentation controls then both the void production and the melt drop solidification

which are the two major limiting effects of the explosion strength. The fragmentation itself occurs primarily from the jet and secondarily from the drops themselves. However, drop fragmentation seems of secondary importance. As can be seen from pictures in Fig. 6, the process of the primary jet fragmentation is very complex. It involves at least three different mechanisms: one large scale instability (asymmetric or not), a stripping of the fluid at the crests of the large instabilities and a further fragmentation of the stripped mass. Describing such complexity is out of reach and simplifications are necessary for a constitutive model.

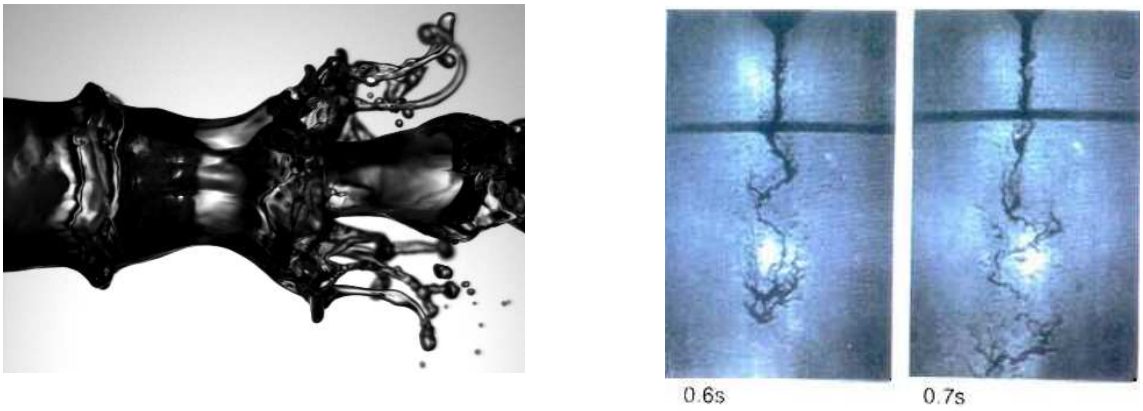

Figure 6: Example of visualisation of experiments of instability and fragmentation of water jet in air (left, [8]) and mercury jet in water (right, [9]).

On the overall, the process is due to tangential frictions and is generally referred to as the Kelvin-Helmholtz (KH) instability. Several complex models for jet instabilities have been developed but they were found of no practical use for modeling since they involve a too fine space resolution. Then the first natural idea for modeling is to use the Kelvin-Helmholtz instability model and transform it to a fragmentation model. In MC3D, this is done by considering that the fragmentation rate (i.e. velocity or erosion) is proportional to the characteristic velocity c_i of the instability defined by $\eta = F(x)e^{kc_i t}$ where η is the height of the instability, F a function describing the modulation of the amplitude, k wave number. From the KH theory, in the case where one fluid has a large density compared to the other one (e.g. $\rho_{amb} << \rho_j$, where subscript *amb* stands for the ambient fluid and *j* for the jet) c_i is given by:

$$c_i = \sqrt{(\beta \Delta V)^2 - \frac{k}{\rho_1}\sigma} \tag{6}$$

with $\beta \approx \sqrt{\frac{\rho_2}{\rho_1}}$ and σ the surface tension. It is worth to notice that the velocity can be further approximated to $c_i = \sqrt{(\beta \Delta V)^2}$ and that the surface tension acts as a low-pass cut-off regarding the wave number, i.e. $(\beta \Delta V)^2 \approx \frac{k}{\rho_1}\sigma$, i.e. $\frac{\rho_2 \Delta V^2}{k\sigma} \approx 1$. Then we see that, with $k \approx 2\pi/D$, D being the diameter of the created drops, the theory is closely linked to the Weber fragmentation criterion. Thus KH theory gives the balance between pressure destabilization forces ($\rho_2 \Delta V^2$) and stabilizing surface tension forces (σ/D). It then happens that finally, KH model is linked to the fragmentation characteristics. Going further, one can recall that dispersion in turbulent jets can be generally described by a law of the form [10]:

$$V_e = E_0 \beta \Delta V \tag{7}$$

E_0 being an entrainment coefficient. $E_0 \Delta V$ is roughly the characteristic turbulent velocity of the flow, i.e. about one tenth of the characteristic flow velocity, $E_0 \approx 0.1$. It appears then that the KH model is also coherent with the experimental observation and that the volumetric fragmentation rate (or entrainment velocity) can be written:

$$\Gamma_v = N_f c_i \tag{8}$$

where, in the MC3D jargon, N_f is called the fragmentation parameter and should be of the order the parameter E_0, i.e. 0.1. Now, the KH model is found to be quite representative of the overall process of instability and fragmentation. A second fitting parameter is needed to obtain the size of the created drops. As we have seen that KH model is closely linked to a Weber criterion, we pose that the diameter is obtained with:

$$D_d = N_d \frac{2\pi}{k} \tag{9}$$

where N_d should be of the order of unity.

However, implementing such model into a CFD premixing code is not so simple and there are several difficulties among which the most important is the account of the multiphase aspects i.e. the fact that several fluids can be close to the interface. This is done in MC3D by considering that we must describe the actual forces acting on the interface. Thus, the mixture flowing along the jet must be defined such that the global pressure forces are conserved i.e. we evaluate a $\left(\rho V^2\right)$ mean ambient quantity, i.e. considering only gas (subscript *g*) and liquid coolant (subscript *l*):

$$V_{amb} = \sqrt{\frac{\overline{\alpha_g \rho_g \left(\Delta \overline{V_g}\right)^2} + \overline{\alpha_l \rho_l \left(\Delta \overline{V_l}\right)^2}}{\overline{\alpha_g}\,\overline{\rho_g} + \overline{\alpha_l}\,\overline{\rho_l}}} + \overline{V_j}, \qquad \rho_{amb} = \frac{\overline{\alpha_g \rho_g} + \overline{\alpha_l \rho_l}}{\overline{\alpha_g} + \overline{\alpha_l}} \tag{10}$$

where $\Delta \overline{V_g} = \overline{V_g} - \overline{V_j}$ and $\Delta \overline{V_l} = \overline{V_l} - \overline{V_j}$ and the overbar denotes an averaging process regarding the mesh (e.g. the gas velocity is a function of the velocities at different faces surrounding the considered mesh). Application of the model on experiments at our disposal leads to fix the parameters N_f at about 0.25 and N_d at about 1. However, several difficulties exist among which we can notice a strong sensitivity to local variations of conditions that might also be largely of numerical nature. Several filtering processes have been envisaged and tested to smooth the solution but none of them was, at the moment, found fully adequate.

4.2 Melt drops solidification

It can be easily understood that, since the explosion is due to a fine fragmentation of the melt drops, solidification of the melt is important for the mitigation of the explosion strength. However, the evaluation of solidification is confronted to various severe difficulties. First of all, the heat transfers must be adequately undertaken, meaning that the melt area must be well captured. In the current version of MC3D, the melt drops are represented by only one numerical field, i.e. with one characteristic diameter (per mesh). It was found that the heat transfers themselves could be quite well represented if the drop diameter is slightly higher than the mean Sauter diameter, i.e. the mean diameter regarding surface area: D_s=6 *V/S* where

V is the total volume and *S* the total surface. The difficulty is then to compute the solidification itself.

The default model in MC3D is simply to use the average drop temperature (or enthalpy) as a criterion for solidification. Recently, a more complex model was introduced [6]: it considers a crust formation and a criterion for fragmentation based on crust thickness. However, this improvement is not sufficient since the solidification is still a binary phenomenon where all drops in a cell are either solid either liquid. To overcome this problem, it is necessary to take into account the fact that the drop size is in reality described by a rather large distribution of diameters, ranging from some tenth of microns to about 1 centimeter. If we consider that the heat transfer coefficient is weakly dependent on the drop size, then the time scale for cooling is proportional to the size of the drop. Thus, considering several size groups for the drops would yield a more efficient modeling of solidification than an improvement of the solidification model itself. Several ways can be envisaged to treat this problem among which the most straightforward is a multiple size groups method (MUSIG). This is currently under way. It is expected that a small number of drop fields will be sufficient so that the CPU cost is not too important.

4.3. Pressurization process during explosion

There are currently two kinds of models in the FCI codes to describe the pressurization. The first models made the hypothesis that the fragment heat was given to a part of the water (micro-interaction model, [11]) which is then heated. The pressurization is due to the expansion of the water. The second series of codes, among which is MC3D, make the hypothesis that the pressurization is due to the direct vaporization at the interface between the fragments and the coolant (non-equilibrium model). It could be stated that both types of model would lead to different behaviors and that experiments should discriminate the most realistic one. However, the experimental support is scarce and, due to the high number of potential differences in modeling, it happens that a fitting process is always possible. However, the implications in real reactor cases are not known and it is clear that additional work is needed to clarify the nature of pressurization. One criticism of the non-equilibrium model used in MC3D is that vaporization processes at large supercritical pressures are far from being clear. This choice was however recently consolidated by the results of the TREPAM experiments [12] that showed that the fragment heat transfer occurs as film boiling even at pressure slightly beyond the critical pressure. Nonetheless, further progresses are needed in order to describe more accurately the different involved processes.

5. CONCLUSIONS - FORESEEN IMPROVEMENTS IN NEAR FUTURE.

We have rapidly presented the architecture of the MC3D software and highlighted the flexibility of the structure which allows fast developments of new applications. We have also discussed some of the major challenges for the modeling of Fuel-Coolant-Interaction. The multiphase multi-scale aspects of FCI problem render the modeling very complex. Indeed, despite the flexibility of the architecture, it is found and an improvement is still necessary in the structure for building applications. We have then recently engaged a task of using a new architecture based on an object oriented approach for building applications. The idea is to build the application one over the other. Each sub-application can always be used and improved in an autonomous way and all upper-applications benefit from the improvements of sub-applications. The first step was to build a single-phase pure gas application. The second step, for the problem of FCI, is to build a 2-phase flow application on top it. The final goal is

to build a general FCI application which will group premixing and explosion physics and high flexibility regarding the number of fields.

Regarding the physics of FCI, further efforts are to be done regarding jet fragmentation, melt solidification and the pressurization process in order to have a more precise modeling. For these all these topics, the code can in fact be helpful to supplement the lack of data since we can use it to make zooms on particular physical processes to model them in a quasi-direct way (e.g. single drop fragmentation and void production under a strong shock wave). Using the code at smaller scale can help building models and constitutive laws at larger scale.

REFERENCES

1. Magallon, D., Huhtiniemi, I. , Hohmann, H., (1999). Lessons learnt from FARO/TERMOS corium melt quenching experiments, *Nuclear Engineering and Design*, **Vol. 189, 1-3**, 223-23.

2. Magallon, D., Huhtiniemi, I. (2001). Corium melt quenching tests at low pressure and subcooled water in FARO, *Nuclear Engineering and Desi*gn, **Vol. 204, 1-3**, 369-376.

3. Huhtiniemi, I. ,Magallon, D., Hohmann, H., (1999). Results of recent KROTOS FCI tests: alumina versus corium melts, *Nuclear Engineering and Design*, **Vol. 189**, **1-3**, 379-389.

4. Ishii, M., Hibili, T. (2006). Thermo-fluid Dynamics of Two-phase Flow. Springer.

5. Leskovar M., Uršič, M., (2009). Estimation of ex-vessel steam explosion pressure loads, *Nuclear Engineering and Design*, **Vol. 239**, **11**, 2444-2458.

6. Uršič, M., Leskovar, M., Mavko B., (2011). Improved solidification influence modelling for Eulerian fuel–coolant interaction codes, *Nuclear Engineering and Design*, in press.

7. Villermaux, E, Fragmentation, (2007). Annual Rev. Fluid Mech.. **39**, 419–46.

8. Marmottant, P., Villermaux, E., (2004). On spray formation, *J. Fluid Mech*, **498**, 73–111.

9. Hall, R.W., Fletcher, D.F, (1995). Validation of CHYMES : simulant studies, *Nuclear Engineering and Design*, **155**, **1-2**, 97-114.

10. Ricou, F. B and Spalding, D. B., (1961). Measurements of entrainment of axisymmetrical turbulent jets, *J. Fluid. Mechanics*, **11**, 21-32.

11. Chen, X., Yuen, W. W., Theofanous T. G. (1997) On the constitutive description of the microinteractions concept in steam explosions *Nuclear Engineering and Design*, **177**, **1-3**, 303-319

12. Berthoud, G., Gros D'Aillon, L. (2009) Film boiling heat transfer around a very high temperature thin wire immersed into water at pressure from 1 to 210 bar: Experimental results and analysis. *International Journal of Thermal Sciences*, **48**, **9**, 1728-1740