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Comparative Review of FCI Computer Models Used in the OECD-SERENA Program

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Abstract – In the frame of the OECD international program SERENA, a comparative review of the main computer models and numerics for both the pre-mixing and the explosion phases has been performed. The present paper is a summary of this review and presents the most important models and differences between the FCI codes. These differences concern: the fuel numerical description; the fuel fragmentation; the flow map for multiphase, multi-component fluid systems; the heat and mass transfers between fuel and coolant. These differences enlighten different opinions and partner's views both on physical and numerical aspects.

I. INTRODUCTION

SERENA is an OECD coordinated program involving 13 organisations whose ambition is to seek for convergence towards a common understanding of FCI for reactor situations (Magallon, 2003). In a first phase, dedicated to establish a state of the art, the program is divided in several tasks, the second of which is dedicated to a comparison of the various approaches for calculating jet break-up and premixing, whereas in third one the explosion phase is studied. In order to reach this objective, comparative calculations of the FARO experiments L-28, L-31, L-33 (Magallon, 2001), KROTOS K-44 (Huhtiniemi, 2001) and TROI-13 (Song, 2003) have been performed. In Task 4, extrapolation calculations for two prototypical reactor situations have been performed (Magallon, 2005).

For the sake of the analysis of the results, we have performed an in-depth comparison of the models and numerics for the codes used in SERENA. Although there are other codes devoted to FCI, the resulting report gives a rather complete state-of-the-art in FCI modelling. It concentrates on the major physical and numerical aspects, i.e. those that are supposed to be the most crucial, and intends to address the three following questions:

- What are the main differences of the codes, relatively to key points of premixing and explosion phenomena?
- How can these differences be understood?
- What should be the consequences of the different choices on the results?

This paper gives an extended summary of this report.

While elaborating the program, some emphasis was put on the fragmentation processes and particularly the jet fragmentation. Therefore, we particularly go into details for the related models. However, from the discussions held all along the SERENA meetings, it appeared that an important and actually more basic emphasis was to be put on the generation of void. Thus, we will also enter in some

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details into the basic phenomena related to the void: flow patterns and heat and mass transfers from fuel to coolant.

Table 1 provides the list of participating organisations and codes used for phase 1. Most of the parties are dealing with premixing and explosion with basically the same code. Nonetheless, for UCSB, premixing is calculated with the 3-D, partly lagrangian code PM-ALPHA-L-3D (hereafter referred to as PM-ALPHA), and explosion with the 2-D Eulerian code ESPROSE-m (simply ESPROSE hereafter). For IKE, premixing is calculated with IKEMIX and explosion with IDEMO[2]. The case of MC3D is in between since both phases are calculated in the same code structure but with two different "applications": MC3D-PREMIX, and MC3D-EXPLO. These two applications have in common the resolution core and lots of constitutive laws. JASMINE was also previously divided into two codes: JASMINE-PRE for premixing and JASMINE-PRO. Since Task 3, it has been decided to maintain only one tool (based on JASMINE-PRE, simply called JASMINE) for the calculation of both premixing and explosion[3]. Finally, it is important to notice that MATTINA does not have any explosion specific model.

Organisation	Code
FZK	MATTINA
IKE	IKEMIX (premix) MC3D 3.2 (task 2 only) IDEMO (explo)
IRSN-CEA	MC3D 3.3.06 (task 2 and 4) MC3D 3.4.02 (task 3)
JAERI	JASMINE-PRE 2.1 (task 2) JASMINE 3.x (task 3 & 4)
KAERI	TEXAS-V
KMU	TRACER-II
NUPEC	VESUVIUS
KINS	IFCI 6.0
UCSB	PM-ALPHA.L.3D (premix) ESPROSE (explo)
UW	TEXAS-V

Table 1: Organisations and codes used for phase 1

EREC also provided the models of the VAPEX code and calculations of FARO L-33, but did not participate directly in the discussions.

Most of the calculations were performed in 2-D, although some codes have 3-D capabilities. However, calculations with PM-ALPHA where made in 3-D (premixing), whereas TEXAS is a 1-D tool.

II. MODELS FOR THE PREMIXING PHASE

II.A. Fuel flow description

There are many flow configurations of concern in the premixing stage. Conceptually:

- the fuel can be in continuous or discrete state;
- the discrete state can have one or two orders of magnitude in characteristic size;
- the fuel can be molten or frozen or in an intermediate state;
- the discrete state can be dilute (during flying) or compact (debris bed);
- The fuel composition is not necessarily homogenous.

Describing all possible configurations and interactions is a challenge that seems a bit unreachable. By the way, extending the number of numerical fields might not be the best choice, due to the resulting complexity in coherence and code maintenance. The major ways explored to capture complexity are:

- Lagrangian description of large particles: PM-ALPHA, TEXAS, VAPEX, JASMINE, IKEMIX;
- Separate continuous field for the jet and partially for the molten debris bed: MC3D (2-D), VESUVIUS (1-D), JASMINE (1-D), IFCI (partially), IKEMIX (1-D);
- Additional small-scale fuel field, fragments or debris (PM-ALPHA, optional in MC3D).

Only the first two points will be discussed here.

Table 2 gives a summary of the fuel descriptions with illustrations.

On the numerical point of view, there is obviously a tendency towards the use of a lagrangian description for the fuel drops. Basically, the drops are grouped according to the desired resolution and each lagrangian particle represents in fact a cluster of identical particles. The major advantages are:

- Improved numerical resolution: convection, length scales;
- Enhanced possibilities for the physical treatment of the drop behaviour (cooling, solidification).

However, the second advantage is challenged by the physical complexity of the various phenomena that it might help to evaluate, such as surface temperature or drop solidification. The later problem will be addressed further.

[2] IKE also provided calculations with MC3D V3.2 for Task-2.

[3] Some important modifications have been made from Task 2 (JASMINE-PRE) to Task 4 (use of a version called JASMINE 3.2). We will describe both codes when necessary.

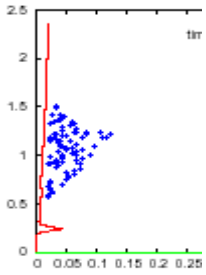
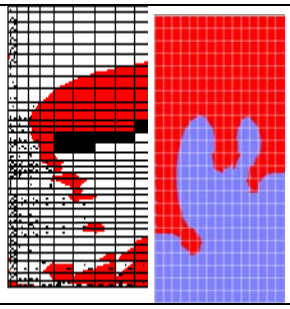
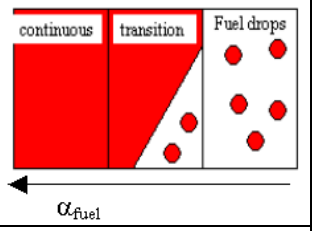
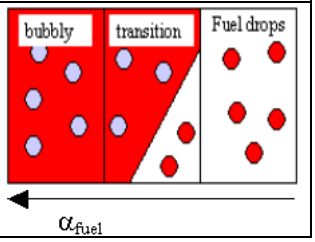
PM-ALPHA TEXAS VAPEX	1 main discrete lagrangian fuel field *ex* : particle flow in PM-ALPHA	
IKEMIX JASMINE	1-D jet + 1 lagrangian drop field *ex* : JASMINE	
VESUVIUS	1-D jet + 1 Eulerian drop field	See JASMINE illustration
MC3D	1 continuous fuel field (VOF) + 1 eulerian drop field *ex* : 2 illustrations of VOF method	
IFCI	1 single eulerian fuel field with interface tracking method	
MATTINA TRACER	1 single eulerian fuel field	

Table 2: Summary and illustration of the fuel fields in the codes used in SERENA

On the physical modelling point of view, the major difference concerns the modelling of large-scale fuel volumes. Of particular interest is the description of jets. A short majority of codes use a special description for this pattern. For most of them, the jet is managed with a special 1-D field, either in lagrangian, either in eulerian way. This concerns VESUVIUS, IKEMIX and JASMINE. In MC3D, there is a special field modelled with a volume tracking method (VOF-SLIC). It is thus not restricted to a special geometry. It is then more generally a continuous fuel field. The case of IFCI is a little special since a jet treatment is included but with no special field. The jet modelling is done through a flow pattern tracking (VOF-SLIC also). The same numerical field describes then alternatively both the drops and the jet. The opposite description concerns PM-ALPHA, VAPEX, and TEXAS. In these codes, the fuel is always in a discrete pattern, i.e. with constitutive laws related to drops. In between are the descriptions of MATTINA and TRACER where the fuel is modelled with one single eulerian field, continuous or dispersed, according to the melt volume fraction.

We could think that these differences are simply different numerical treatments. This is not true: they lead to real fundamental differences in behaviours. As this phase is the beginning of the FCI, theses discrepancies control the rest of the calculation. Taking into account the actual mechanisms of fragmentation[4] and dispersion introduced in codes, the two different options are schematically pictured in Figure 1. Promoters of the purely drop flow (TEXAS, PM-ALPHA) argue that the jet break-up is mainly due to fragmentation at the leading-edge through Rayleigh-Taylor mechanisms (Figure 1, A). With this hypothesis, the use of drops is legitimate and leads effectively to a leading-edge fragmentation. The opposite point of view makes the hypothesis of a small-scale fragmentation all along the jet column, through Kelvin-Helmholtz mechanisms (Figure 1, B, MC3D, IKEMIX, VESUVIUS, JASMINE, IFCI). In that case, with the drop break-up process, two different fragmentation mechanisms are considered.

Mechanisms A and B lead of course to radically different patterns of fragmentation, i.e., in drop size distribution and fuel dispersion. With jet fragmentation, a radial dispersion is naturally included. This is not the case for drop break-up, although explicit mechanisms of dispersion could be included[5].

[4] It might be important to clarify the sense of the expressions "break-up" and "fragmentation". The fragmentation involves a small-scale disintegration. The term break-up is more general and expresses the idea of a complete splitting of the considered object. The fragmentation generally leads to a break-up but not necessarily. When specifying large-scale disintegration, we will also use the term break-up. Following this idea, for most of the jet models, as only a small-scale disintegration is considered, it is better to refer to jet fragmentation. Fragmentation can also be understood as atomization (although atomization might express the idea of a very fine fragmentation).

[5] An implicit dispersion is ensured by friction with the ambient fluid as well as possibly turbulence and numerical diffusion.

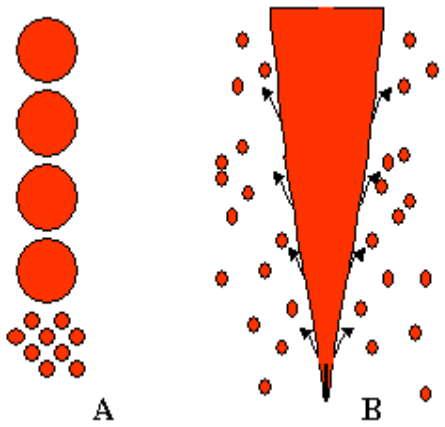


Figure 1: Conceptual picture depicting the two different jet break-up mechanisms: A : leading-edge break-up, B: continuous jet column fragmentation

The cases of MATTINA and TRACER are not so explicit. However, fragmentation can occur only in a discrete state, i.e., only in meshes with small or moderate melt volume fraction. Fragmentation mechanisms are then very near to the case A.

It is thus obvious that very different ways are used to model the fuel and, although it exists a consensus on the importance of a precise description of the fuel area, this dispersion of the descriptions gives the flavour of the discussions that exist in the FCI community.

Considering the reactor situations, the existence of a real large jet (stream, not necessarily on the axis) seems likely for the ex-vessel situation. On the contrary, in the in-vessel situation the occurrence of real 1-D continuous jets is more questionable due to a probable multi-jet situation: this may add supplementary mechanism(s) for break-up. The question is now obviously whether the differences in modelling contribute significantly to energetics of FCI in reactor situations.

II.B. Flow map

We will now consider the description of the coolant flow and its interaction with the discrete fuel particles. We will only describe the case where the fuel fraction is low enough so that it cannot be considered as packed or dense. Generally, this is the case for fuel volume fractions lower than 0.3. The eventual presence of a continuous jet does not modify the flow map as it is based on relative volume fractions. We firstly have to note that all codes have in common the fact that the description is characterized in a geometrical way, considering only the local volume fractions of the gas and of the water. This means that:

- there is no transportation of configurations
- there is no consideration of the neighbouring cells in the flow characterization.

Note also that only MATTINA uses a transport equation for the coolant areas, i.e. for liquid drops and gas bubbles.

There are two main types of configuration for the coolant flow, with differences laying mainly in the treatment of the transitional configuration. For all codes but MATTINA, with α being the relative void fraction (i.e. without considering the fuel), and α_B , α_D some limiting values explained hereafter:

- if $\alpha < \alpha_B$: bubbly flow, liquid coolant is continuous and all fuel drops are in contact with water (typically in film boiling)
- if $\alpha > \alpha_D$: droplet flow, gas is continuous with liquid droplets. Fuel drops are in general considered in contact with the gas (although heat transfer by direct contact with impinging water drops is possible and treated in various ways).

In-between is the transitional flow and there are the main differences. The most usual values for the transition bounds are $\alpha_B = 0.3$, $\alpha_D = 0.7$. For MATTINA there is a sharp transition : $\alpha_B = \alpha_D = 0.52$.

Now, a first group of codes considers, in one way or another, that the transitional flow is a composition of a bubbly part and a droplet one: MC3D, JASMINE, VESUVIUS and IKEMIX (Figure 2, top). The fuel drops are distributed, at first order, proportionally into water and gas. There is either a real description of a bubbly and a droplet part, as in MC3D, or simply modifications of the constitutive laws by essentially linear interpolations, to account for the transition (MATTINA, JASMINE, VESUVIUS, IKEMIX).

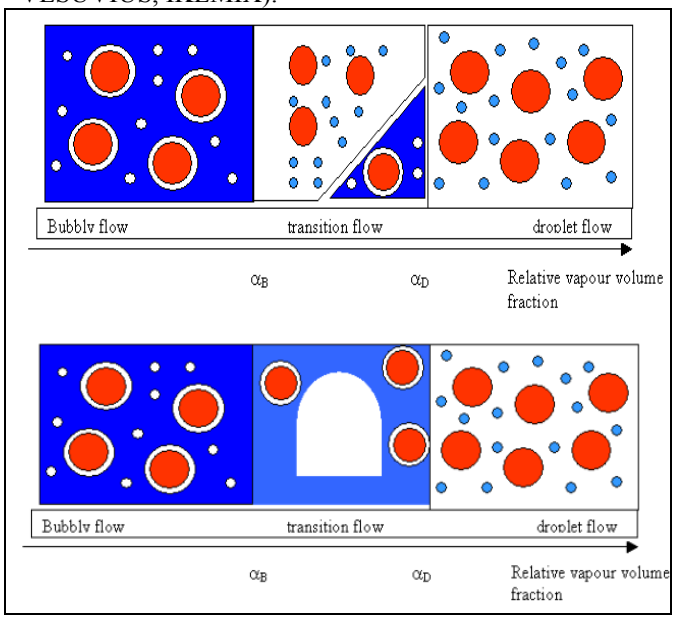


Figure 2: Comparison of the flow maps. Top: composition of bubbly and droplet flow. Bottom: gas slug flow

In the second approach (Figure 2, bottom), the transition part is considered as a specific configuration: the churn flow. It is supposed that the flow is made of gas slugs, with adapted friction laws (churn regime for the Ishii's law), and a prescribed length scale for the slugs (i.e. the Taylor diameter). The codes using this description are: PM-ALPHA, TRACER, VAPEX and IFCI. In this regime, all fuel droplets are in contact with water (in film boiling state).

Both approaches have their drawbacks and make assumptions that need experimental confirmations. The churn description is based on stationary 1-D, 2-phase flow observations. The 3-D extension in transient situations is far from being obvious, particularly if we consider the presence of fuel drops. The interpolation option of the first approach is more satisfactory from the point of view of continuity between flows. However, some additional physics is needed because of the mechanical coupling between phases, which is complicated by the presence of four effective different physical fields described with only two numerical fields.

In view of the high importance of void generation, the most important aspect is the effective partition of the fuel in the coolant, i.e. relative amount of fuel supposed to be in interaction with either the liquid or the gas. Figure 3 gives a picture of the disparity in the way this is done. It gives, approximately, the fraction of the fuel that is supposed to be in contact with water. This partition can also be given by weight factors applied to individual interactions. This picture is somewhat simplifying as:

- additional heat transfer from fuel to water might modify the picture (for example drop-drop impact heat transfer);
- the transition might not be linear (for example it is a law in the form of $(1-\alpha)^{1/4}$ for PM-ALPHA).

It is firstly to be remarked that the drop to water heat transfer is not necessarily in line with the flow maps. As an example, for PM-ALPHA, for the friction, drops are supposed to be in water even in the transition flow, whereas for the heat transfer the void effect begins with the transition region. Also, in IFCI, film boiling (heat transfer?) is reduced from $\alpha_g = 0.75$, i.e., inside the droplet flow pattern. MATTINA shows similar trends.

Figure 3 emphasizes very important differences between the codes. Heat transfer to coolant and vaporization should be very different between, for example, IKEMIX and IFCI. It is suspected that, for similar conditions, IFCI leads to far more important vaporization than IKEMIX.

The reason for this discrepancy is probably the lack of experimental data for these kinds of flow. The global experiments like FARO or QUEOS (Meyer, 1999) are not sufficient in the complete resolution of the problem. Now, it is clear that an important effort is to be done in this area. This need is emphasised by the conclusions presently done from SERENA calculations (all tasks) on the importance of reducing uncertainties on void predictions (Magallon et al., 2005).

The flow map has also an important influence on dynamical aspects, thus influencing fragmentation and then heat transfers. This specific effect is however more difficult to analyse as it occurs through indirect mechanisms.

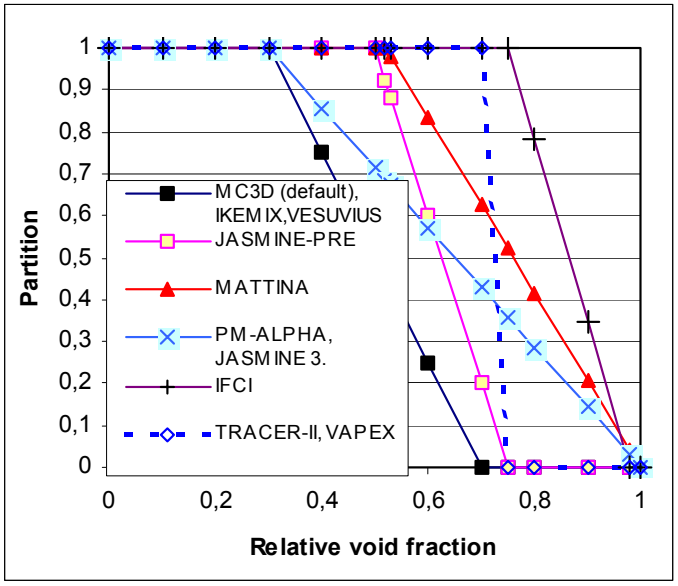


Figure 3: Simplified representation of the fraction of fuel in direct contact with the water relatively to heat transfer, as a function of the void fraction. The transitions are not necessarily linear.

II.C. Melt fragmentation

The crucial role of melt fragmentation is recognized by most of the participants. However, large discrepancies exist on primary fragmentation, i.e. fragmentation from large-scale (~ continuous) melt stream to discrete particles in stable state (some millimetres). Codes with a specific continuous field (or simply jet) use specific fragmentation laws or models, whereas the others use drop fragmentation models whatever the conditions (see description of these models in Section II.C.2). As already pointed out (Figure 1) this makes an important difference for the dispersion of the melt as only the jet models include a specific radial dispersion.

II.C.1 Jet fragmentation models

For the jet fragmentation physics, there has been a consensus towards a simplified approach.

JASMINE and VAPEX use the global Saïto (1988) correlation, giving the break-up length of a boiling jet as:

(1) $$\frac{L}{D} = 2.1\left(\frac{\rho_j}{\rho_l}\right)^{0.5} Fr^{0.5} \qquad Fr = \frac{V_j^2}{gD}$$

For corium jets in water, the correlation leads to

(2) $$\frac{L}{D} \approx \frac{6V_j}{\sqrt{gD}}$$

For FARO L-28 and L-31, with diameters at impact of the order of 4 cm, we have $\frac{L}{D} \approx 10.V_j$. The Saïto correlation should overestimate the experimental results by a factor of 2.

The Saïto correlation does not provide any information about the fragmentation process, i.e. the particle diameter and the ejection velocity. Constant parametrical values are used.

MC3D also uses a global correlation as the default model, but a different one, deduced from a theoretical work (Meignen, 1997). It is based on an Orr-Sommerfeld type formulation, taking into account the velocity profiles and the viscosity. The conclusions of the model are:

- The fragmentation is driven by the pressure head in the vapour film around the jet; the ambient pressure and the jet velocity are of very low influence;
- The fragmentation rate can be deduced from comparison to a standard case, denoted with a subscript 0:

(3) $$\Gamma = \Gamma_0 \left(\frac{T_0}{T_j}\right)^{0.75} \sqrt{\frac{\mu_g}{\mu_{g,0}}\bigg|_{p=1bar} \frac{\sigma_0}{\sigma_j}\left(\frac{\rho_0}{\rho_j}\right)^{0.5}}$$

where the standard case is chosen as the FARO corium approximate properties, at 3000 K:

(4) $T_0 = 3000$ K, $\mu_{g,0} \sim 10^{-3}$ kg/m/s, $\rho_0 = 8000$ kg/m^3, $\sigma_0 = 0.5$ N.m.

For the standard corium case, the reference fragmentation leads to a break-up length approximately given by

(5) $$\frac{L}{D} \approx C_s\, V_{jet} \qquad C_s = 5.5\ m^{-1}\ s.$$

In comparison with (2), the break-up length does not depend on the jet diameter. For the diameter of the resulting drops, the model did not provide a correlation easy to compute. So this one is an input parameter (4 mm is the default value)

A second optional model was also used in addition in Task-4. It calculates a fragmentation rate according to local conditions. Theoretically, there is then no special limit in the use of this second model. It is based on the Kelvin-Helmholtz theory for the tangential instability. In this model, we write that the volumetric rate of fragmentation is given by:

(6) $$\Gamma_f = N_f c_i$$

where

- $$c_i = \frac{1}{\rho_1+\rho_2}\sqrt{\rho_1\rho_2\left(V_1-V_2\right)^2 - \sigma k\left(\rho_1+\rho_2\right)}\bigg|_{k=k\max}$$ is the characteristic velocity of the instability.
- N_f is a fragmentation parameter with expected value around 6. In the calculations, $N_f = 2$ was used
- $$k_{\max} = \frac{2}{3}\frac{\left(V_1-V_2\right)^2}{T}\frac{\rho_1\rho_2}{\rho_1+\rho_2}$$

In this model, the diameter of the created drops is related to the wavelength λ of the instability so that:

(7) $$d_d = N_d \lambda$$

N_d is a parameter with expected value between 0.1 and 0.5. In calculations, $N_d = 0.2$ was used.

IKEMIX uses a correlation deduced from a separate model also using Kelvin-Helmholtz theory. Local fragmentation rates and fragment sizes are determined from stripping of waves on a 1-d cylindrical jet driven by steam relative velocities. These are determined from local axial pressure gradients. Under the approximation of a constant relative velocity driven by hydrostatic head, a correlation for the global break-up length can be derived giving:

(8) $$\frac{L}{D} = 2.38\left(\left(\frac{\rho_j}{\rho_l}\right)^{0.5} Fr^{0.5}\right)^{2/3}$$

Then, compared to (2) and (5), we obtain again a slightly different formulation with different dependencies on velocities and jet diameter. The diameter of the created drops is a prescribed constant value. Note however that for Task-2, a constant fragmentation rate was used, based on an analysis of the experiment L-28.

Finally, VESUVIUS uses a separate model based on calculations of a separate film model with the Epstein-Fauske (1985) instability model. This model is an extension of Kelvin-Helmholtz theory to stratified 3-phase flows. The correlation proposed by Epstein-Fauske is in fact a fitting between two opposite situations of thick and thin film. Due to the included film model, it is not possible to compare directly the results with other models. Here also, the size of the resulting drops is specified as a parameter.

It is obvious that the jet fragmentation is a task that is not resolved. Although the models are fitted on experiments like FARO, the different dependencies show that extrapolations to reactor conditions will necessarily lead to different results. Also, only the KH model in MC3D uses a non-constant prescribed drop diameter. The results obtained for Task-4 with this model cannot then be compared to others.

II.C.2 Drop fragmentation.

For codes not using jet fragmentation (PM-ALPHA, MATTINA, TRACER and TEXAS), the drop fragmentation (or break-up) is then also the primary fragmentation mechanism. For the others, the drop fragmentation is only used as the secondary mechanism. This feature is then less critical. However, it is important to notice, that in Task-4 in-vessel calculations, the jet models could not be used as in Task-2 for different reasons. Then, even for MC3D and JASMINE, drop fragmentation mechanisms are important in some situations inadequate for the jet models. Even where jet model could be used (IKEMIX, VESIVIUS) the occurrence of several jets unperturbed each other, i.e., keeping a 1-D configuration, is questionable. If this is not the case, the jets might break by large-scale mechanisms, thus giving more importance to the drop fragmentation.

Five of the SERENA codes use a local correlation formulated by Pilch (1986) (TRACER, VESUVIUS, IFCI, MC3D, IKEMIX). This correlation is a linearization of a model describing the coarse fragmentation by Rayleigh Taylor instabilities (acceleration induced). Strictly speaking, this model should hold only for Weber numbers larger than 350. Except for MC3D, the correlation is however extended to smaller Weber numbers. This is due to the fact that the dimensionless break-up time

$$\tau = t_b \frac{\Delta v}{D}\sqrt{\frac{\rho_c}{\rho_f}} \quad (9)$$

is always of the same order of magnitude whatever the break-up process. However, the diameter of the resulting fragments or drops is sensitive to the process and this should lead to a modification of the global correlation. Expressed in area variation, we have :

$$dA/dt = C_0 \frac{A}{D}\sqrt{\frac{\rho_c}{\rho_f}}\Delta v. \quad C0 = 0.245 \text{ to } 0.29 \quad (10)$$

JASMINE and MATTINA use of the Pilch & Erdman correlation (Pilch and Erdman, 1987). This correlation is supposed to take into account the different mechanisms occurring at different Weber numbers. So there is no restriction regarding the Weber number. However, the use of this correlation in codes is questionable as the correlation contains quantities prior to the fragmentation process:

$$\frac{dD}{dt} = \frac{d_{s,\max} - D}{t_b}, \text{ with} \quad (11)$$

$$d_{s,\max} = \frac{We_c \sigma}{\rho_c v_0^2}\left(1 - \frac{v^*}{v_0}\right) \quad (12)$$

v^* is an estimate of the velocity at the break-up time, and v_0 the initial velocity. The dimensionless break-up time is:

$$\tau = \begin{cases} 6(We-12)^{-0.25} & 12 \le We \le 18 \\ 2.45(We-12)^{0.25} & 18 \le We \le 45 \\ 14.1(We-12)^{-0.25} & 45 \le We \le 350 \\ 0.766(We-12)^{0.25} & 350 \le We \le 2670 \\ 5.5 & 2670 \le We \end{cases}$$

So, this correlation does not use local and temporal variables but the initial conditions prior to the fragmentation. Indeed, the introduction of parameters as v^* in (12) is due to this restriction, in order to take into account the variation of the flow conditions during the process. The use of this kind of correlation, with local conditions, might not be appropriate in global codes.

TEXAS[6] (Tang, 1993) uses an original correlation, developed by Chu and Corradini, still assuming that the fragmentation is due to Rayleigh-Taylor phenomena. This leads to a formulation similar to the Pilch one:

$$dD/dt = -f_0\sqrt{\frac{\rho_c}{\rho_f}}\Delta v \quad (13)$$

$$f_0 = \left(0.1093 - 0.078\sqrt{\frac{\rho_c}{\rho_f}}\right) We^{0.246}$$

The factor f_0 varies from 0.16 at We = 12 to 0.4 at We ~ 1000, so it compares rather well with the Pilch formulae for the Weber numbers involved in premixing. Note also that TEXAS has another fragmentation model, based on the stripping model of Epstein-Fauske. This model is however not recommended by Corradini (although used with equal importance by KAERI).

Finally, only PM-ALPHA does not use a correlation but a parametrical model. The user input parameter β_b is the dimensionless break-up length L/D. However, it is important to notice that for Task 4, no break-up was used. The particles were injected with a bimodal spectrum (20% at 3 mm and 80% at 10 mm) for both cases and the diameters were kept unchanged during pre-mixing

The stable size of the drop is supposed to be obtained for Weber = 12 (gravitational Bond = 1 for PM-ALPHA). Looking at the experimental data, this critical Weber number, in conjunction with the models used is in fact questionable. If We = 12 is effectively a local limit for fragmentation, this does not mean that the final average diameter is given by this criterion. This is clear from Pilch & Erdman data. This is why JASMINE has been recently modified so that the critical Weber number is 6.

[6] And optionally IKEMIX

II.D. Heat and mass transfer

Heat transfers from the fuel to the coolant and the subsequent coolant mass transfers are obviously very important features. The two major mechanisms are film boiling and radiation.

Concerning the film boiling, there is a relative agreement and all codes use correlations derived from the Epstein-Hauser correlation (1980). Only MATTINA uses a different correlation, i.e. Dhir & Purohit (1978). However, the correlations only give the heat removed from the drop. Important discrepancies exist regarding to the part of the flux used directly for vapour production. For PM-ALPHA, all film boiling energy is deposited at the liquid/vapour interface and used for vapour production. The vapour produced is supposed (eventually) to condense further while in the state of bubbles. On the contrary, for JASMINE and VESUVIUS, only a small fraction (2 to 3 %) is used for vaporization. The others are using various methods for correlating the vaporization to the subcooling. As this is one of the key points in FCI, it appears that there is an important lack of understanding.

Concerning radiation, only PM-ALPHA uses a complete model (zonal method). All other codes calculate a local radiation heat transfer only (inner-cell radiation). Note that MC3D has developed an inter-cell radiation model (however less elaborate than the PM-ALPHA model), but this model is still under qualification. As quite little effort (except for these two codes) has been put on the subject, it is not currently clear whether or not such a complicate modelling is needed. At least, some clarifications are needed to evaluate such a necessity.

III. MODELS FOR THE EXPLOSION PHASE

All the codes, except MATTINA, use special physics and numerics for the description of the explosion phase. It is however recognized by Jacobs, in charge of MATTINA, that this is not a real choice. For the other codes, the basic aspects of the flow patterns established for premixing are conserved for the explosion phase with however the important following differences:

- Addition of a fragment (debris) field for most codes (some codes are dealing with debris during premixing but in a different way);
- No continuous fuel field (~jet). For codes using a jet field in premixing this one is transferred in fuel drops in various ways;
- Use of simplifying assumptions of homogeneity for the calculation of the interaction for ESPROSE, IDEMO and VAPEX (the micro-interaction concept);
- The lagrangian description of the fuel is sometimes abandoned for a more classical eulerian description (ESPROSE, IDEMO).

III.A. Micro-Interaction versus non-equilibrium

There are currently two important concepts for the modelling of the explosion. We will refer to them as the micro-interaction and the disequibrium concept.

The first concept is called the micro-interaction concept. It was introduced by Theofanous for ESPROSE, but it is in fact a development of the concept used by earlier analytical tools. It makes the hypothesis that:

- the fragments (debris), of the order of 100 μm,
- the vapor (hot fluid),
- a given amount of the cold fluid,

are mixed together to form a (more or less) homogeneous state, generally named mixed fluid or m-fluid. This comes from the idea that only a limited amount of water participates in the interaction. This modelling is also adopted by IDEMO and VAPEX[7].

Although they are based on the same principles, ESPROSE and IDEMO have slightly different formulations. Both have four fields: fuel drops, fuel debris, liquid (cold) coolant, vapour (hot coolant). The differences come from the mechanical and thermal couplings. In IDEMO, all fields but the drops are mechanically coupled, whereas in ESPROSE, the liquid coolant that does not participate directly in the interaction has its own momentum balance. This simplification in IDEMO allows ignoring the basic difficult problems of flow patterns and interactions between the fields. The second important difference in IDEMO is that it is made the hypothesis of a finite time scale for heat transfer from debris to coolant (the m-fluid), whereas in ESPROSE, fragments are in an homogeneous state with the m-fluid (instantaneous heat transfer). The debris in IDEMO has thus its own energy balance. With a heat transfer coefficient of, say, 10^5 W/m².K, and a fragment of, say, 100 μm, the time scale for heat transfer is of the order of 1 ms. Thus, the debris is actually not instantaneously quenched. However, here again, the implication of assuming instantaneous equilibrium is difficult to establish. The assumption of equilibrium is questionable only if the fragmentation time scale is smaller or of the same order than the time scale for quenching each individual fragment.

The non-equilibrium approach is addressed in fact in a very classical manner, where the fragments give heat to the coolant in a finite time scale, according to the local conditions and some assumptions. This heat is transferred into vapour generation either by a non-equilibrium balance

[7] Note that VAPEX is constructed in a way very similar to ESPROSE. We will thus compare only ESPROSE and IDEMO.

at the coolant interface (or a parametric partition). This is the way followed by MC3D, IFCI, JASMINE, VESUVIUS, TEXAS. Then, these codes deal all with basically 4 fields, each one having its own momentum and energy balance (drops, debris, liquid coolant, vapour or gas).

The two descriptions have their drawback and difficulties. In the micro-interaction concept, the main difficulty comes from the entrainment rate of cold water in the mixed fluid. This cannot be extracted directly from experiments. In the desequilibrium approach the major difficulty comes from the amount of heat giving directly vaporization. In both cases, exists the additional difficulty of the heat transfer time scale (null for ESPROSE, finite for the others).

III.B. Drop fine fragmentation

All codes but IFCI use a mechanistic law to describe the fragmentation during the explosion. In IFCI, the fragmentation is given by a simple parametric model with user-defined parameters.

It is now recognized that two types of fragmentation can be involved in an explosion: the so-called thermal fragmentation and the standard hydrodynamic fragmentation.

In the first one, fragmentation is believed to be due to instability of the vapour film around the drops but the actual mechanism of drop instability is still an area of research. The first model developing this idea was proposed by Kim (1988) and further adapted for TEXAS. The conceptual picture is that the film destabilization leads to the development of small liquid jets under the influence of Rayleigh-Taylor instabilities. These jets are able to penetrate the melt drop before vaporization. When the latter occurs, a superficial part of the drop is ejected. Since then, this work has been extended in several ways, mainly following the idea of Inoue (1995) for whom the destabilization leads to local contact between the liquid coolant and the melt. These contacts induce a strong local pressurization which lead to the destabilization of the drop itself and thus to its fragmentation. Whatever the real mechanisms, it is quite widely accepted that the thermal fragmentation should be influent mostly at the beginning of the explosion, during the triggering and the escalation. However, the model developed for TEXAS is used in all conditions, according to the characteristic time:

$$\tau = \frac{D_f}{6 C_{fr}} \left(\frac{\rho_c}{(P - P_{th})} \right)^{0.5} \quad (14)$$

P_{th} is a threshold pressure, taken to be the initial pressure. The parameter C_{fr} is taken to be around 0.001-0.002. It represents the ratio between the initial instability amplitude and the wavelength. Thus small values of C_{fr} are expected.

MC3D also use a mechanism to initiate the fragmentation, but it is purely parametric.

Except TEXAS and IFCI, it is considered for all other codes that the driving mechanism for the explosion is an hydrodynamic fragmentation. Here also, the actual process is still not resolved. Whatever the process, the characteristic time for fragmentation is still of the order of

$$t^+ = \sqrt{\frac{\rho_f}{\rho_a}} \frac{D}{\Delta v} \quad (15)$$

as for premixing, the difference being on the kinetics of debris area creation. The dimensionless time, t_b/t^+, is either:

- τ = constant ~1 : formulation from Carachalios et al (1983), and also from Pilch: MC3D, IDEMO, IFCI, VESUVIUS, TRACER-II;
- τ =Cte. $Bo^{-1/4}$, formulation obtained by Theofanous from SIGMA experiments (Theofanous, 1997), used by ESPROSE, VAPEX.

The latter formulation is also consistent with the experimental results of Reinecke & Waldman (1970) who gave $t^*=48.\ We^{-1/4}$, and the theoretical work of Harper et al.(1972). From their SIGMA experiments, UCSB suggests a value of about 13 for the constant (termed β_f). However values going from 9 to 200 where used in the interpretation calculations of Task-3 and 4 (9 for alumina tests, 200 for corium tests and reactor calculations).

Comparison of TEXAS formulation with the others shows that there is nearly an order of magnitude in the time scale for fragmentation. For characteristic choc conditions, the fragmentation takes some tenth of millisecondes (except may be with β_f = 200 in ESPROSE) with the hydrodynamic formulation whereas is takes some millisecondes with TEXAS formulation.

Last, it is important to notice that in none of the codes, the debris size is calculated and dependent on the local conditions. In all cases the debris size is constant going from 10 µm to 100 µm. In ESPROSE and VAPEX, with the assumption of local equilibrium this is of no concern.

III.C. Heat and mass transfer

The energy transfer question is the core of the differences between the two approaches of modelling: micro-interaction and non-equilibrium. It is also the core of the explosion process and probably the most difficult feature to model. This will become quite evident, as we will observe the disparities in the different approaches.

The non-equilibrium approach is simpler from the conceptual point of view. It assumes that the fragments are giving their energy at a specified rate. Part of this energy goes to water, the rest going to evaporation.

In MC3D, a constant heat transfer (5.10^4 w/m².K) from debris to water is assumed. Part of this energy goes to the water, calculated form a conduction-limited transfer

law. The rest (the largest part actually) goes to vaporization. In VESUVIUS, the model is even simpler with a "direct vaporization model" where the energy for vaporization is a given amount of the instantaneous available energy from fragmentation. The fraction is 2 % in Task 3 calculations but has been raised to 5 and 10 % in Task 4 calculations for the ex- and in-vessel cases, respectively. The approach in TEXAS and JASMINE is less parametric for the global heat transfer. It is assumed that heat loss is controlled by internal conduction and thus released in a time scale:

$$t_h = C_h \frac{R^2}{a_t} \quad (16)$$

where R is the radius, and a_t the thermal diffusivity. The coefficient C_h is 0.1 in TEXAS and 0.045 in JASMINE. For a "standard" corium fragment of 100 µm, this gives approximately 0.1 to 0.2 ms. This value is the same as for a constant heat transfer coefficient of ~ 10^6 W/m²/K. This shows that this modelling gives a nearly instantaneous quenching. Concerning the associated mass transfer, JASMINE makes the hypothesis that all the energy is used for vaporization.

In the micro-interaction method, the heat transfer rate is instantaneous in ESPROSE, while IDEMO uses a constant heat transfer coefficient, ranging from 5.10^4 to 5.10^5 w/m².K. However, the main idea of the concept is the rate of input of fresh water into the mixed-fluid. Theofanous has proposed to express this rate as directly proportional to the fragmentation rate itself.

$$E = f_e.F \quad (17)$$

The proportionality constant, i.e. the entrainment factor f_e, is found, from SIGMA and KROTOS experiments to be bounded by 5 and 15, and a value of seven is recommended. All along phase 1 calculations a constant value of 7 has been used in ESPROSE. In IDEMO, values between 5 and 12 are recommended. Calculations were made with the conservative choice $f_e = 5$.

III.D. The role of void in the models

The role of void on the explosion was constantly highlighted in SERENA meetings, and particularly in the Task-4 meeting where very different behaviours in the calculation were evidenced with similar initial conditions. We will thus address this point in details.

III.D.1. Fragmentation

We have seen that for fragmentation, most of the codes deal with almost the same law. However, the transposition in multiphase flows can be very different, and this makes the difference.

For ESPROSE, VAPEX and TRACER, a linear interpolation according to the void fraction is done. The formulation for the volumetric fragmentation rate is thus:

$$F = \alpha_f \left(\frac{\alpha}{t_g^+ \tau_g} + \frac{1-\alpha}{t_l^+ \tau_l} \right) \quad (18)$$

where each characteristic and dimensionless time is calculated as if the drop were in the considered fluid (gas or liquid coolant). Such simple linear interpolation might lead to some problem because it is not legitimate to use the formulations for fragmentation when the ambient fluid is in a dispersed state. It is obvious that fragmentation is much more effective in the liquid: 10 % of water in a 90% void region can have a significant impact on the fragmentation. This impact should even be enhanced by the fact that the liquid velocities are higher while in dispersed state.

The second method is to use one average ambient fluid. This is the line followed in IDEMO, VESUVIUS and JASMINE (Task-3). In fact, this formulation should lead to similar trends (to be verified) since an averaged formulation tends to give rather high densities due to the water and possibly some strong velocities if gas is dominant.

The third method consists of introducing a strong dependency according to the flow pattern. This is the case in MC3D, TEXAS and JASMINE (new version, Task-4). In these codes, the fragmentation occurs only for drops in continuous water. Then, basically, the fragmentation rate can be written as:

$$F = \alpha_f \left(\frac{C}{t_l^+ \tau_l} \right) \quad (19)$$

where C = 1 up to a given void and then decreases to 0. For MC3D and JASMINE, C equal 1 in bubbly zone, and decrease to 0 in the transition. For TEXAS, the decrease occurs (more sharply) around a 50 % void. In contrast with the two other methods, this one provides a real cut-off of the fragmentation for region with high void.

III.D.2. Heat and mass transfer

Concerning the heat and mass transfer, similar trends are obtained.

For code using the micro-interaction concept, the heat and mass transfer is driven by the entrainment factor. It has been seen that this factor is taken as a constant, i.e., not a function of void. This means that the entrainment rate is directly proportional to the fragmentation rate. Again, the expression (17) might be suited for continuous medium, but should be taken with caution in dispersed flow with high void. In the case of IDEMO, VAPEX and PM-ALPHA, the role of void is unclear, without any real heat transfer cut-off for high voids.

In MC3D, as for the all other constitutive laws, everything is driven by the flow pattern. Then again, heat and mass transfer are maximized in purely bubbly flow, and decrease to zero at the end of the transition flow. So taking into account the fragmentation characteristics, the role of void is clear. High voids lead to a clear cut-off of the transfer and so no explosion is possible in such context.

In JASMINE and VESUVIUS, it is made the hypothesis that all fragments are in contact with water, thus allowing fast heat transfer and resulting vaporization. However, in VESUVIUS, there is a sharp cut-off of the transfer at 70 % void (~ droplet flow), whereas in JASMINE, as we have just seen, the fragmentation is reduced to zero from 30 % to 70 % void. So, in these two codes, there should be some cut-off of the explosion process for high voids, probably less pronounced in VESUVIUS.

IV. OTHER UNRESOLVED ISSUES

Beside the general difficulties previously discussed, there exist at least two supplementary issues that are far from being resolved: the drop solidification effect, and the hydrogen generation.

IV.A. Drop solidification

The drop solidification influences the whole FCI process through the limitation of the fragmentation. In principle, the solidification of the drops is numerically far easier to compute in a lagrangian description. However, only PM-ALPHA proposes a model for computation of the solidification of the drops[8]. This is probably because, physically, the problem is not obvious. Because of the rather low conductivity of the fuel and of the very different conditions that can be met by the drop during its history, the computation of the temperature profile is rather difficult without an adequate meshing of the drop. Furthermore, a way to take account of the fragmentation of a solidifying drop in a simple model seems, at present, rather difficult to find. At last, the material effects should also be considered (chemicals, phase diagram). This seems to be a huge task and the necessity of such modelling is clearly to be discussed.

IV.B. H2 generation

A second important issue that needs further clarification is the role of hydrogen generation (oxidation) both during the premixing and the explosion. Only MC3D and IFCI can handle the presence of non-condensable and an oxidation. It is well known that in FARO, some non-negligible amounts of hydrogen are created, but only MC3D proposed a calculation of this aspect in Task-2. The result is that for high subcooling (FARO L-31), nearly all the pressurization (i.e. the void) is done by the hydrogen.
The influence of oxidation on the energetics is also a real open issue. The ZREX and ZRSS experiments (Cho, 1998) showed the influence of oxidation of metallic zirconium on explosion energetics. This effect is not accounted for currently in the FCI codes.

V. CONCLUSIONS

We have tried in this paper to review the most important physical and numerical models included in FCI codes used for SERENA program. Although other codes exist for this purpose, this review gives a good general picture of the state of the art. In contrast with what is often heard, the modellings in these codes are rather different. They are the mirrors of the subjective views and perspectives of the persons and experts in charge of their development. Then, analysing the codes in details, together with the discussions held all along the meetings, allows a better understanding of the differences in views and descriptions.

However, beside the clear code differences and expert opinions, for which discussions, the first stage of collaboration, should help to find the most reliable picture of the phenomenon, we must admit that very strong difficulties are encountered. Most of these are related to the extrapolations of most of the theoretical models to a very complex multiphase environment. As an example, we can emphasize the problems of the fuel primary fragmentation, and the drop thermal fragmentation. Very detailed modellings have been provided for these too phenomenon, leading probably to quite clear global pictures. However, these models are found to be very difficult to include in FCI codes. The two major reasons are the necessary numerical simplifications that are to be done for this purpose, and the necessity to extend the studies to the actual conditions found in the multiphase environments considered.

This review clearly shows that there exist some major differences. Some of these differences reflect real controversies on some specific features. The primary fragmentation is one of them. But most of them simply reflect a limited knowledge of very complex multiphase phenomena involving orders of magnitude in pressure, temperature and scales. The most important aspects have been discussed in details and this should help in the understanding of the behaviours of the codes with, (at least) three important pending questions:

- Are the differences on fuel break-up mechanisms during premixing leading to significant differences in the energetics of FCI?

[8] Except by comparison of the mean temperature with the solidus and liquidus.

- What is the fundamental mechanism responsible for the differences in voiding during premixing?
- What is the exact role of void during the explosion?

NOMENCLATURE

Standard scientific notation with:

α	volume fraction (void if no subscript)
β_f	fragmentation parameter in ESPROSE
D,R	diameter, radius.
f_e	entrainment factor (17).
k, λ	wave number, length.
Γ	volumetric fragmentation rate
N_f	fragmentation parameter (6)
T	temperature
t	time
t^+	characteristic time
τ	dimensionless time = t/t^+
Δv	velocity difference
σ	surface tension
Bo	Bond number
We	Weber number

Subscripts:

0	standard corium case in Meignen correlation (3)
a	ambient fluid
d	drop
c	coolant or critical
j	jet
g	gas
l	liquid

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