DE LA RECHERCHE À L'INDUSTRIE

TECHNICAL MEETING ON PHENOMENOLOGY AND TECHNOLOGIES RELEVANT TO IN-VESSEL MELT RETENTION AND EX-VESSEL CORIUM COOLING

SHANGHAI, 18/10/2016, TECHNICAL SESSION 1C

CORIUM PROPAGATION MODELLING WITH THE PROCOR SOFTWARE – APPLICATION TO CORIUM VESSEL LOWER HEAD

CEA/DEN/DTN/SMTA/LPMA
S. BAJARD, B. HABERT, R. LE TELLIER, L. SAAS

October 18th, 2016

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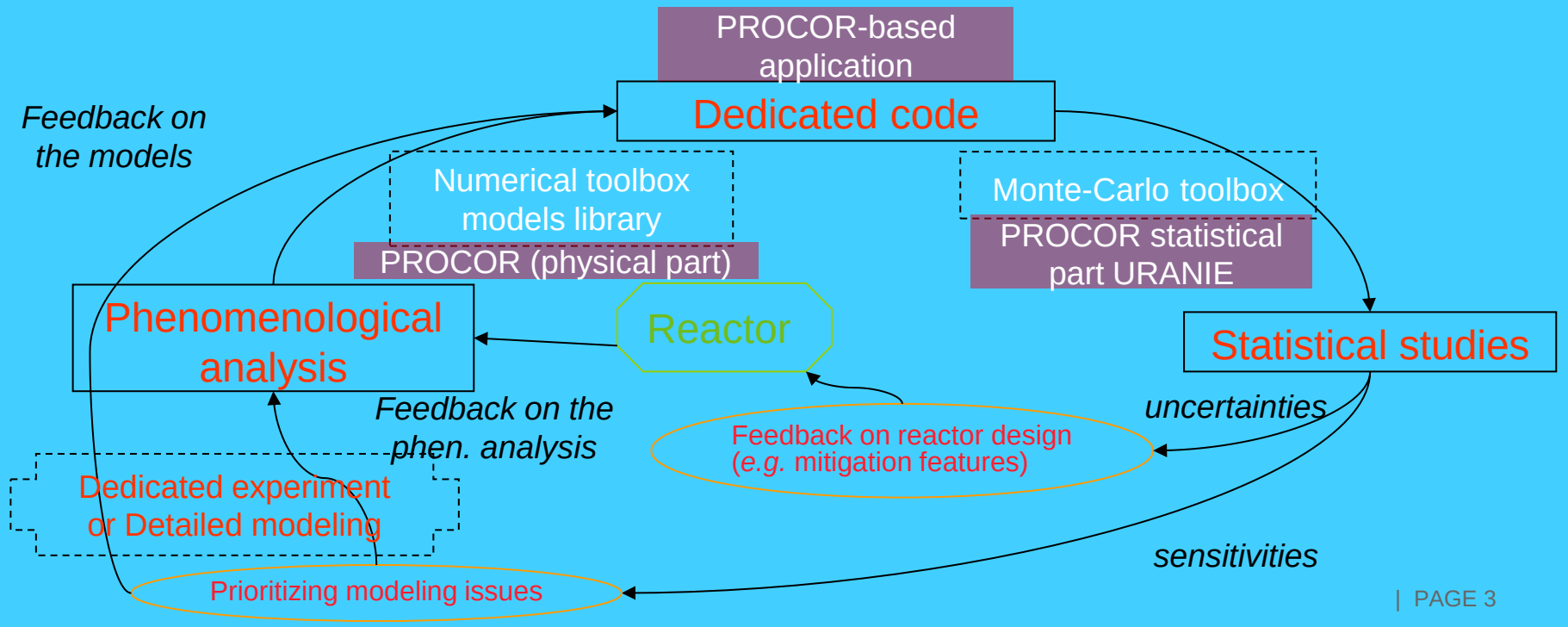
Outlines

- **PROCOR software (PROpagation of CORium) : a short description**
- **Modelling of the corium pool propagation in lower head (in PROCOR for IVR study)**
- **Results : 2 modes of vessel rupture by focusing effect**
- **Current improvement/R&D using fine modelling :**
  - Analytical work preamble to CFD simulations of the light metal layer responsible for the focusing effect
  - Multicomponent multiphase diffusion modelling in a liquid miscibility gap : corium pool stratification phenomenology

PROCOR : short description

- **PROCOR stands for PROpagation of CORium: its objective is to simulate the transient of severe accidents phenomena**
  - Only propagation of corium and its interactions are modeled (no Fission Products or H2 release);
  - A software platform composed by a kernel, a library of models, and different reactor applications;
  - A PROCOR application is an assembly of models of the library that use the services of the kernel;
  - PROCOR is composed of two parts :
    - a physical part (models and applications) : to simulate corium propagation (deterministic part)
    - a statistical part (based on URANIE (CEA), Monte Carlo method) : to perform studies on the physical part
  - PROCOR has an associated work cycle in order to enhance the modelling



PROCOR application : for IVR

- **Simplified modelling is used but parameters associated to the models (lumped parameter models) and applications are used to take into account uncertainties of physical phenomena**

- **Parameters allow to perform sensitivity or statistical studies (statistical studies not presented here).**

- **Different PROCOR applications have been developed : an application is dedicated to a type of PWR reactor (In-Vessel Retention, Ex-Vessel Retention…).**

- **a PROCOR application dedicated to the lower head propagation used for IVR study :**
  - take into account the transient corium transfer from the core to the vessel lower head : evaluation of corium mass flow rates in the vessel lower head (external computations not managed by PROCOR)
  - compute corium pool behavior in the vessel lower head : corium pool stratification that evolves through time, heat flux evaluation, ablation of internal structure and of vessel wall
  - the reactor pit is flooded : Critical Heat Flux (CHF) is a parameter : $CHF = CHF_{max}\ f(z)$

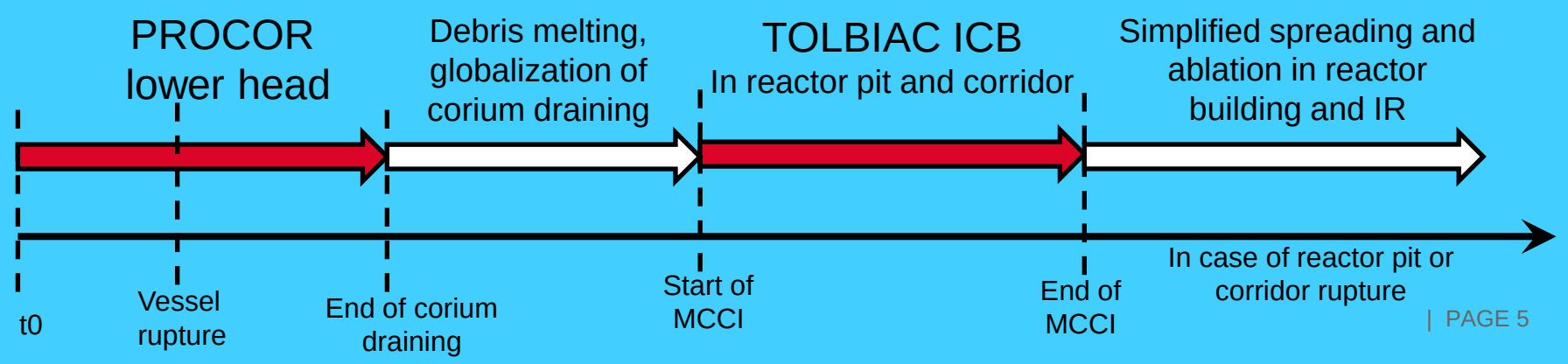
Objective of this application → Evaluation of the vessel failure
Thermal failure only : major risk is failure by focusing effect

PROCOR ex-vessel application

- **the PROCOR ex-vessel application** is composed of a chaining between PROCOR lower head application and TOLBIAC-ICB code (CEA software)
  - The PROCOR lower head application computes the corium propagation in the vessel, the ablation of the vessel lower head and the corium and debris draining through the vessel rupture hole into the reactor pit;
  - Then debris melting/cooling is computed and start of Molten Corium-Concrete Interaction (MCCI) is evaluated using a 1D simplified model;
  - if MCCI starts the TOLBIAC-ICB code (software) computes more accurately the MCCI in the reactor pit and in the corridor;
  - Simplified models of spreading and ablation are used for the instrumentation room (IR) and/or for reactor building in case of lateral rupture of the reactor pit and/or the corridor;
  - Wet and dry reactor pit can be considered.

Objective of this application → Evaluation of the reactor building failure

PROCOR ex-vessel



PROCOR modelling in the lower head (1/2)

- Corium flow rates from the core are input data for the lower head (timing, mass flows, temperatures, species compositions, corium/debris ratio…)

- An Energy/Mass 0D model for each corium layer:
  - transient mass and energy equations formulation: specific heat no Equation of State
  - Stationary heat transfer correlations for natural convection, heat flux profile, radiative transfer (stationary model)
  - the crust is seen as boundary thermal conditions (liquidus temperature)
  - transient added mass is taken into account (corium flows from core + ablated steel)

$$\frac{dm}{dt} = \sum_j \frac{dm^{\mathrm{in,j}}}{dt}$$

$$mC_p \frac{dT}{dt} + \sum_j \left(\frac{dm^{\mathrm{in,j}}}{dt} \int_{T^{\mathrm{in,j}}}^{T} C_p^{\mathrm{in,j}} dT' \right) = \sum_i \phi^i S^i + \dot{q}^{\mathrm{mass}} m$$

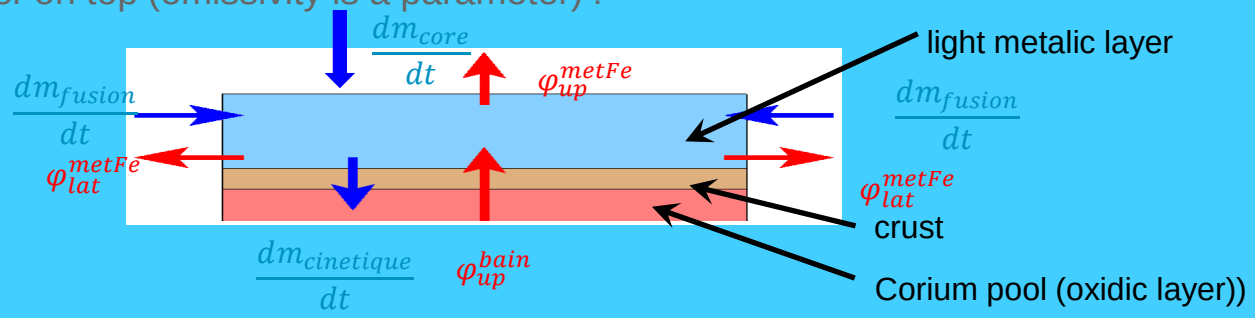
Mass transfer between layers, corium from the core, and ablated materials

- A corium pool stratification model based on species diffusivity :
  - the stratification evolves during the transient (heavy metal layer/oxidic layer/light metal layer)
  - Use an equilibrium model (Salay-Fichot model);
  - Use a kinetic model (Le Tellier-Saas) : Uranium diffusivity is a parameter D_u ;
  - upper crust is stable but totally permeable to mass transfer;

→ **all the hypotheses on phase segregation and thermal balance are consistent**

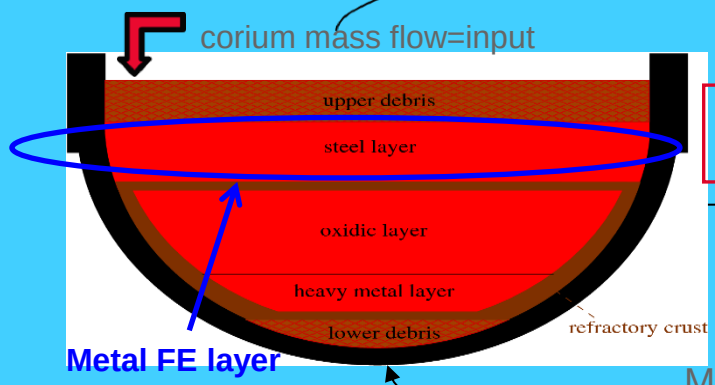
PROCOR modelling in the lower head (2/2)

- The light metal layer is responsible for the focusing effect:
  - Transient mass and energy equations formulation (0D)
  - “Classical stationary” correlations : Globe&Dropkin (h_{up}) , Chawla&Chan or Chruchill&Chu (h_{lat})
  - Radiative heat transfer on top (emissivity is a parameter) :



- Ablation model for the vessel=1D mesh (water level, with maximal **Critical Heat Flux 1,5 to 2 MW/m2**)
- Ablation model for internal structures
- A heating/cooling and melting model for each debris bed

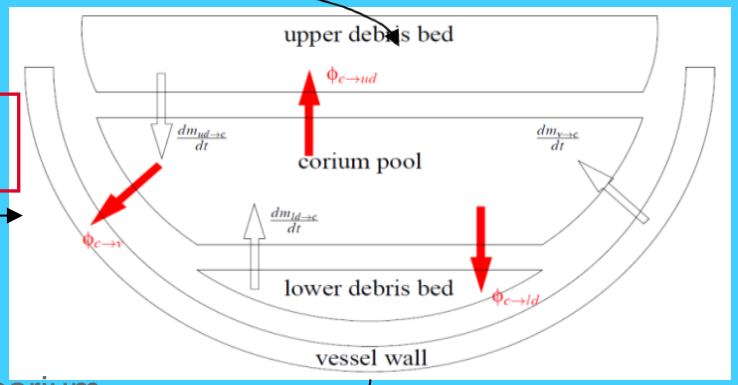
CHF= CHF_{max} f(z) is parameter



Vessel integrity ?

Heat fluxes to the surroundings

Corium pool stratification

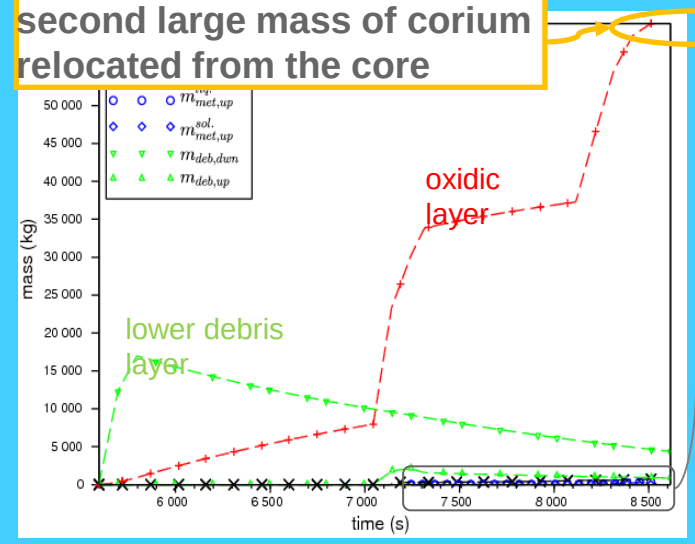


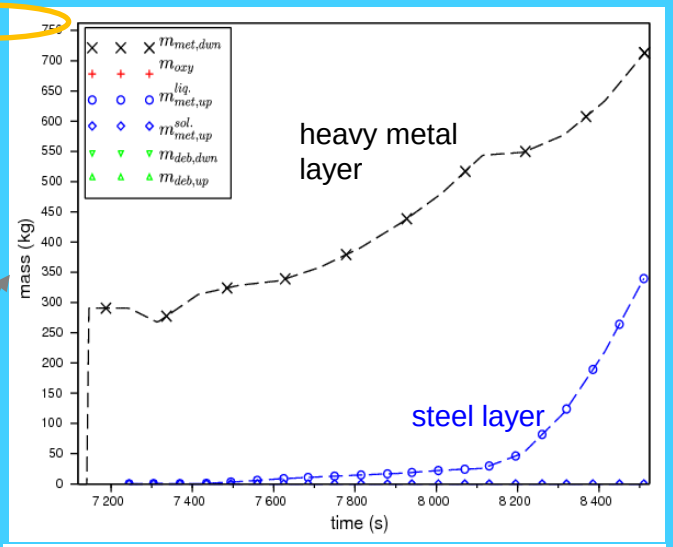
Mass addition to the corium pool

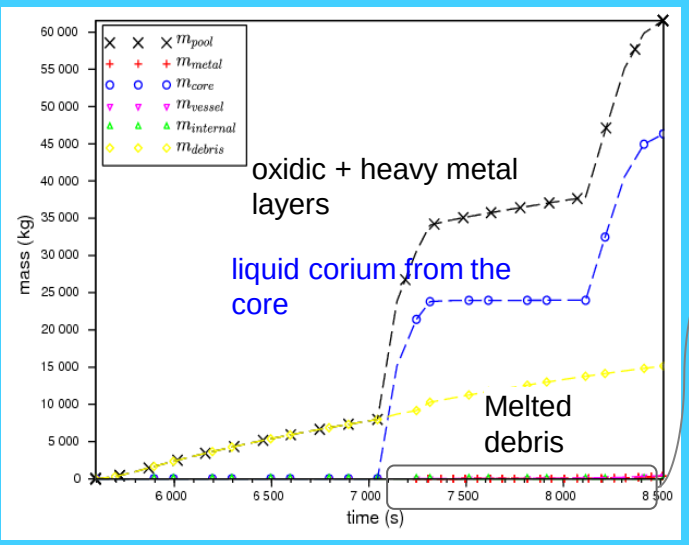
PROCOR :Sensitivity analyses regarding the vessel failure

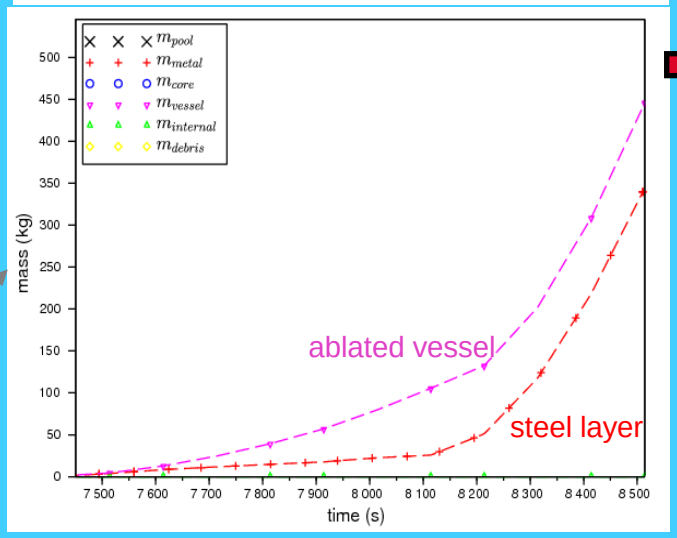
Transient focusing effect : early “mode”

second large mass of corium relocated from the core









Early mode : thickening of the light metal layer : few centimeters, with time system is going out of the focusing effect zone

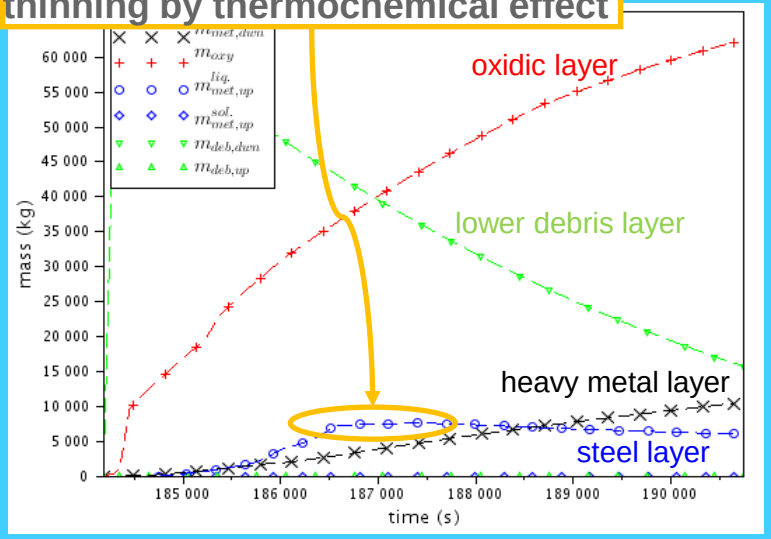
Thermal behavior during the formation of a thin steel layer ?
→ inadequacy of the 0D axisymmetric stationary model

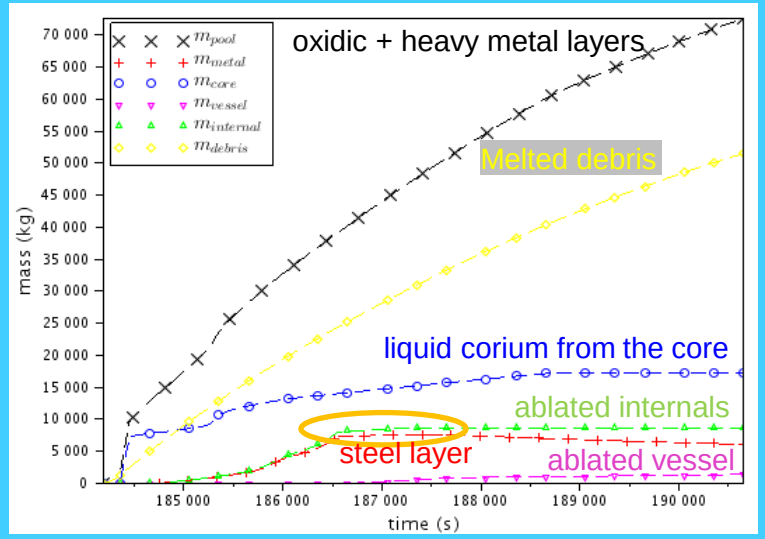
Lack of knowledge : need of a finer (scale) modelling in support of simplified thermalhydraulics modelling

PROCOR : Sensitivity analyses regarding the vessel failure

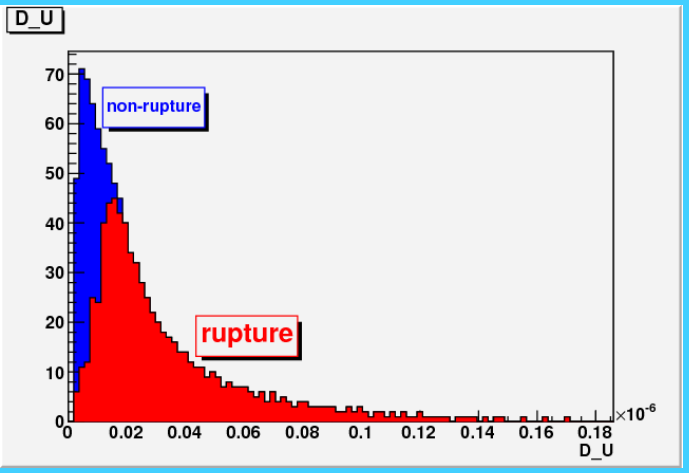
Transient focusing effect : thermochemically-driven “mode” (late mode)

thinning by thermochemical effect





- Important parameter regarding this mode of vessel rupture : D_u parameter (U diffusivity in the oxidic layer)



- log-triangular law [1.8E-9, 1.8E-8, 1.8E-7]

(Stokes-Einstein formula : 1.81E-8 m2s-1)]

- lower value → slower thinning of the steel layer

2nd mode : thinning of the light metal layer : decimetric thickness, with time system is going in of the focusing effect zone

Lack of knowledge :
Need of finer modelling support of simplified modelling of stratification evolution

Finer modelling : analytical work preamble to CFD for fhe thin metallic layer thermal-hydraulic

R&D Objective : have a finer modelling to gain in knowledge using experimental and/or numerical approach

In this presentation, we focus on two points based on CFD approach

- Use CFD computations for corium pool : presented in this conference by EDF (C. Le Guennic)

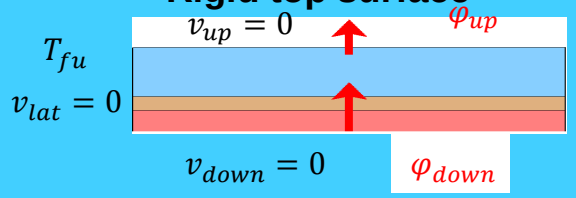
- **1st point : Thin metallic layer thermal-hydraulic modelling :**
  - Goal : gain margin to focusing effect in time and in the level on the lateral heat flux ;
  - CEA is participating with Trio CFD code (CEA) to "Benchmark on thin metallic layer" (IVMR project)
  - we present hereafter only analytical work preamble to CFD simulations of the thin metallic layer : what are the boundary conditions that we have to consider on top of the thin metallic layer

- **2nd point : Corium pool stratification modelling : kinetic stratification model**
  - Goal : enhance the mass transfer modelling between layers, and have a better coupling between thermal-hydraulic and thermochemistry of corium;
  - To complete the CFD modelling multiphase and multi-component modelling is needed ;
  - CEA is developing a multicomponent (*i.e. «multi-species»*) multiphase diffusion modelling in a liquid miscibility gap (Phase Field method in Ph.D. C. Cardon) that will be integrated in a CFD code to simulate the stratification : presented hereafter;

Finer modelling : analytical work preamble to CFD for fhe thin metallic layer thermal-hydraulic

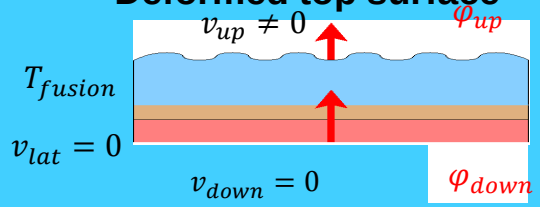
- **Questions to be answered regarding the top boundary treatment in CFD code for thin metallic layer computations : how is upper heat transfer affected by top free surface boundary condition?**
  - Gain margin : what is the natural convection regime? Marangoni-Bénard (thermal gradient acting on surface tension on top surface) convection vs. classical Rayleigh-Bénard convection or both convection
  - When Marangoni-Bénard convection is of importance, how large is the free surface deformation?

Rigid top surface



- **the crust separating the steel layer from the pool imposes a rigid BC with an imposed heat flux from the pool**
- **top BC : radiative heat transfer**

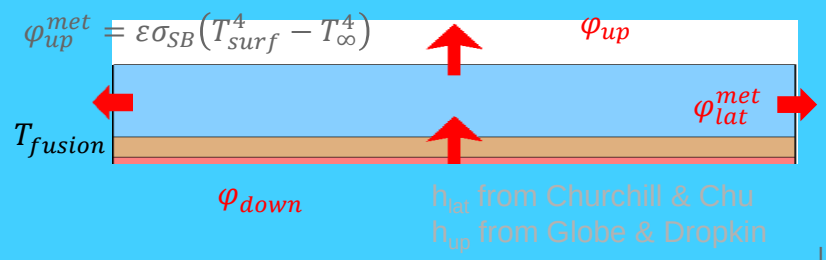
Deformed top surface



- **Some answers to these questions can be found by using results from the literature for the 1D axial problem (adiabatic lateral BC):**
  - *Gain margin : Linear stability analysis D.A. Nield, "Surface tension and buoyancy effects in cellular convection", Journal of Fluid Mechanics, 19(3), pp 341-352, 1964*
  - *Numerical simulations T. Boeck, "Bénard-Marangoni convection at large Marangoni numbers: results of numerical simulations", Advances in Space research, 36, pp 4-10, 2005*

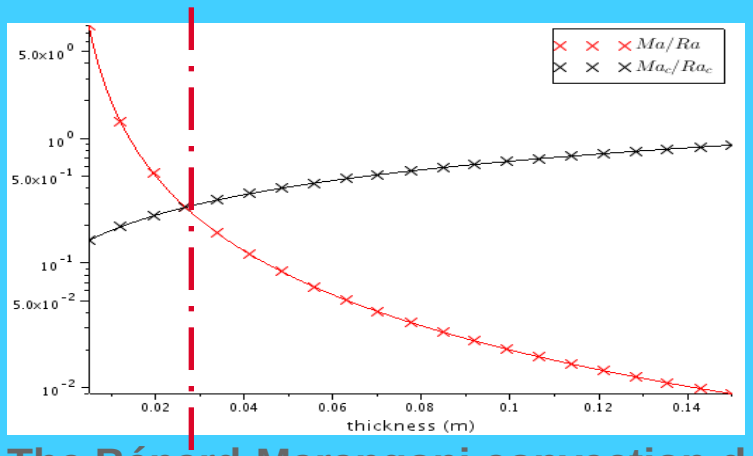
- **In order to do so, we use stationary solutions of the thermal problem for the metal layer as modelled in S.A. integral codes : $\rightarrow T, T_{surf}$**
  - The thickness varies from 0.5cm to 15cm;
  - For instance, for $\mathrm{R} = 2.0m$, $\varphi_{up}^{pool} = 1\ MW.m^{-2}$

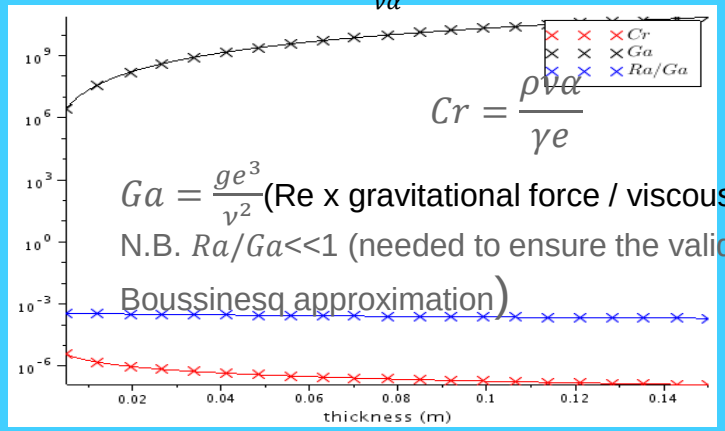
$T_{\infty} = T_{fusion}$, $\varepsilon = 2/3$



Finer modelling : analytical work preamble to CFD for fhe thin metallic layer thermal-hydraulic

- **<u>Objective:</u> Questions to be answered regarding the top boundary treatment: top free surface**
  - We have done an evaluation of Ma, Ra and associated critical values → relative importance of Marangoni-Bénard convection vs. Rayleigh-Bénard convection
  - Comparison of Nu_{up} w.r.t. Nu_{up} =f(Ma) for pure Marangoni-Bénard convection → **how is upper heat transfer affected?**
- **From linear stability analysis:** $\frac{Ma}{Ma_c} + \frac{Ra}{Ra_c} \cong 1 + \varepsilon$ with $Ma = \frac{\gamma_T e \Delta T}{\rho \nu \alpha}$, $Ra = \frac{g \beta \Delta T e^3}{\nu \alpha}$ and (Ma_c, Ra_c) critical values depending on $Bi = \frac{e \varphi_{up}}{\lambda}$





$Cr = \frac{\rho \nu \alpha}{\gamma e}$

$Ga = \frac{g e^3}{\nu^2}$ (Re x gravitational force / viscous force)

N.B. Ra/Ga<<1 (needed to ensure the validity of the Boussinesq approximation)

- **The Bénard-Marangoni convection dominates for thicknesses below 3cm:**

→ this free surface effect should be taken into account in detailed CFD for thicknesses ≈ 5cm

- **In any case, the Crispation number Cr (resp. Galileo number Ga) is <<1 (resp. >>1) indicates that the free surface deformation is small**

→ CFD calculations with a non deformed boundary and modified boundary conditions :

$$\frac{\partial v_x}{\partial z} + Ma \frac{\partial T}{\partial x} = 0 \qquad v_z = 0 \qquad -\lambda \frac{\partial T}{\partial z} = \varphi_{up}$$

Finer modelling : modelling multicomponent multiphase diffusion modelling in a liquid miscibility gap

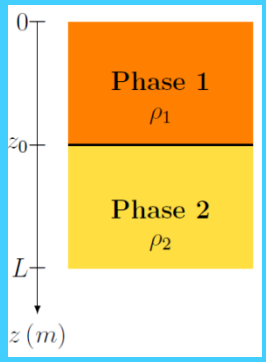
- **Objective:** a mesoscopic model for the multicomponent multiphase diffusion in a liquid system with a miscibility gap that meets the following criteria:
  - "compatible" with CFD (tractable coupling with Navier-Stokes equation)
  - consistent use of thermodynamic database (to ensure consistency in the steady-state, isothermal case with thermodynamic equilibrium calculations)
  - The model parameters has to be fitted on meso/macro properties/observations (in particular surface tension)

- **Consistency properties that the overall multicomponent diffusion model should exhibit** (x_i element molar fraction, y_j species molar fraction) **:**
  - Ternary case U-O-Zrmodel should be consistent in the limiting binary cases U-O, U-Zr, Zr-O;
  - The values of x_U, x_{Zr}, y_{ZrO_2} (species molar fractions) are constrained so that $y_{j\neq O}(\mathrm{t},\vec{r}) \geq 0$;

- **Phase-field approach:** complete in-vessel corium system (suboxidized corium + steel) N-component system (example of U-O-Zr):
  - Use analytical derivation of Free Energy Functional to define diffusion mobility ($\tilde{\mu}_j$)
  - Fix evolution of element molar fractions by N-1 **Cahn-Hilliard (CH)** equations (diffusion equation of $x_i$that depends on $\tilde{\mu}_j$) to ensures conservation (example $\rightarrow \boldsymbol{x_U}, \boldsymbol{x_{Zr}}$);
  - Add hypothesis of instantaneous local equilibrium of redox reactions to deduce species molar fraction evolution (example $\boldsymbol{y_{ZrO_2}}$, from redox process UO_2+Zr ↔ U+ZrO_2)

Stratification kinetics modeling

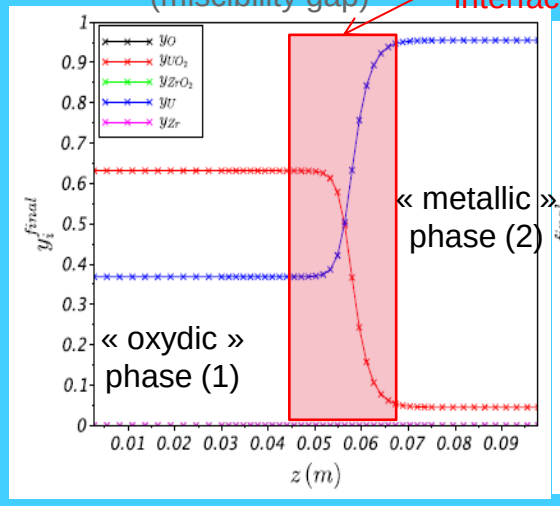
- **Model implementation of this model has been done (mock-up)**
  - interface with U-O-Zr-Fe database using the OpenCALPHAD code
  - C-H coupled equations : finite difference scheme in space (staggered grid for degenerate mobility coefficients) + theta-scheme in time + Newton-Raphson iterative method



- **Numerical result examples: verification of steady-state w.r.t. thermodynamic equilibrium calculations on 1D slabconfigurations**
  - when in the miscibility gap, we obtain a two-phase configuration and, away from the interface equilibrium, $y_i^{oxy,eq}$, $y_i^{met,eq}$
  - when out of the miscibility gap, homogeneous y_i configuration consistent with $y_i^{hom,eq}$

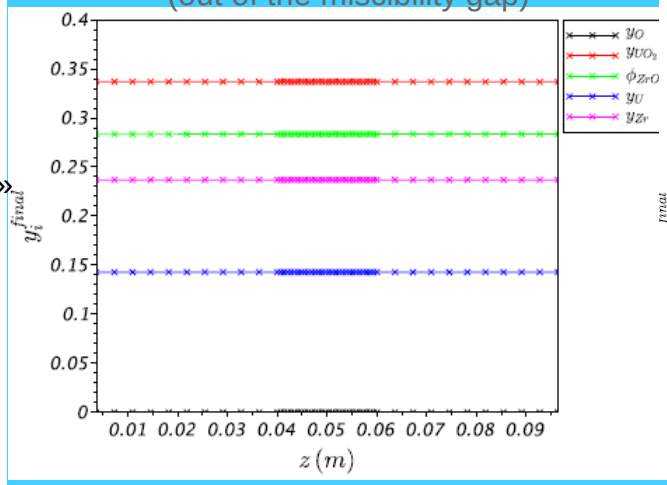
U-O case (miscibility gap)

Diffuse interface



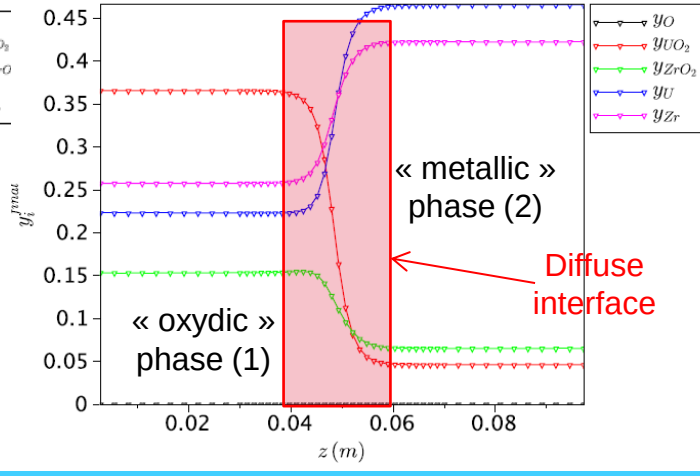
two phases in the U-O miscibility gap

U-O-Zr case (out of the miscibility gap)



One homogeneous phase

U-O-Zr case (global inventory corresponds to miscibility gap)



two phases in the U-O-Zr miscibility gap

Summary/Conclusion

- **Two modes of vessel rupture by focusing effect computed with PROCOR software but the model are too conservative.**

- **Need of finer deterministic modelling to support simplified modeling for IVR in PROCOR software (in order to reduce conservatism and gain margin on focusing effect) : deduced from statistical studies**

- **Two points of finer modelling have presented :**
  - Analytical work preamble to CFD simulations of the light metal layer responsible for focusing effect → to be continued in IVMR project : CFD on thin metallic layer
  - CFD-compatible modeling of multicomponent multiphase diffusion related to stratification kinetics → to be pursued as a part of a Ph.D. thesis to start in fall 2016 (now).

- **These detailed/fine scale simulations (CFD) should be complementary to dedicated experiments in the overall process of improving in-vessel corium behavior integral models.**

- **From these finer modelling, some simplified modelling has to be built to be introduced in PROCOR software (deterministic part) and statistical studies has to be done (probabilistic part) to deduce new R&D issues to have better modelling (a new PROCOR methodology round trip)**