Assessment of advanced corium-in-lower-head models in MAAP and PROCOR codes

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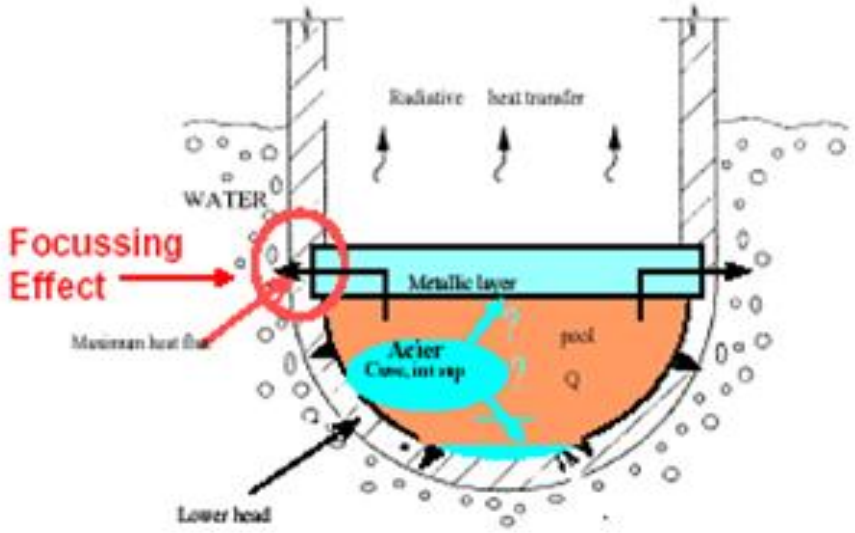
Outline

- **Context and issues**
- Original corium pool modeling in MAAP4 and MAAP5
- Advanced corium modeling
- CEA/EDF teamwork
- Benchmarking
- Results
- Conclusions

Context and issues

- Conceptual Design for future generation of PWR:
  - EVR (Ex-Vessel recovery)
    - Corium flooding in the reactor pit after the vessel rupture
  - IVR (In-Vessel Retention)
    - External cooling of the vessel to evacuate corium decay heat



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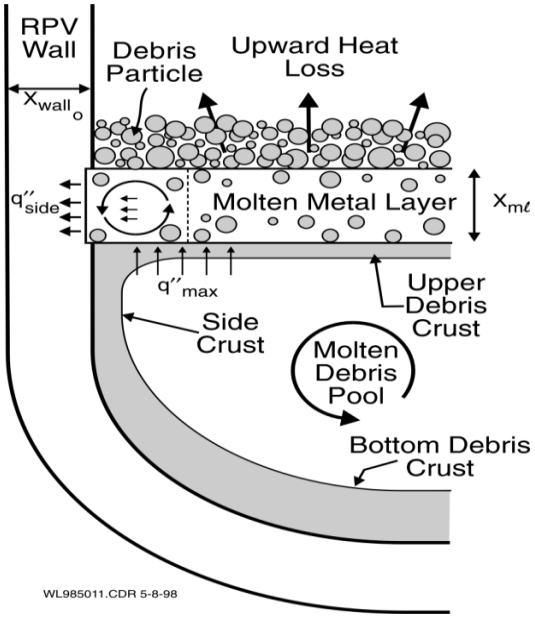
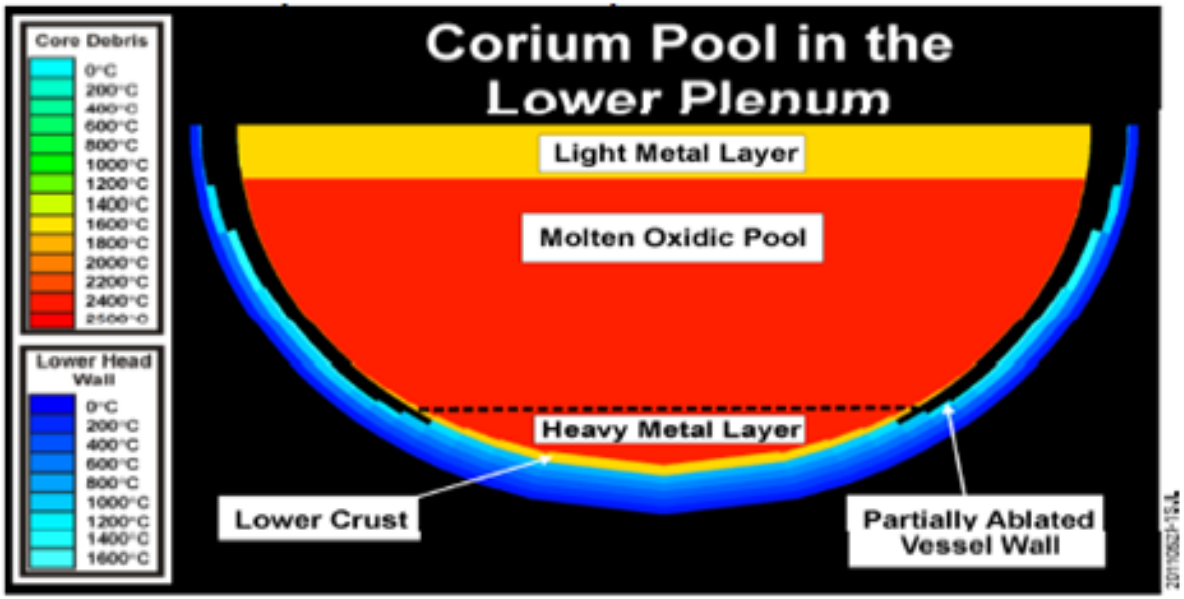
Original corium pool modeling in MAAP4 and MAAP5

"Boundary" stationary calculation



MAAP4



MAAP5

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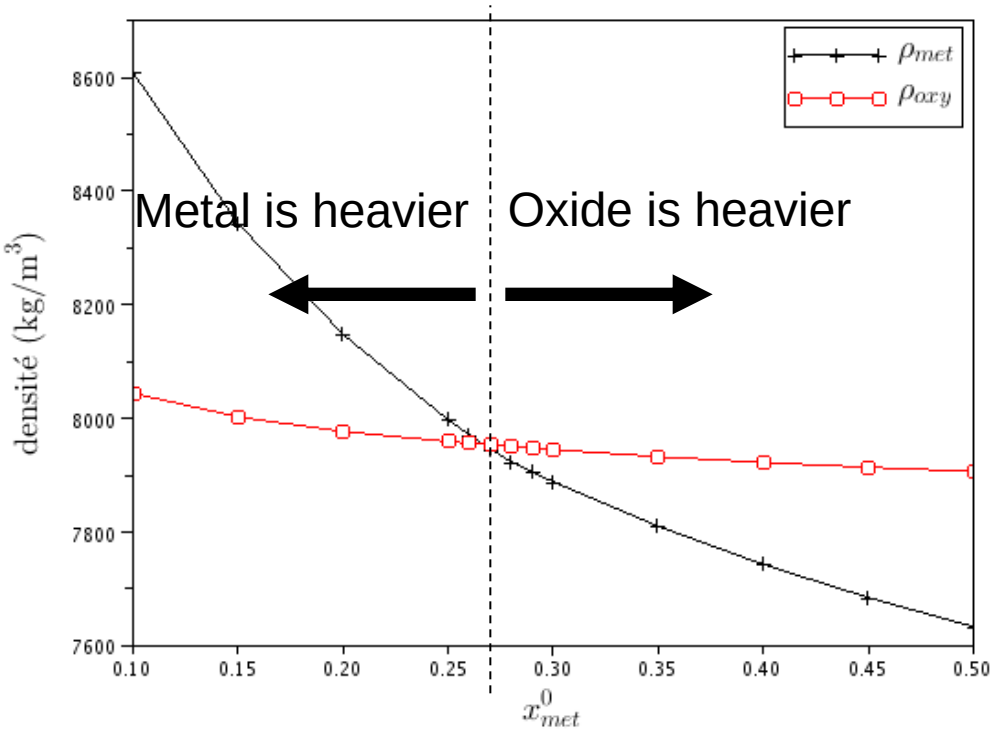
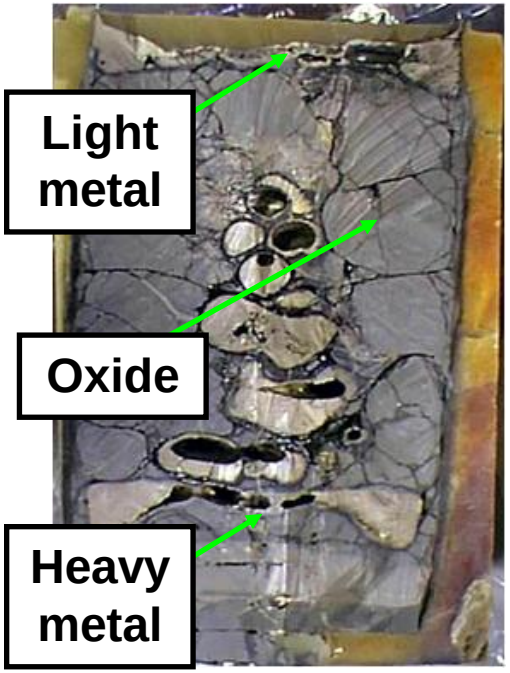
Advanced corium modeling: first glance

The stationary calculation cannot be guaranteed to be most penalized => transient metal stratification



Density evolution in MASCA experiments depending on steel mass ratio $X°_{met}$

T=3000K, C_n=32%, $R_{U/Zr}$=1.2

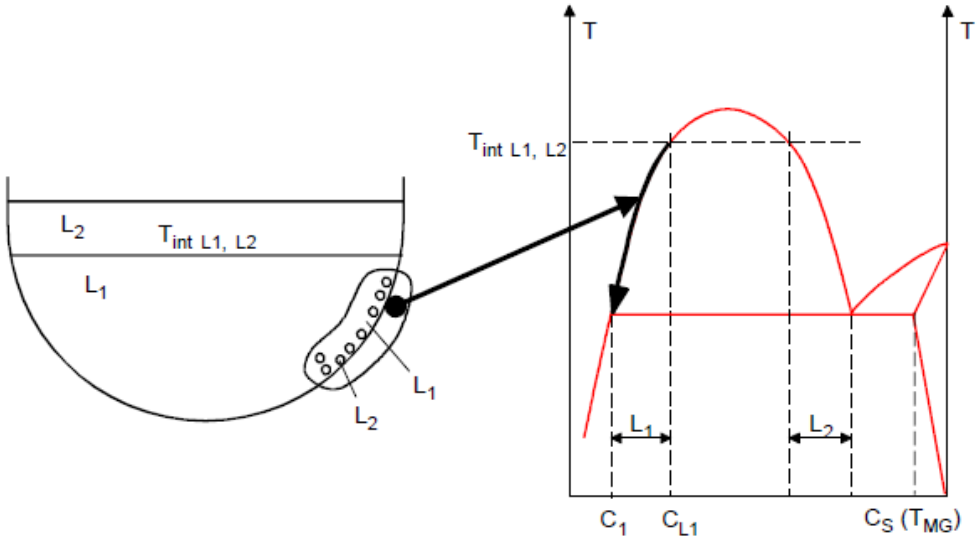


MASCA-RCW final ingot:

$R_{U/Zr}$=1.2, C_n=32%, X_{met}=0.095

Advanced corium modeling: hypothesis 1

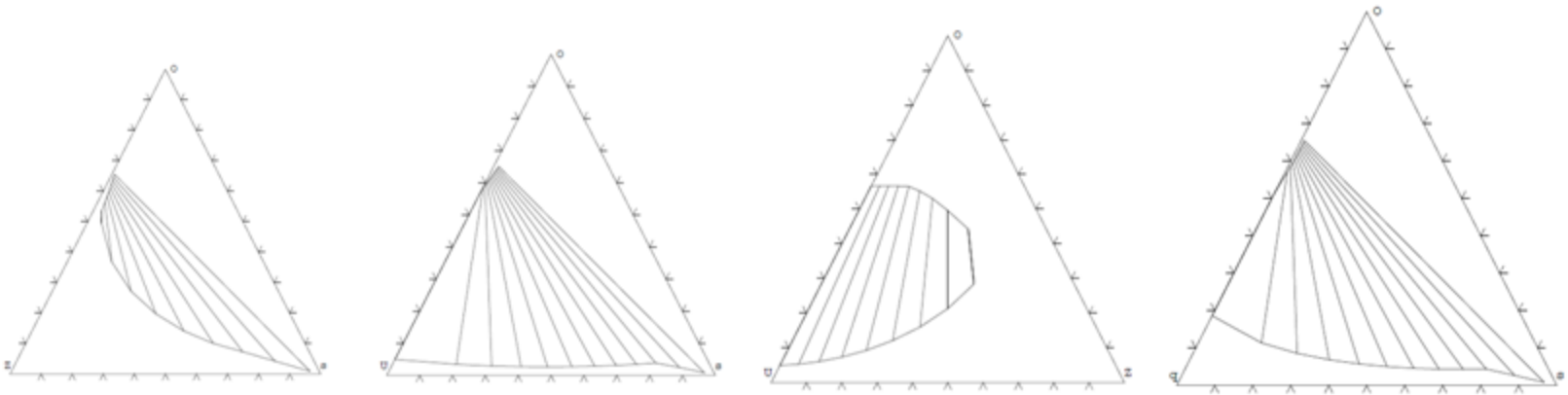
Corium pool with a miscibility gap - the corium pool in equilibrium is expected to be surrounded by the refractory crust



JM Seiler et al., The thermalhydraulics of corium pools undergoing a miscibility gap. Model development and reactor applications. OECD MASCA Seminar 2004 Aix-en-Provence, France 10-11 June 2004

Advanced corium modeling: hypothesis 2

A fast equilibrium model which provides the compositions of the oxide and metal phases in (U-Zr-O-SS) system

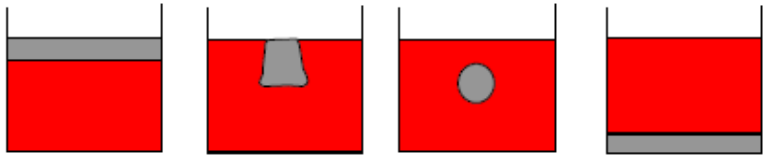


U, Z, O, SS masses ⟶ mass fractions into phases

M. Salay, F. Fichot, Modelling of metal-oxide corium stratification in the lower plenum of a reactor vessel, in: Proc. of Int. Topical Meeting on Nuclear Thermal-Hydraulics (NURETH-11), Avignon, France, 2005

Advanced corium modeling: hypothesis 3

Kinetics of the layer inversion – 0D mass transfer model obtained from MASCA-RCW experiment analysis



This model is based on transfer by diffusion in sub-layers whose thicknesses are controlled by Grasshof and Schmidt numbers: $Sh=Nu\ Gr^{1/12}(Sc/Pr)^{1/3}=(kc\ D_{ab})/L$, where $\mathbf{D_{ab} = 2.10^{-8} m^2/s}$ is diffusion coefficient of Uranium in oxide.

Variation of the atomic concentration of species y(t) to reach a final state corresponding to the equilibrium (with atomic concentration y_{eq}):

$$y(t) = y_{eq} - (y_{eq} - y(0))\ \exp(-kc\ S_{int}\ t/Vol)$$

Gilles Ratel, et al., « Considerations on mass transfer kinetics for layer inversion and layer oxidation » MASCA2 SEMINAR Cadarache, France, October 11-12, 2007

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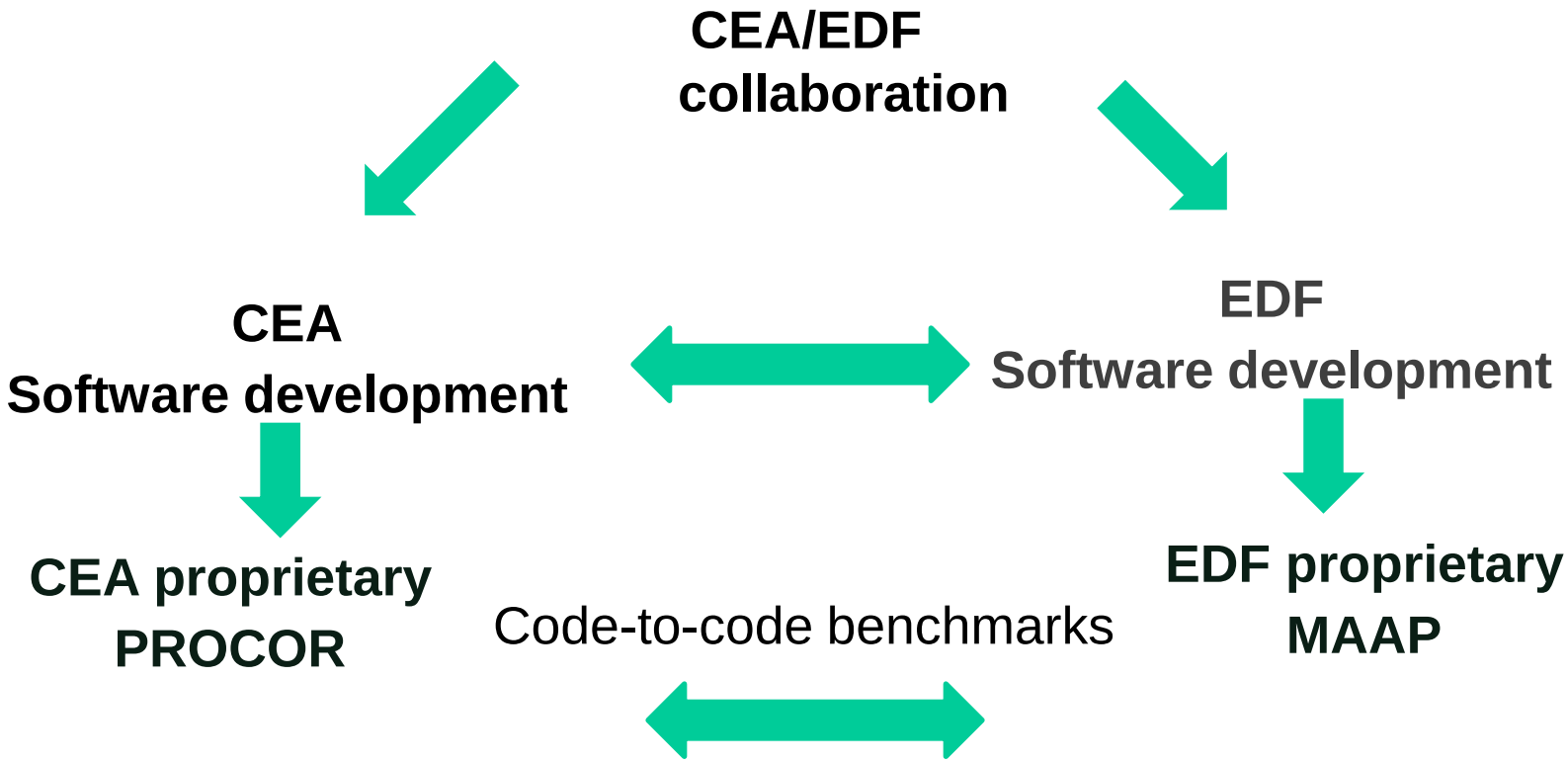
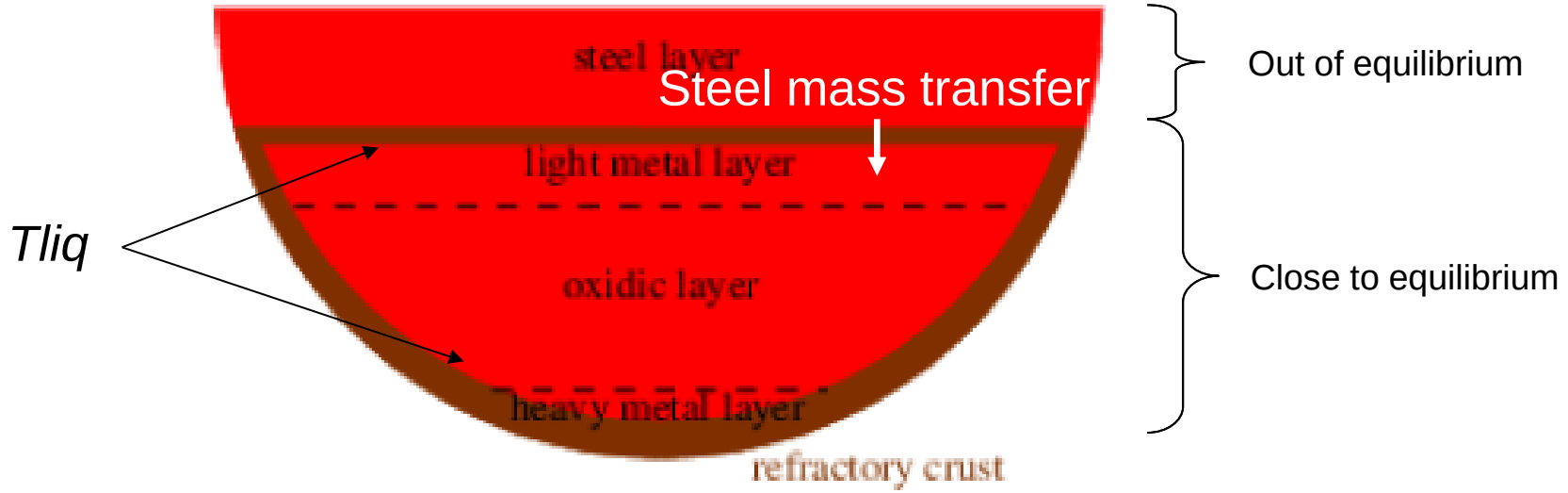
CEA/EDF teamwork: setup



CEA/EDF teamwork: codes PROCOR & MAAP (EDF)

- metal and oxide layers in equilibrium are surrounded by a refractory crust
- fast model providing compositions in equilibrium
- kinetic of inter-layer mass transfer
- out-of-equilibrium steel goes to the pool across the crust
- 0D mass and energy conservation equations of the layers



R. Le Tellier, L. Saas, S. Bajard, “Transient stratification modelling of a corium pool in a LWR vessel lower head”, to be submitted to Nuclear Engineering and Design

CEA/EDF teamwork: thermal modeling in codes based on 0D energy balance

- PROCOR $$mCp\frac{\partial T}{\partial t} = -\sum_j \frac{\partial m_j}{\partial t}\int_{T_j}^{T} Cp_j(T)dT + \sum_i Q_i + Q_v V$$

- MAAP (EDF) $$\frac{\partial H}{\partial t} = \sum_i F_i\left(\frac{H}{m}\right)_i + \sum_i Q_i + Q_v V$$

Where heat rate across interface *i* defined as $Q_i = S_i h_i (T_i - T)$

Thermal modelling relies on closure laws describing the layer boundary heat transfers in terms of Nusselt correlations for h_i coefficients. The choices of these correlations are based on an available experimental data base.

The vessel external cooling is out of scope due to the constant limit condition temperature T_{liq}.

CEA/EDF teamwork: first calculation

Initial **reactor case** code-to-code calculation showed many **divergences** of the results which are **difficult to explain** due to complexity of the reactor case.

Adapted strategy consists in **simplifying** the problem and carrying out a set of standalone calculations (**benchmarks**) with identical initial and limit conditions.

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Benchmarking

The basic concept is:

- To start from **simplest case** to identify the causes of **divergence**.
- To introduce specific user parameters in order to converge to **closest** best estimate **results**.
- To go on with more and **more complex** benchmark starting from the final “state” of the previous one.

Benchmarking

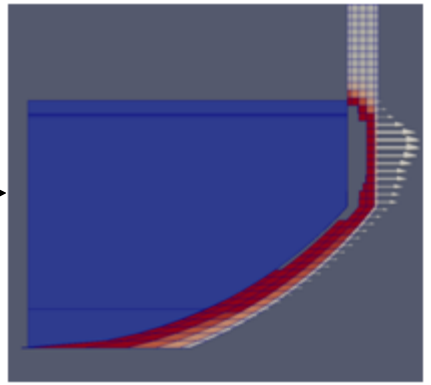
Advanced benchmark mode in MAAP developed at EDF

Used to create and to tune a complex initial pool configuration and to elaborate a transient scenario.

My_benchmark.exe

A separate FOTRAN code, governs the calculation calling MAAP's routines

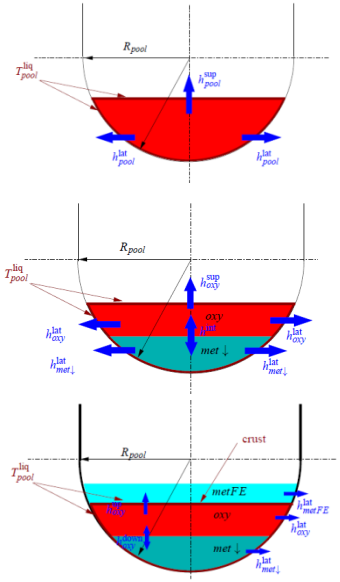
maaplib.so
MAAP compiled routines



Benchmarking: the studied cases

Three cases with increasing complexity with the last one being quite similar to the reactor case:

- Steady state of an initially liquid bulk oxide pool.
- Heating of an initially solid pool up to fusion and then thermal calculation of the resulting two-layers stratified pool up to steady state.
- Add-on of liquid steel over the top of the previous benchmark pool.



We deal with quasi steady state melt pool with different melt stratification configurations: the thickness of the layers, melt composition and the liquid temperature of the system stay constant.

No crust modelling has been involved.

Benchmarking: variables of interest and differences

The calculations have been carried out in such a way that it will be possible to estimate a maximum difference of variables of interest: heat rates Q^{lat} *and* Q^{sup} *and temperature* T_{pool} *.*

The differences between the results for a quantity of interest *G* between two series G_i and G_i^{ref} are defined as follows (*i* is the index referring to a common time grid t_i used for the comparison):

$$\varepsilon_{L_1} = \frac{\left\| (G_i - G_i^{ref})_i \right\|_{L_1}}{\left\| (G_i^{ref})_i \right\|_{L_1}} \quad \text{and} \quad \varepsilon_{L_\infty} = \frac{\left\| (G_i - G_i^{ref})_i \right\|_{L_\infty}}{\left\| (G_i^{ref})_i \right\|_{L\infty}}$$

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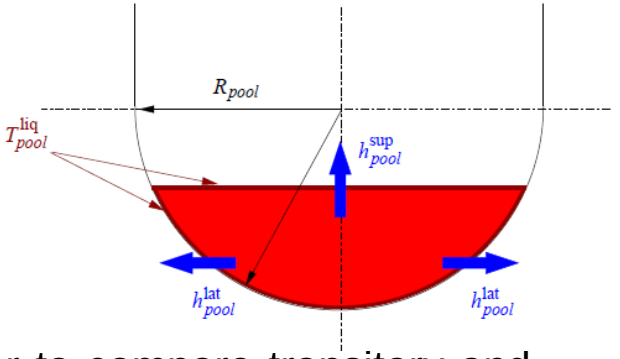
Benchmark1: bulk oxide pool

Statement

A bulk oxide pool is considered in a truncated spherical cap geometry.



Subjects of study:

- Oxide pool correlations
- Pool temperature T_{pool} calculation
- Physical properties sensibility

Method: The code-to-code calculations will be carried out in order to compare transitory and steady state pool temperatures as well as deviations related to the benchmark inputs variations. Firstly, we will realise the base case calculation. Secondly, we will run a set of complementary calculations with a variation of only only one parameter at each time to fulfil a sensibility study.

Base case properties and variations

	R_{pool}	m	Q_{pool}		ρ	Cp	λ	μ	β	$T°_{pool}$
Base case	1.84	$81.9 \cdot 10^{3}$	$15 \cdot 10^{6}$	2500	8600	570	6.3	$6 \cdot 10^{-3}$	$1 \cdot 10^{-4}$	2800
Variations	2.00	$73.7 \cdot 10^{3}$	$18 \cdot 10^{6}$	2600	8000	500	4.0	$8 \cdot 10^{-3}$	$2 \cdot 10^{-4}$	2900

Benchmark1: bulk oxide pool

Analytical solution to be compared with calculated temperature profile:

$$T_{pool} = T_{pool}^{0} \exp\left(-\frac{t}{\tau}\right) + \left(T_{pool}^{liq} + \frac{Q_{pool}}{(h^{lat}S^{lat} + h^{\sup}S^{\sup})}\right)\left(1 - \exp\left(-\frac{t}{\tau}\right)\right)$$

Original correlations

	PROCOR	MAAP (EDF)
Nu^{lat}	$0{,}131(Ra_i)^{0,25}\left(\frac{L_{pool}}{R_{eq}}\right)^{0,08}$	$0{,}131(Ra_i)^{0,25}\left(\frac{2L_{pool}}{3R_{pool} - L_{pool}}\right)^{\frac{19}{3}}$
Nu^{sup}	$0{,}381(Ra_i)^{0,234}$	$0{,}466(Ra_i)^{0,229}$

Benchmark1: results

Four calculations are compared:

- MAAP-INI – MAAP4EDF with original correlations
- MAAP-MOD – MAAP4EDF with oxide correlations from PROCOR
- PROCOR-INI – PROCOR with the state equation $\Delta H_{pool} = (m\ Cp\ \Delta T)_{pool}$
- PROCOR-MOD – PROCOR with the state equation from MAAP4EDF

Results: there is no notable impact due to differences in the correlations (case 1). Instead, the differences related to a state equation are more substantial (case 2).

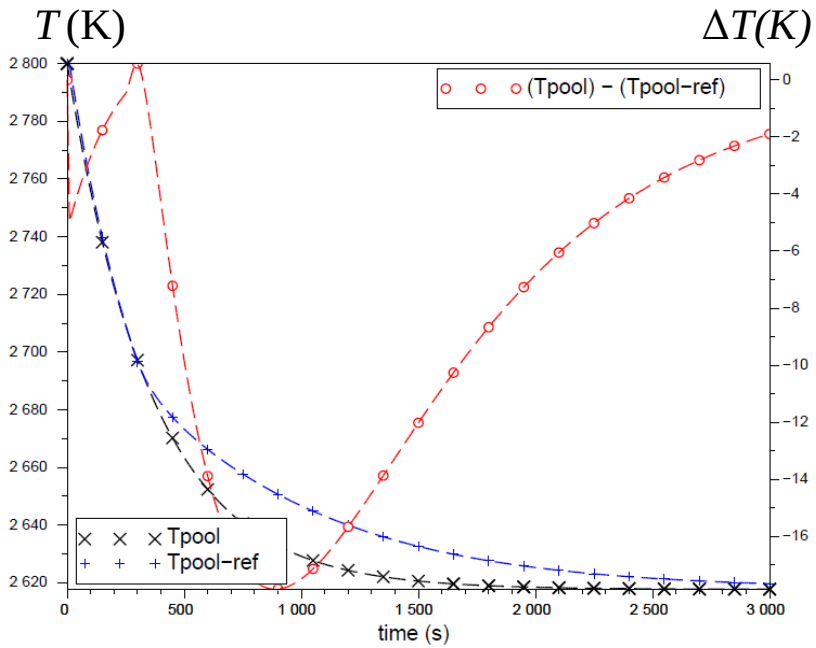
Maximal difference $\varepsilon_{L_1}(\varepsilon_{L_\infty})(\%)$

Case ↓	Variable of interest →	Q^{lat}	Q^{sup}	T_{pool}
1	MAAP-INI vs MAAP-MOD	2.22 (1.78)	2.24 (2.68)	0.04 (0.07)
2	**PROCOR-INI vs PROCOR-MOD**	**6.97 (7.45)**	**6.97 (7.45)**	**0.41 (0.77)**
3	MAAP-MOD vs PROCOR-MOD Best estimate	0.01 (0.04)	0.01 (0.04)	0.04 (0.28)

MAAP state equation has been put in PROCOR for further benchmarks. PROCOR correlations for oxide layer will be used in MAAP.

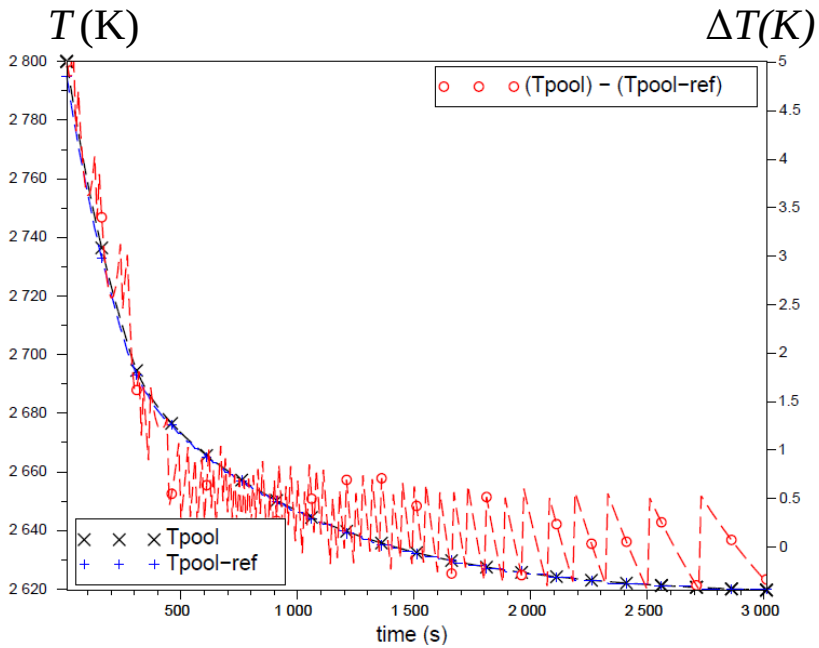
Benchmark1: results

Original state equations



PROCOR-MOD (Tpool-ref) vs PROCOR-INI (Tpool)

MAAP state equation used in both codes



PROCOR-MOD (Tpool-ref) vs MAAP-MOD (Tpool)

left scale : temperatures Tpool & Tpool-ref
right scale : difference of temperatures ΔT = (Tpool)-(Tpool-ref)

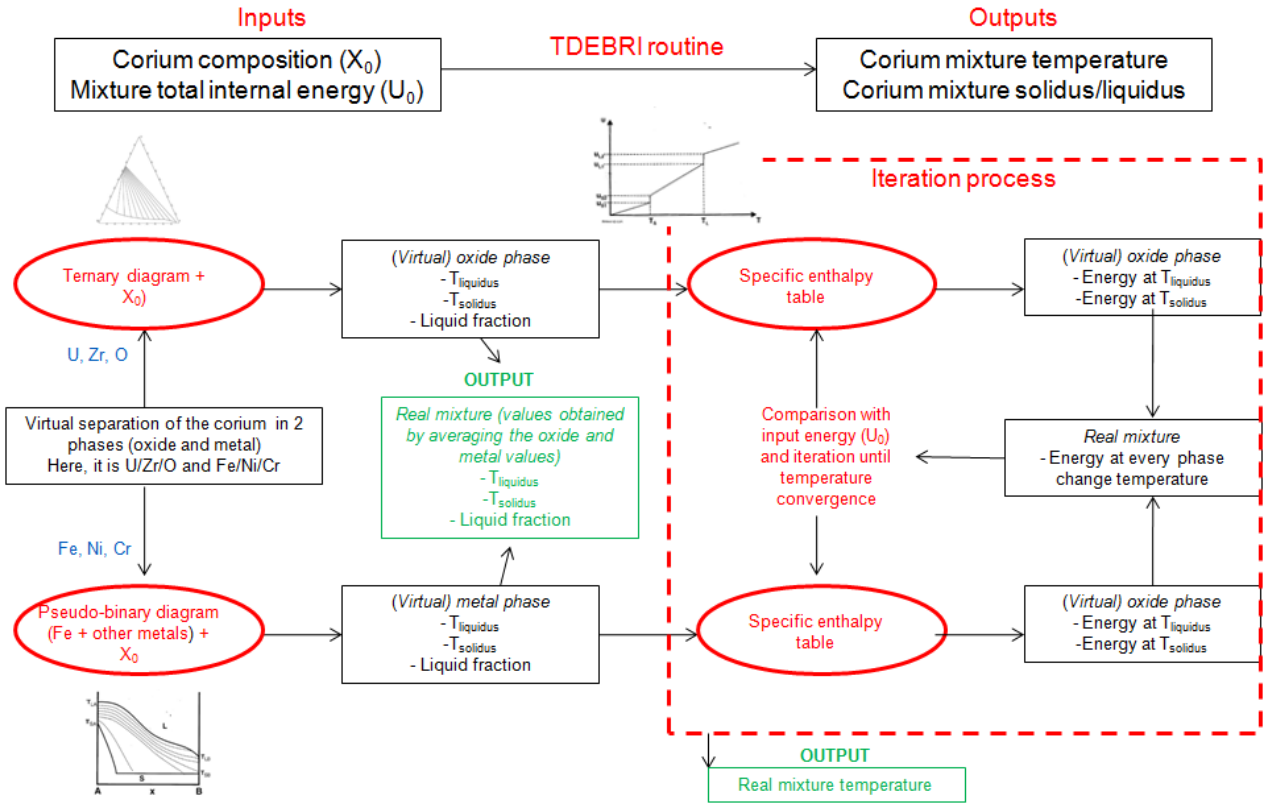
Pool temperature profile at T_{liq}=2500K

Benchmark1: state equation in MAAP

Pool is separated into oxide phase (combination of U-Zr-O, steel oxides and concrete slag oxides) and metallic one (B-C-Fe-Cr-Ni-Zr).

Ternary diagram(U, Zr, O) and pseudo-binary one (Fe + other metals) are used to get T_{liq}, T_{sol}, F_{sol} for each phase.

Iterative procedure is applied to link current pool enthalpy and temperature.

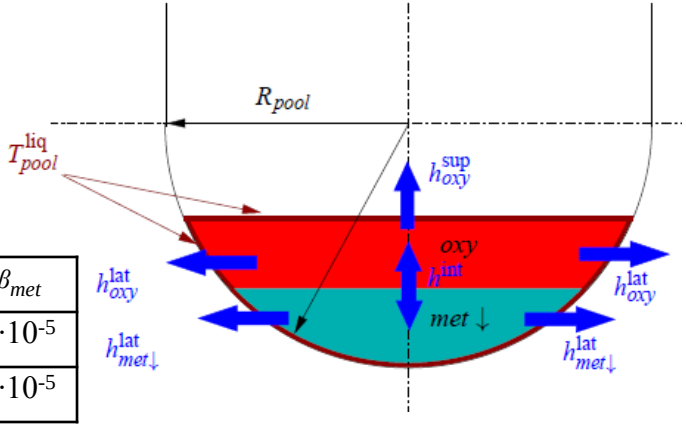


Benchmark2: two layer pool thermal exchange

Statement: An initially solid bulk pool is considered in the same truncated spherical cap geometry. It is assumed that the pool will separate into two layers when its average temperature T_{pool} reaches T_{liq}.

Initial pool parameters

R_{pool}	m	Q_{pool}		ρ	Cp	λ	μ	β	$T°_{pool}$
1.84	$81.9 \cdot 10^{3}$	$15 \cdot 10^{6}$	2500	8000	530	12	$1 \cdot 10^{-2}$	$2 \cdot 10^{-5}$	2000



base case properties and variations

	ρ_{oxy}	Cp_{oxy}	λ_{oxy}	μ_{oxy}	β_{oxy}	ρ_{met}	Cp_{met}	λ_{met}	μ_{met}	β_{met}
Base case	8000	510	7	10^{-2}	$3 \cdot 10^{-5}$	8400	530	35	10^{-2}	$4 \cdot 10^{-5}$
Variations	7600	600	5	$5 \cdot 10^{-3}$	$6 \cdot 10^{-5}$	9000	600	40	$5 \cdot 10^{-3}$	$6 \cdot 10^{-5}$

Subjects of study:

- Fusion delay
- Heavy metal correlations and inter layer interface condition
- Physical properties sensitivity for the heavy metal layer

Benchmark2: two layer pool thermal exchange

Original correlations for heavy metal layer

	PROCOR	MAAP4EDF
Nu^{lat}	BALI downward $0{,}131(Ra_i)^{0,25}(\frac{L_{pool}}{R_{eq}})^{0,08}$	Churchill & Chu $Gr > 10^9 : 0.15(Ra_e \sin(\Theta))^{1/3} / ((\frac{0.492}{\Pr})^{\frac{9}{16}} + 1)^{\frac{16}{27}}$ $Gr <= 10^9 : 0.68 \Pr^{0.25} (\Pr + \frac{20}{21})^{-0.25} (Ra_e \sin(\Theta))^{0.25}$
Nu^{sup}	Adiabatic	Globe-Dropkin $1 + 0.174 Ra_e^{\frac{1}{3}} \Pr^{0.074}$

The Churchill & Chu and Dlobe-Dropkin are original MAAP correlations for the metal layer. Their use for the heavy metal leads to an overestimated heat flux.

Alternative correlations to investigate →

Nu^{lat}	Nu^{sup}
BALI downward $0{,}131(Ra_i)^{0,25}(\frac{L_{pool}}{R_{eq}})^{0,08}$	Fieg & Werle $\max(1, 0.748 Ra_i^{0.127})$

Benchmark2: results

Four calculations are carried out:

- MAAP-INI – MAA4EDF with original correlations
- MAAP-MOD – MAA4EDF with Fieg & Werle and BALI downward correlations
- PROCOR-INI – PROCOR with adiabatic condition on the heavy metal oxide interface
- PROCOR-MOD – PROCOR with the same correlations and interface condition as MAAP-MOD

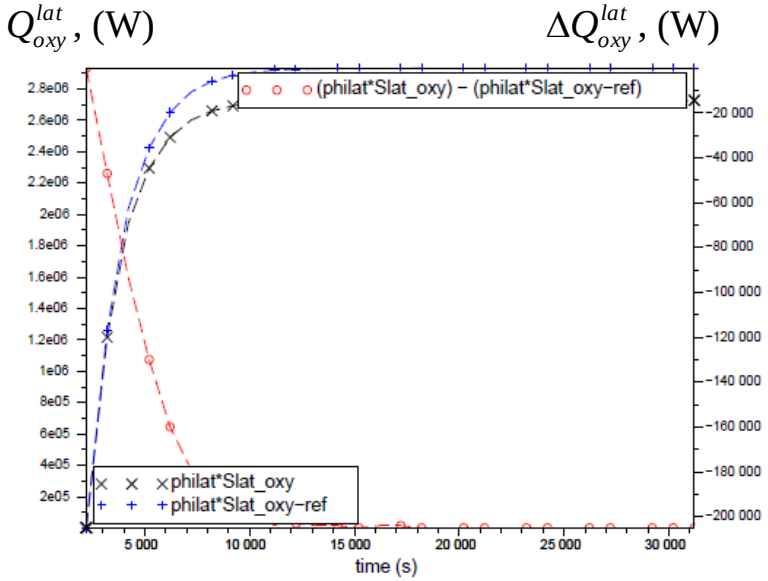
Maximal difference $\varepsilon_{L_1}(\varepsilon_{L_\infty})(\%)$

Variable of interest → / Case ↓		Q^{lat}	Q^{sup}	T_{pool}
1	**MAAP-INI vs MAAP-MOD**	**4.24 (6.84)**	**129.23 (122.27)**	**2.15 (2.24)**
2	PROCOR-INI vs PROCOR-MOD	3.76 (4.92)	100.00 (100.00)	0.12 (0.17)
3	MAAP-MOD vs PROCOR-MOD Best estimate	0.08 (0.10)	1.91 (2.09)	0.02(0.11)

The choice of correlation as well as a condition on the interface is the principal source of differences. The best estimated results (case 3) are very close => will be used in the next benchmark.

Benchmark2: results

Heat rates with original and best estimated correlations in MAAP



Oxide layer lateral heat rates

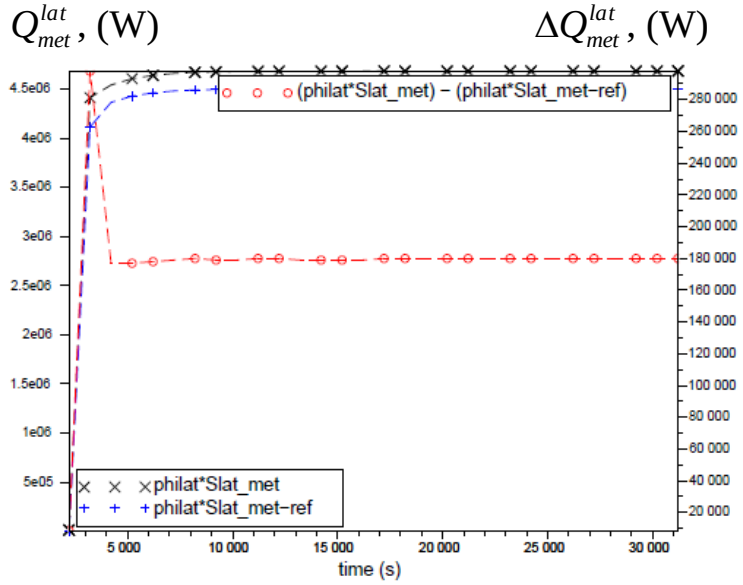
left scale:

Q^{lat}_{oxy} in MAAP-MOD = philat*Slat_oxy-ref

Q^{lat}_{oxy} in MAPP-INI = philat*Slat_oxy

right scale :

ΔQ^{lat}_{oxy} = (philat*Slat_oxy) -(philat*Slat_oxy-ref)



Heavy metal layer lateral heat rates

left scale:

Q^{lat}_{met} in MAAP-MOD = philat*Slat_met-ref

Q^{lat}_{met} in MAPP-INI = philat*Slat_met

right scale:

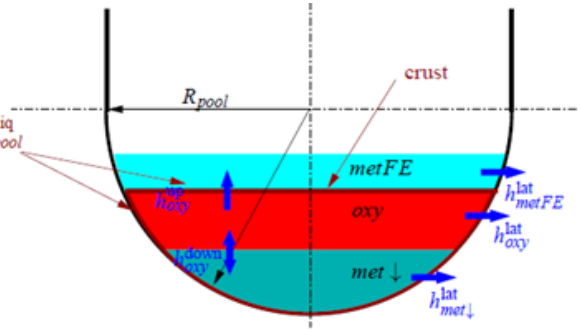
ΔQ^{lat}_{met} = (philat*Slat_met) -(philat*Slat_met-ref)

Benchmark3: three layer pool thermal exchange

Statement: This benchmark will be focused on the thermal exchange of the top steel layer (noted "*metFE*"). The starting point for this case is the steady state of the two layer pool from the previous benchmark with the addition of 10 t of steel.

Properties of the layers

	m	ρ	Cp	λ	μ	β	ε	T^0
Steel (metFE)	$10 \cdot 10^3$	6995	750	33	$5 \cdot 10^{-3}$	$3 \cdot 10^{-5}$	0.8	1800
Oxide (oxy)	$50.2 \cdot 10^3$	8000	510	7	$1 \cdot 10^{-2}$	$3 \cdot 10^{-5}$	0.9	2725.8
Heavy metal (met)	$31.7 \cdot 10^3$	8400	530	35	$1 \cdot 10^{-2}$	$4 \cdot 10^{-5}$	0.8	2631.2



Subjects of study:

- Steel layer correlations
- Calculation mode of h_{sup} for steel
- Heat radiation model

Method: No steel properties sensitivity is reported here. The transient calculations will be made in order to analyze the steel layer correlations as well as the upper interface condition. As for the other layers, the best estimated correlations above will be used.

Benchmark3: three layer pool thermal exchange

Original correlations for the steel layer

	PROCOR	MAAP4EDF
Nu^{lat}	Chawla & Chan $Gr > 10^{10} : \frac{0.16}{(1+(\frac{0.492}{\Pr})^{\frac{9}{16}})^{\frac{16}{27}}} Ra_e^{\frac{1}{3}}$ $Gr < 10^{8} : 0.508 \left(\frac{\Pr Ra_e}{\frac{20}{21}+\Pr} \right)^{\frac{1}{4}}$ Logarithmic interpolation in $10^8 \leq Gr \leq 10^{10}$	Churchill & Chu $Gr > 10^{9} : 0.15(Ra_e \sin(\Theta))^{1/3} / ((\frac{0.492}{\Pr})^{\frac{9}{16}}+1)^{\frac{16}{27}}$ $Gr <= 10^{9} : 0.68 \Pr^{0.25} (\Pr + \frac{20}{21})^{-0.25} (Ra_e \sin(\Theta))^{0.25}$
Nu^{sup}	Globe and Dropkin written for half of the layer thickness $1 + 0.174 Ra_{ext}^{\frac{1}{3}} \Pr^{0.074}$	Globe-Dropkin $1 + 0.174 Ra_e^{\frac{1}{3}} \Pr^{0.074}$

Benchmark3: three layer pool thermal exchange

Steel layer upper flux

MAAP: a flux between two parallel plans with emissivity ε_1 and ε_2 and the heat sink temperature T_{hs}

$$q^{sup}_{metFe} = \frac{1}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1} \sigma (T^{sup}_{metFe}{}^4 - T^4_{hs})$$

Emissivity
$\varepsilon_1 = \varepsilon_2 = 0.8$

$$\varepsilon_{metFe} = \frac{1}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1}$$

PROCOR: the emissivity to the black body

$$q^{sup}_{metFe} = \varepsilon_{metFe} \sigma (T^{sup}_{metFe}{}^4 - T^4_{hs})$$

Emissivity
$\varepsilon_{metFe} = 0.667$

Benchmark3: results

Four calculations were carried out:

- MAAP-INI – MAAP4EDF with original steel correlations
- MAAP-MOD – MAAP4EDF with steel correlations from PROCOR
- PROCOR-INI – PROCOR with T_{metFe}^{fus}, ε_{metFe} = 0.8
- PROCOR-MOD – PROCOR with T_{metFe}^{sup}, ε_{metFe} = 0.667

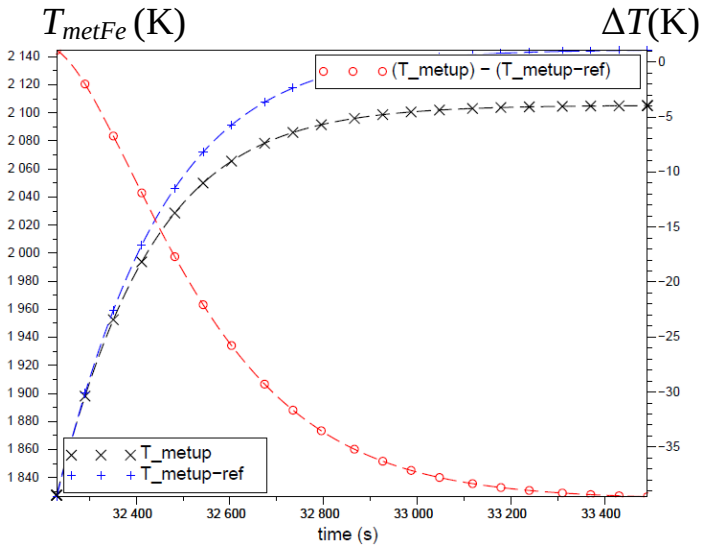
Differences $\varepsilon_{L_1}(\varepsilon_{L_\infty})(\%)$ in the steel layer relatives to PROCOR-MOD

Variable of interest → / Case ↓		Q^{lat}	Q^{sup}	T_{pool}
1	**MAAP-INI**	**20.70(18.87)**	**11.42(13.25)**	**1.39(1.84)**
2	PROCOR-INI	3.76(4.55)	4.79(4.52)	0.4(0.58)
3	MAAP-MOD Best estimate	0.01(0.13)	0.01(0.13)	0.01(0.06)

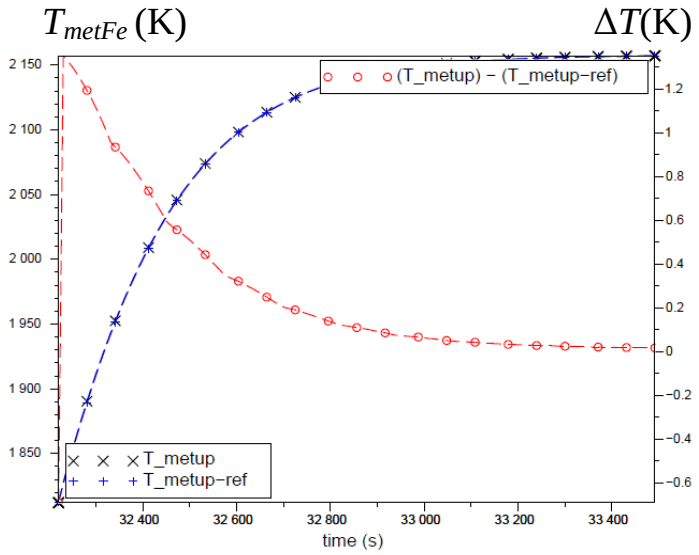
The choice of correlation is the principal source of differences.

Benchmark3: results

Temperature difference rises up to the 40K due to the different correlations. In the best estimated case, the maximum deviation is close to zero.



PROCOR-MOD (T_metup-ref) vs MAAP-INI (T_metup-ref)



PROCOR-MOD (T_metup-ref) vs MAAP-MOD (T_metup)

left scale : temperatures T_metup & T_metup-ref
right scale : temperature difference ΔT = (T-metup)-(T_metup-ref)

Temperatures of the steel layer *metFe*

Outline

- Context and issues
- Original corium pool modeling in MAAP4 and MAAP5
- Advanced corium modeling
- CEA/EDF teamwork
- Benchmarking
- Results
- **Conclusions**

CONCLUSIONS

Despite the key elements of the modelling shared by the codes, the calculation results could be quite different due to other specific code approaches. Such a unitary **benchmarking** approach makes it possible to **identify the sources of difference**.

In this first set of benchmark dedicated to the thermal modelling of a stratified corium pool, the **differences** are essentially due to the **heat transfer correlations**, the **enthalpy equation of state** and the **physical properties** data.

Necessary **adjustments** have been carried out in the codes in order to converge to close results. As a result, two **best estimate** versions (MAAP-MOD and PROCOR-MOD) are now available and could be used in the **future benchmark programme** which can contain **more complex** cases including a simultaneous heat and mass exchange.

Beyond the validation itself, a development of a **coherent equation-of-state** (EOS) in enthalpy has been identified as **medium-term objective** of research in order to replace the original EOS of MAAP in which supposed phase compositions do not match the miscibility gap conditions.

Thank you for your attention