Numerical Modeling of Leading-Edge Ceramic Oxidation in Inductively Coupled Plasma Facility

Vincent Le Maout*, Matthew Konnik, Alison E. Rzepka, Francesco Panerai, and Kelly Stephani

Materials for Hypersonic Applications and Extreme Environments
Illinois University at Urbana-Champaign (UIUC)
Illinois, USA

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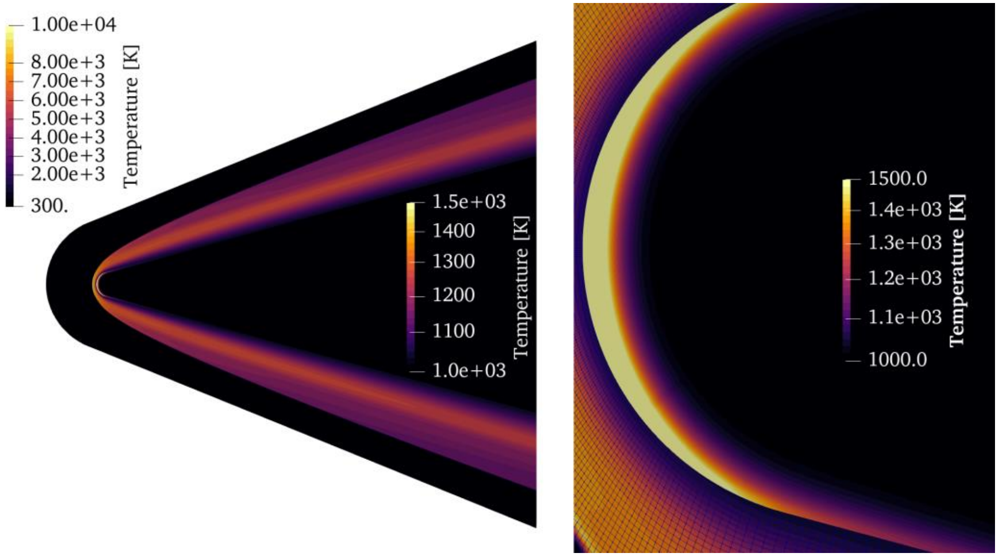
Ablation Workshop
November 9th-10th 2022

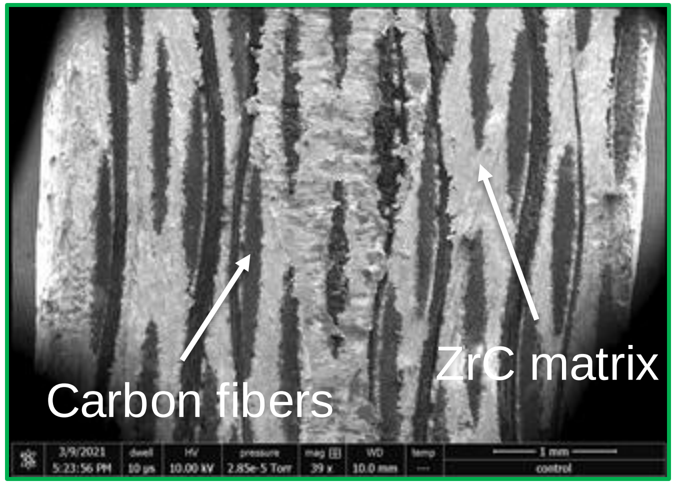
Ceramics Usage for Hypersonic Applications

Thermal Protection Systems for atmospheric reentry necessitates high temperature and stress resistance.



Hypersonic reentry simulation at **Mach 26**.

C/ZrC ceramics composite



Scanning Electron Microscopy

Furnace experiment in an oxygen rich environment

Medium temperature : powdered oxide layer

High temperature : dense oxide layer

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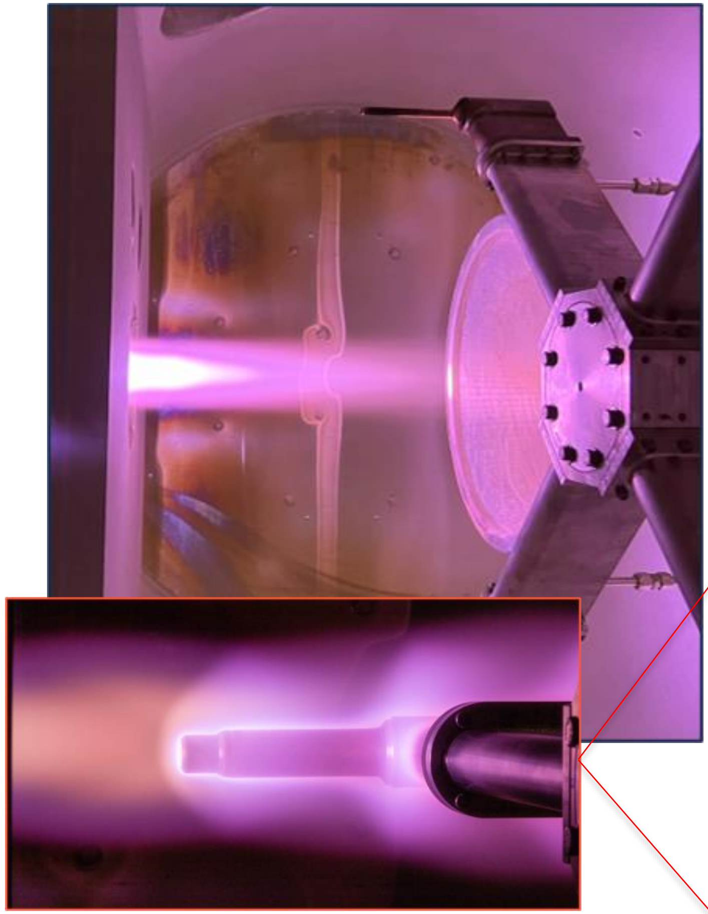
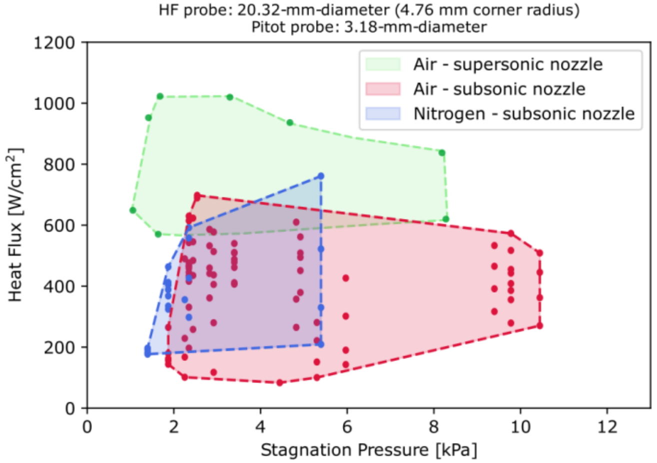
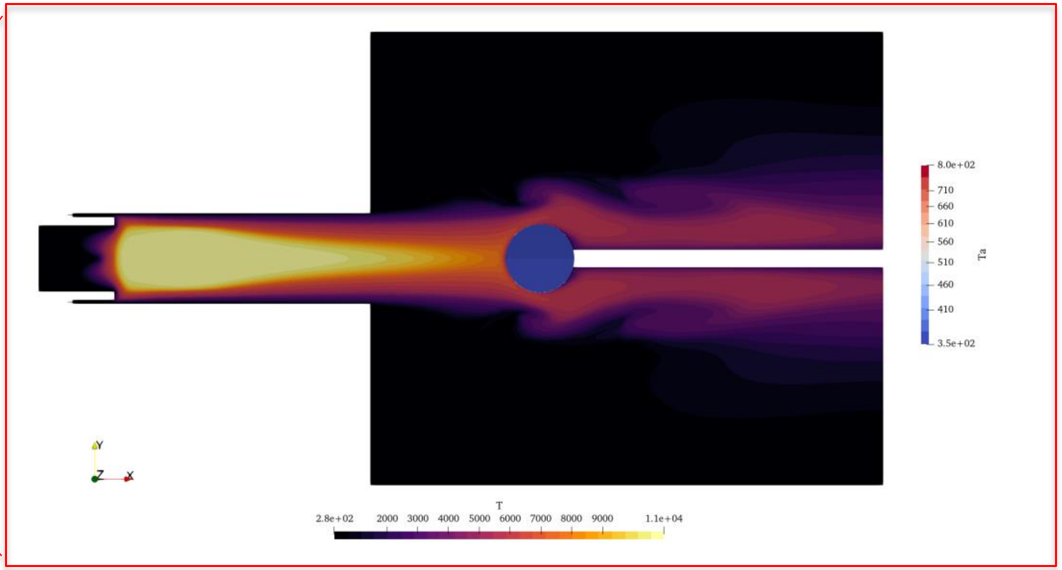
Thermal Protection System Testing



- **Inductively Coupled Plasma** (ICP) technology
- **350 kW** Radio-Frequency Generator (2.1 MHz)
- **Maximum performances:**
  - Mach 4
  - Stagnation Enthalpies up to 36 MJ/kg
  - Pressure up to 5 bar



Specification overview of some materials testing facilities



Digital tween of ICP experiment (Non-Equilibrium Flow) 2D axisymmetric

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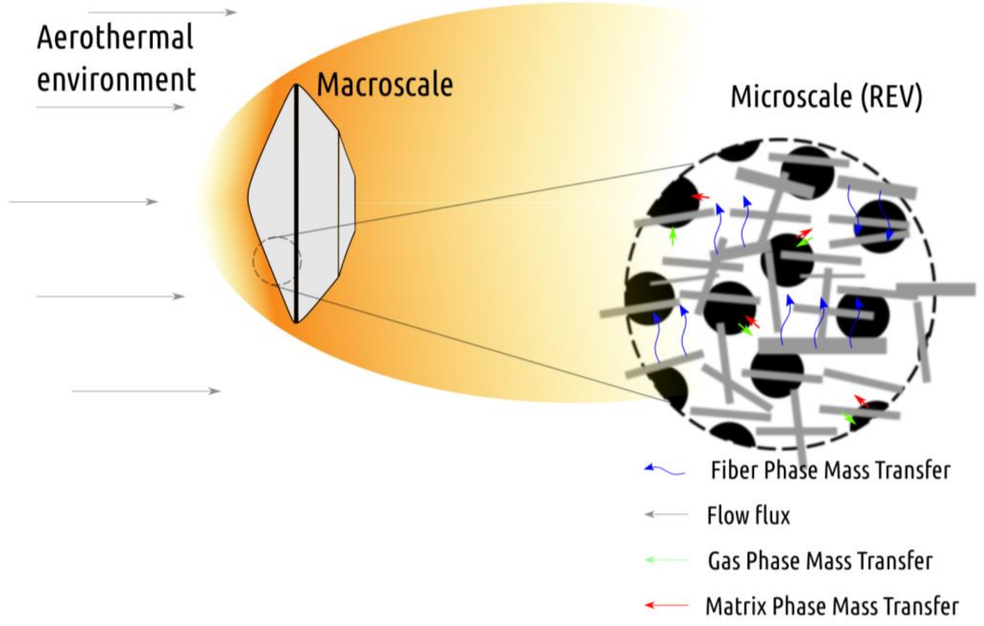
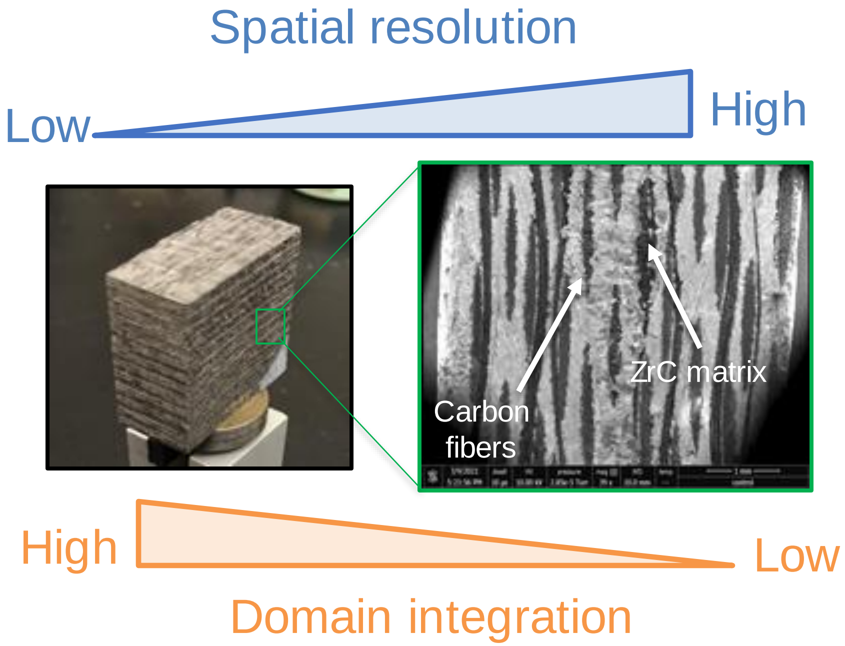
CMC Thermophysical Model



Thermal Protection Systems for atmospheric reentry necessitates high temperature and stress resistance.

The **design of protection material** is critical to assess the **safety** of the **payload**.



Simulation of Material Response in Aerothermal Environment necessitates :

- Ablation arbitrary number of solid phases,
- Heterogeneous mass exchange,
- Gas species diffusion through the material,
- Global mass and energy conservation.

How to leverage the loss of information on large scale modelling ?

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Multiscale Description of TPS

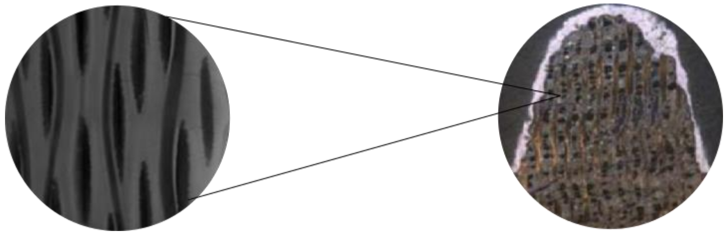
Detailed microscopic mass, momentum and energy balance at the scale for the **Representative Elementary Element** (REV)

$$< x^p >= \frac{1}{V_{REV}} \int_{D^p} x^p \, dV \quad \forall p \in \mathcal{P}$$

Mathematical Average of microscale governing equations on the **REV**

Microscale

Macroscale



x^p

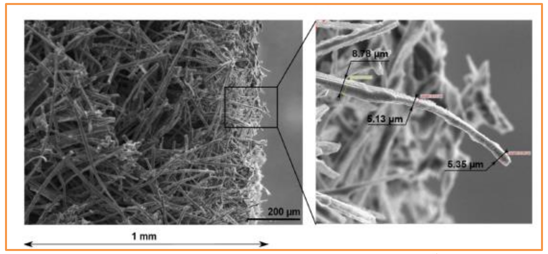
Explicit property

$< x^p >$

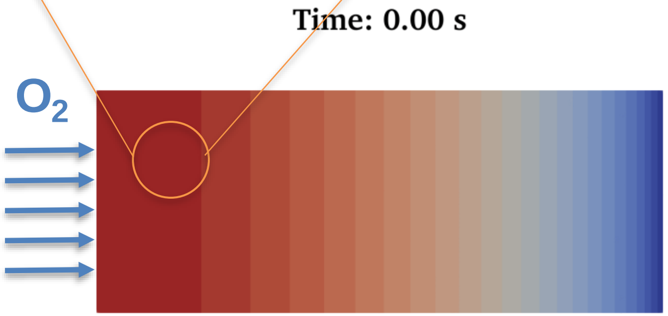
Averaged property

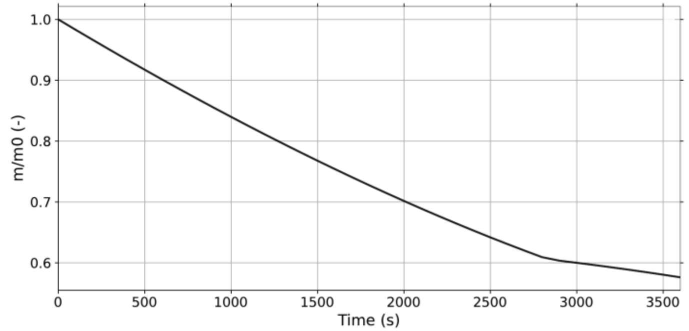
Numerical approximation of resulting **PDE** on the **domain of interest**

Multiscale ablation of carbon fibers

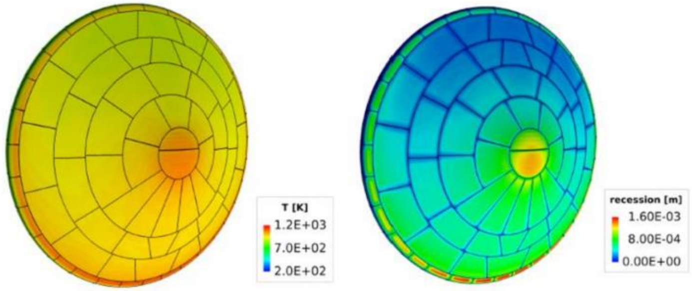


Cylindrical Shrinkage Fiber Model





e.g., Thermochemical simulation of MSL heatshield [1] :



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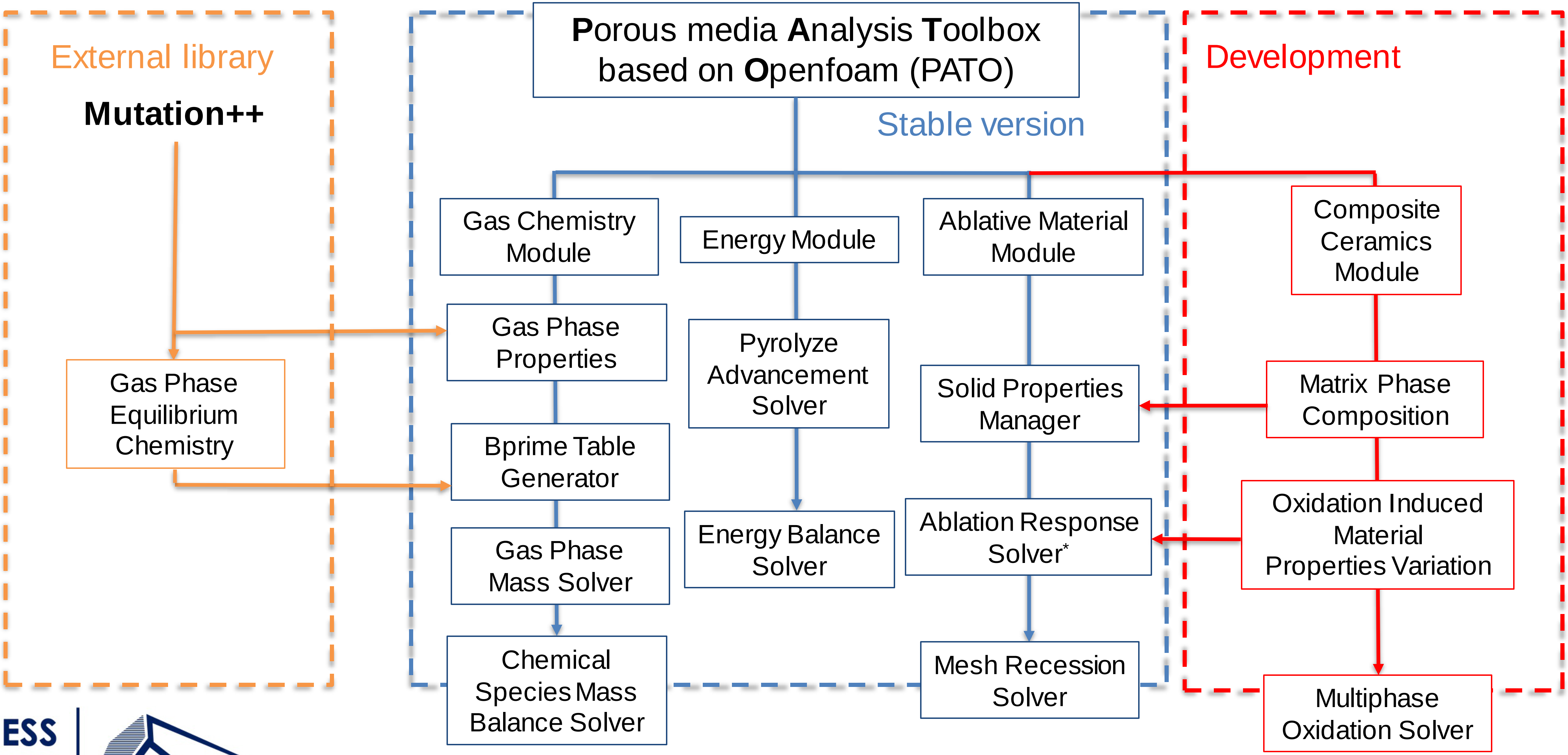
[1] Jeremie B.E. Meurisse *et al.*, Multidimensional material response simulations of a full-scale tiled ablative heatshield, Aerospace Science and Technology, Volume 76, 2018

PATO code overview



*Concern only carbon fiber shrinkage module

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Mathematical Model for Reactive Porous Ceramics

Mass Conservation in the Gas phase :

- The perfect gas law is assumed for the gas phase $\bar{\rho}^g = \dfrac{\bar{p}^g R T^g}{M^g}$
- Velocity of gas is computed using the Darcy-Klinkenberg law $\bar{\mathrm{v}}^g = -\dfrac{1}{\epsilon^g}\left(\dfrac{\mathrm{K}^g}{\mu^g} - \dfrac{\beta}{\bar{p}^g}\right)\nabla \bar{p}^g$
- This allow to define the mass conservation equation of the phase solely as a function of pressure :

$$\frac{\partial}{\partial t}\left(\epsilon^g \frac{\bar{p}^g R T^g}{M^g}\right) - \nabla\cdot\left(\frac{\bar{p}^g R T^g}{M^g}\left(\frac{\mathrm{K}^g}{\mu^g} - \frac{\beta}{\bar{p}^g}\right)\nabla \bar{p}^g\right) = \sum_{ns=1}^{N_s} \underbrace{\left(\theta^{ns}\sum_{k}^{\mathrm{I}_g} \dot{\omega}_k^{g,ns}\right)}_{\text{Heterogeneous reactions for all solid phases}}$$

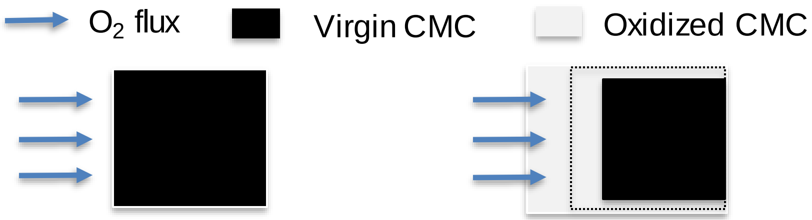
- And for gas species k :

$$\frac{\partial}{\partial t}\left(\epsilon^g (\rho^g y_k^g)^{\bar{g}}\right) + \nabla\cdot\left(\epsilon^g (\rho^g y_k^g)^{\bar{g}} \mathrm{v}^{\bar{g}}\right) - \nabla\cdot\underbrace{\left(\mathrm{D}^g_{k\,\mathrm{eff}}\nabla(\rho^g y_k^g)^{\bar{g}}\right)}_{\text{Diffusion in porous media}} = \underbrace{\epsilon^g \dot{\omega}_k^{\bar{g}}}_{\text{Homogeneous reactions}} + \sum_{ns=1}^{N_s}\underbrace{\left(\theta^{ns}\dot{\omega}_k^{g,ns}\right)}_{\text{Heterogeneous reactions}}$$

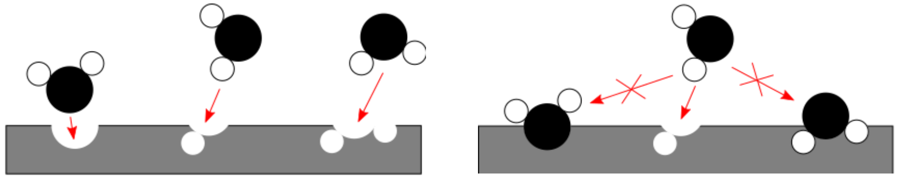
PATO Oxidation Solver Extension

Accounting for **multiphase oxidations** necessitates to extend **heterogenous reactions solver** to keep track of **gas/surface interactions and their effect on solid mass balance.**

Oxidation of CMC

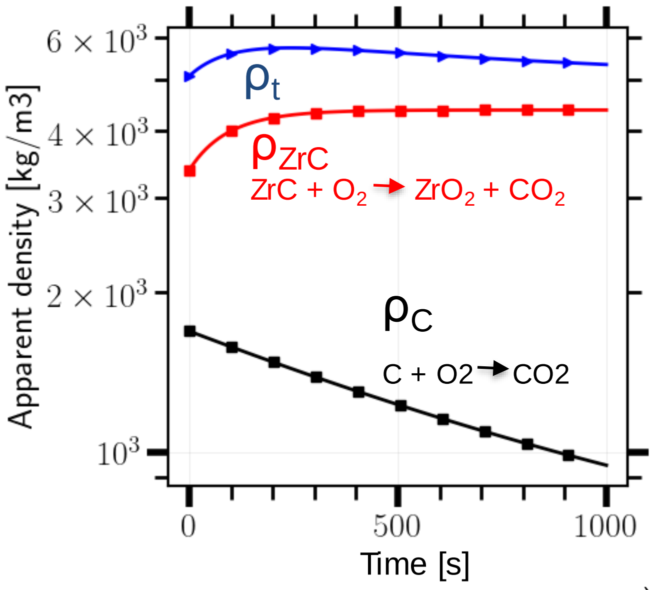


Example : adsorption on a surface

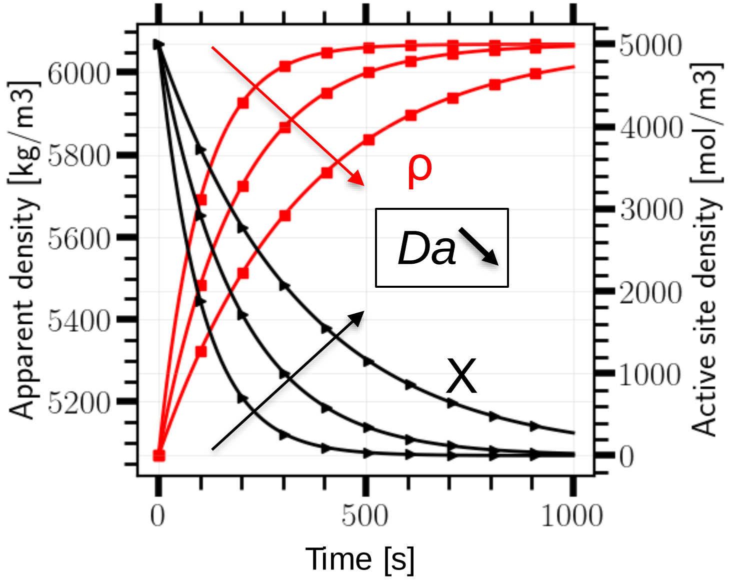


Depths of O2 penetration is a competitive process between diffusion and surface reactivity measured by the number *Damköhler*:

OD composite oxidation



OD oxidation regime



Heterogeneous source term :

$$\frac{\dot{\omega}_k^{g,ns}}{M_k} = \sum_{r=1}^{N_r} \left(\underbrace{k_r^f (\nu''_{r,k} - \nu'_{r,k}) \Pi_{j=1}^{I_g \cup I_{ns}} (x_j^{g,ns})^{\nu'_{r,j}}}_{\text{mass production by forward reaction}} - \underbrace{k_r^b (\nu''_{r,k} - \nu'_{r,k}) \Pi_{j=1}^{I_g \cup I_{ns}} (x_j^{g,ns})^{\nu''_{j,r}}}_{\text{mass destruction by backward reaction}} \right)$$

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Mathematical modelling

Energy Conservation in the porous media :

– Thermal Equilibrium is supposed to hold in the entire domain $T^g = T^{ns} \quad \forall ns \in [1, N_s]$

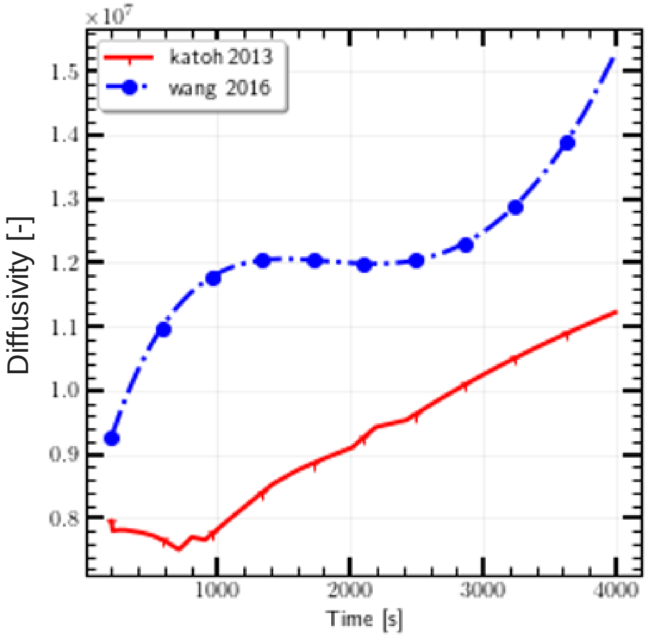
– The conduction parameter is an average of gas and solid phases thermal properties

$$\underbrace{\sum_{ns=1}^{N_s} \left(\epsilon^{ns} \rho^{ns} c_p^{ns}\right) \partial_t T}_{\text{Temperature time variation (heat storage) in solid phases}} + \underbrace{\partial_t \left(\epsilon^g \rho^g h^g - \epsilon^g p^g\right)}_{\text{Energy time variation in gas phase}} - \underbrace{\nabla \cdot \left(\underline{\lambda} \nabla T\right)}_{\text{Heat conduction}} + \underbrace{\nabla \cdot \left(\epsilon^g \rho^g h^g \mathrm{v}^g\right)}_{\text{Heat convection}} - \nabla \cdot \underbrace{\sum_{k}^{\mathrm{I}_g} \left(\mathrm{D}_{k,\mathrm{eff}}^g \nabla (\rho^g y_k^g)^{\bar{g}} h_k^g\right)}_{\text{Heat diffusion}} = \underbrace{\dot{E}_\Omega + \bar{h}\pi_{tot}}_{\text{Heat source}}$$

Material and Gas Phase Properties :

– Material parameters are function of pressure, temperature and pyrolysis rate

– Gas transport properties are computed using Mutation++



Wei, X. *et al.*, Zirconium Carbide Produced by Spark Plasma Sintering and Hot Pressing: Densification Kinetics, Grain Growth, and Thermal Properties. *Materials* **2016**, *9*, 577.

Katoh, Y. *et al.*, Properties of zirconium carbide for nuclear fuel applications. Journal of Nuclear Materials, **2013**, 741, 1.

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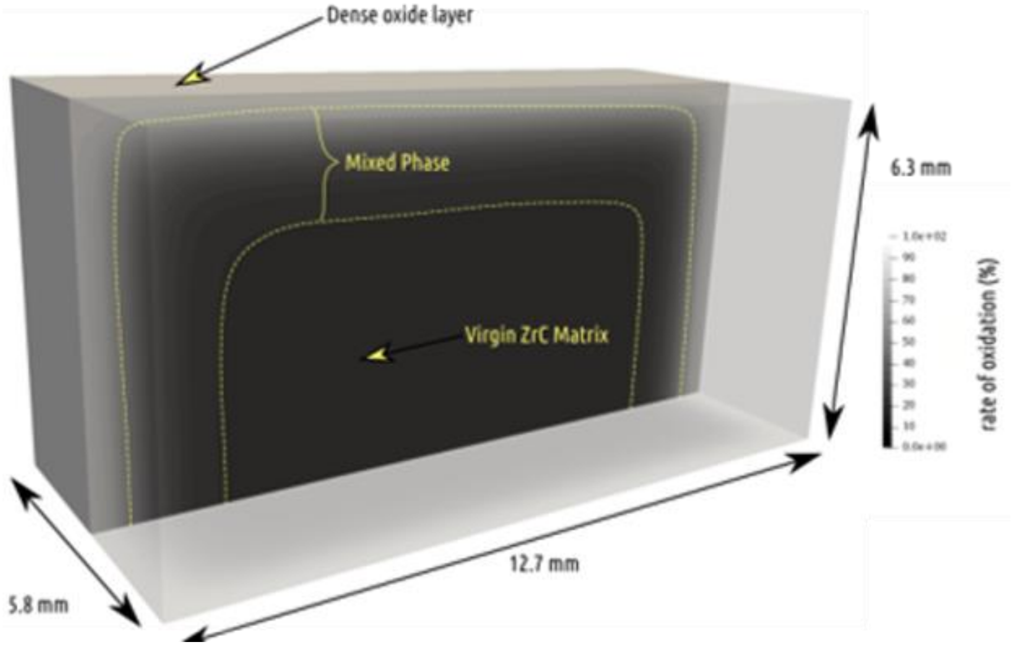
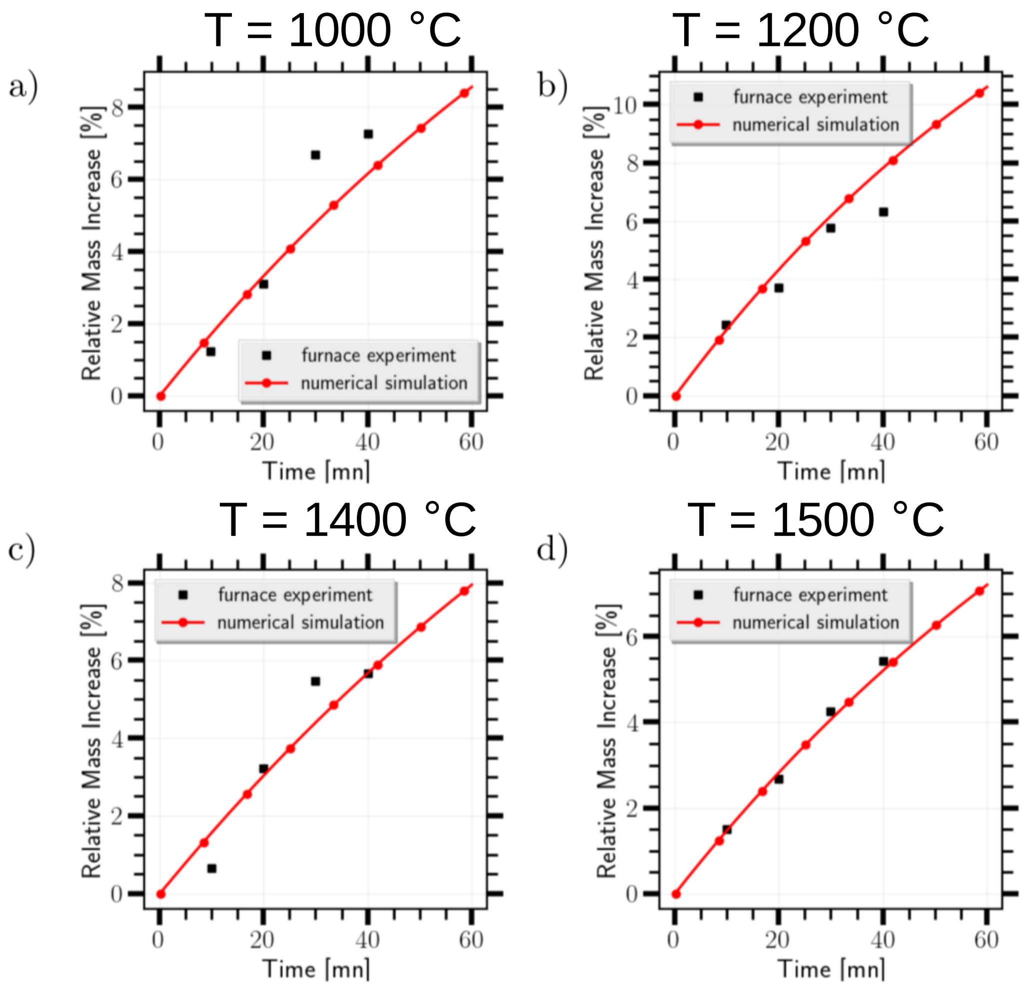
Multidimensional Oxidation

The model is applied to **predict the mass variation of pure ZrC ceramics** exposed to constant **high temperature at atmospheric pressure environment**.

Oxidation of ZrC ceramics at 1400 °C after 20mn

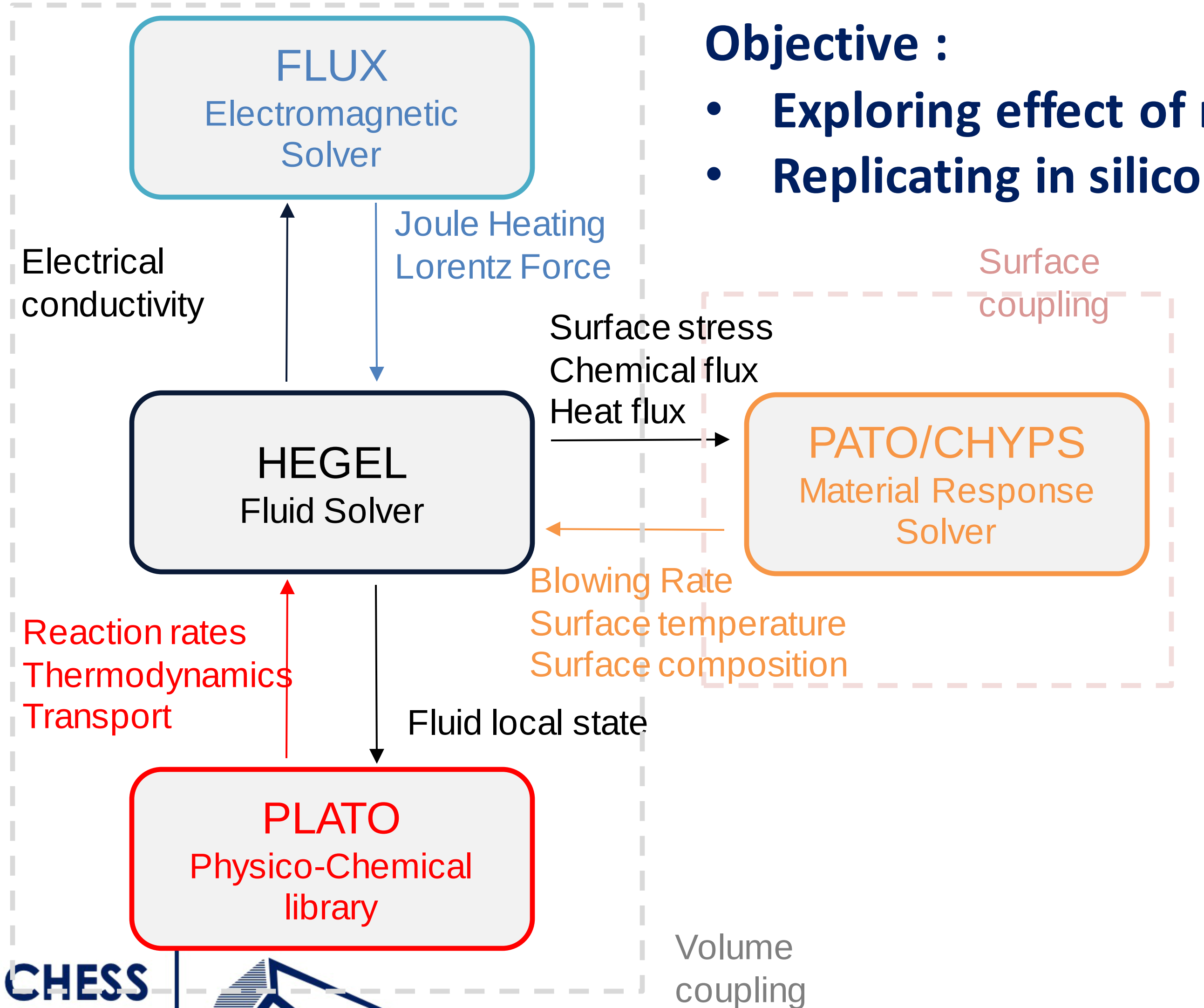




Kinetics rate are obtained from re-characterization of Rama Rao oxidation :

$ZrC + 2O_2 => ZrO_2 + CO_2$

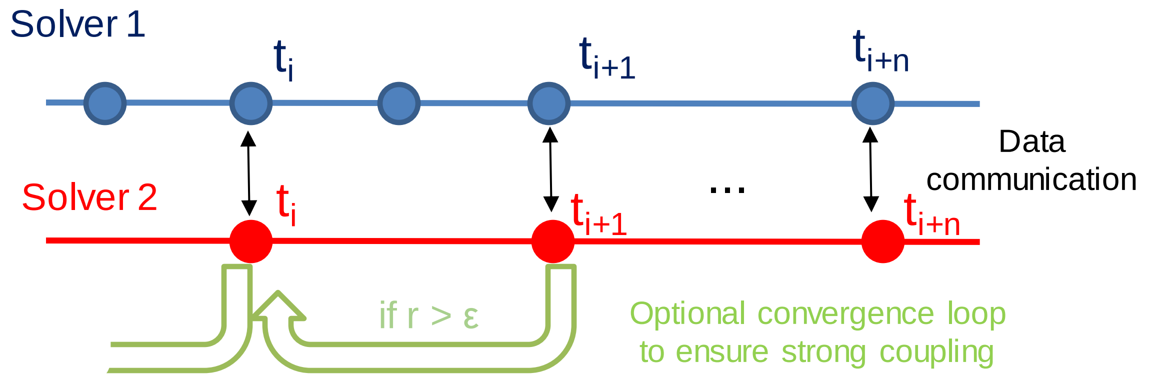
CHESS Numerical Program for Multi-Solver Coupling



Objective :

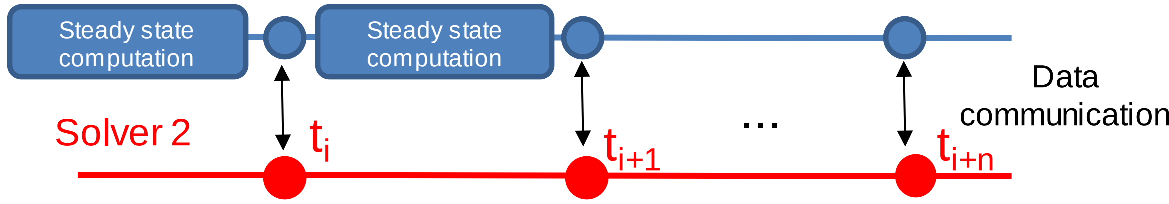
- **Exploring effect of material response on aerothermal environment,**
- **Replicating in silico experimental facility for code validation.**

Time accurate simulation :



Steady Simulation

Solver 1 (successive steady state – time is only for synchronization)



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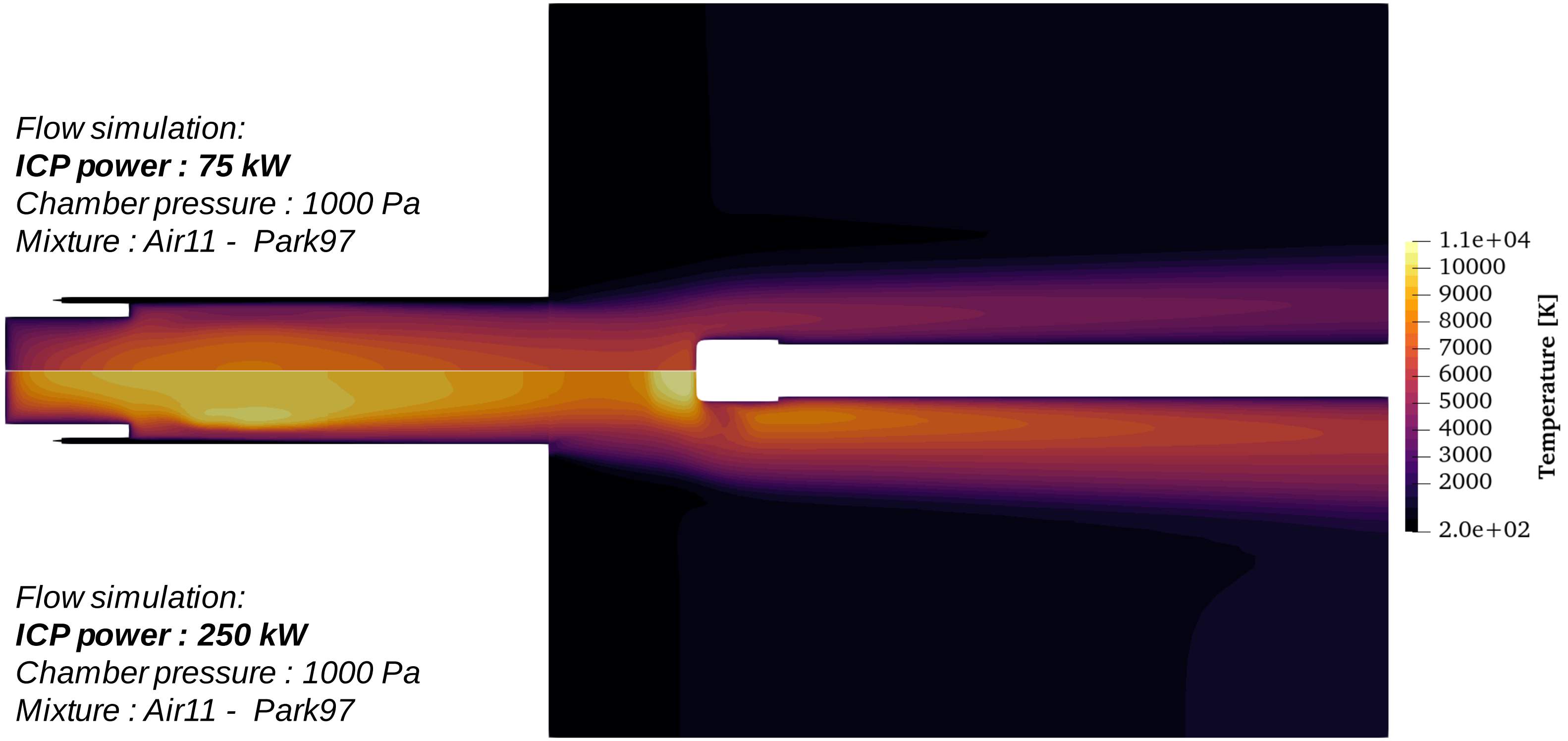
Oxidation in Inductively Coupled Plasma Facility

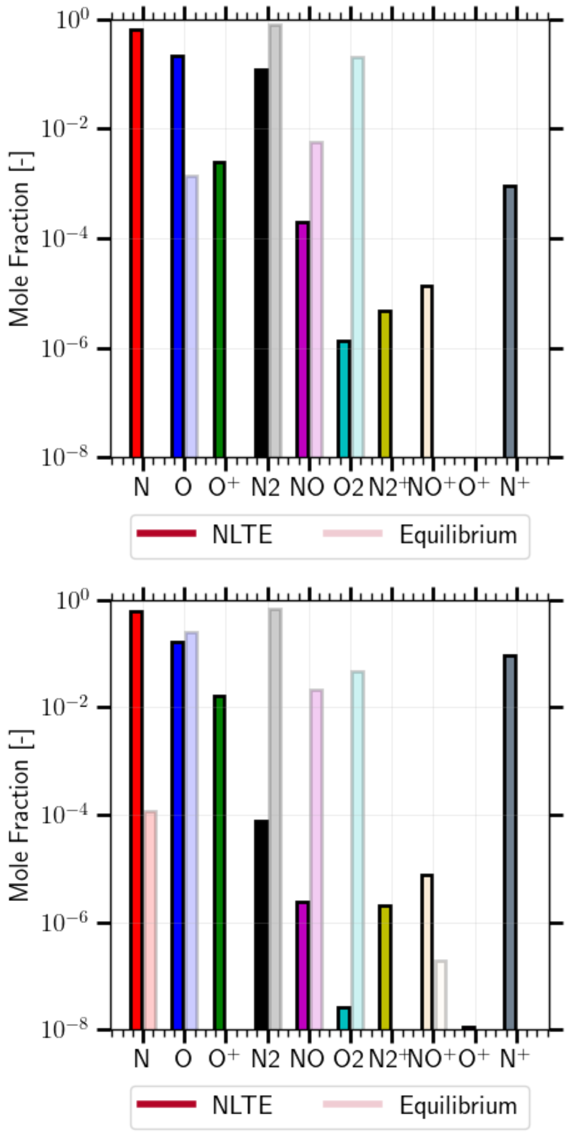
The numerical experiments have shown the sensitivity of material response on oxidation rate. **How numerical simulations can help to characterize this parameter ?**

Characterizing aerothermal environment :

Flow simulation:
ICP power : 75 kW
Chamber pressure : 1000 Pa
Mixture : Air11 - Park97



Flow simulation:
ICP power : 250 kW
Chamber pressure : 1000 Pa
Mixture : Air11 - Park97



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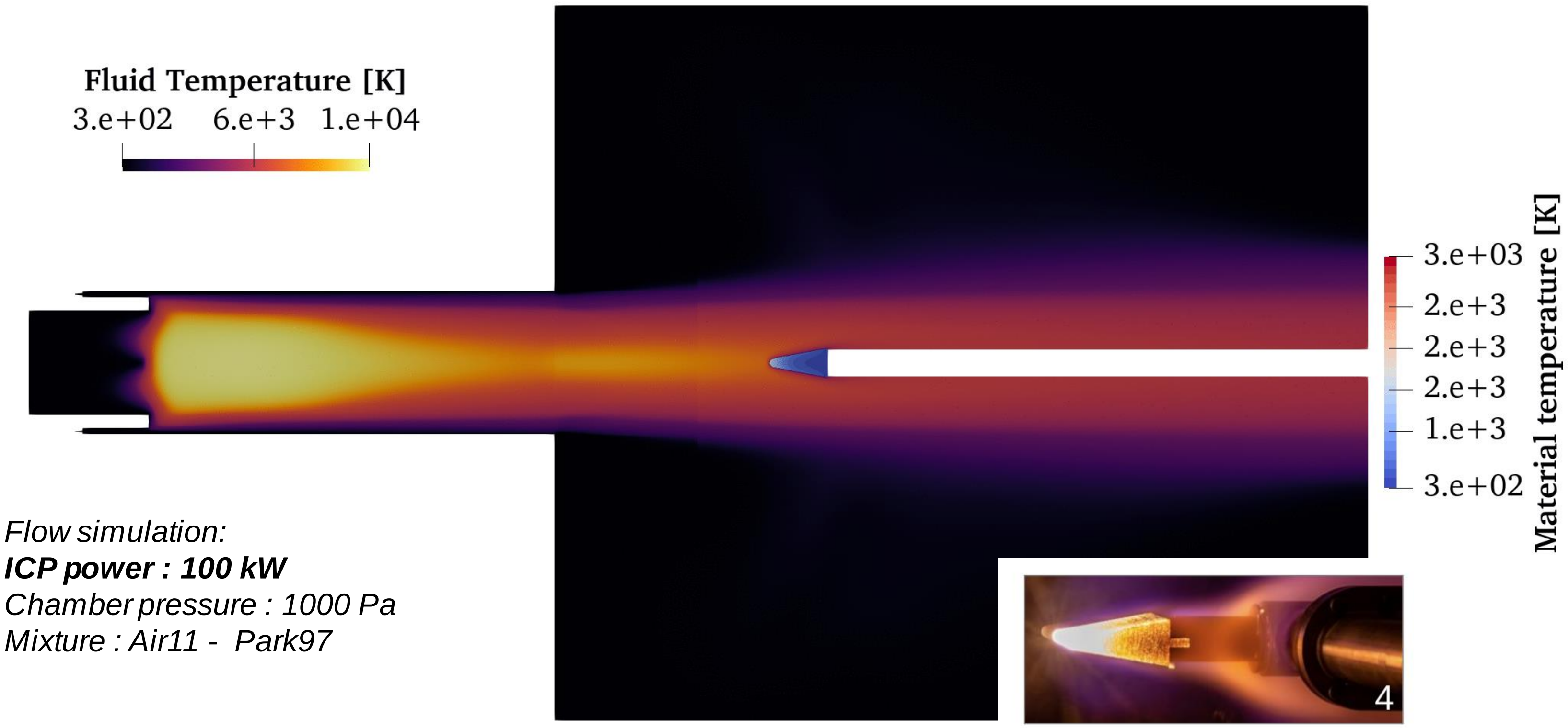
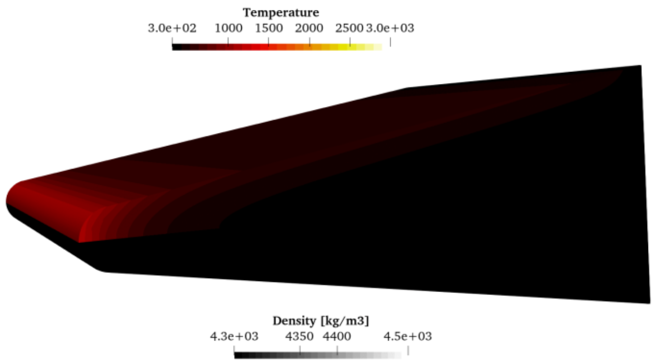
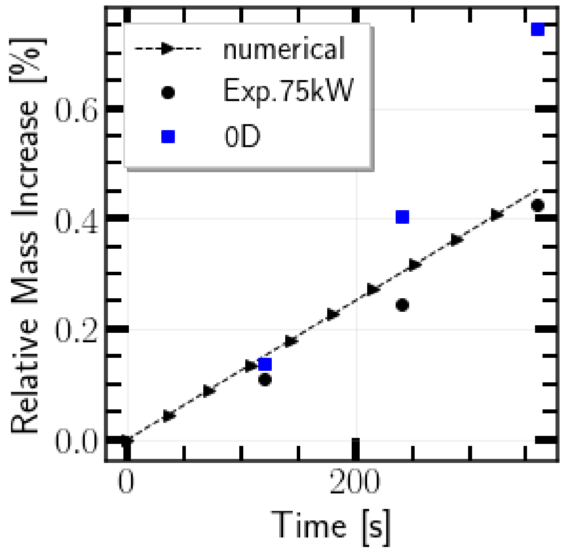
Wedge Probe Geometry

The **developed framework** has then been applied to **study material response in ICP flow experiments**:



Flow simulation:
ICP power : 100 kW
Chamber pressure : 1000 Pa
Mixture : Air11 - Park97





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Conclusion & Perspectives

Studies of UHTCs at UIUC as lead to :

- Experimental structural characterization of material (µCT, XRD surface analysis),
- Oxidation kinetics characterization of ceramics in isobar isothermal furnace experiments,
- Adaptation of ablation module within PATO numerical frameworks for numerical modelling.

Short and mid-term objectives :

- Characterization of UHTC thermo-physical response inside ICP facility,
- Comparison with numerical model developed in UIUC,
- Development of microscale model oxidation model using SPARTA DSMC code to enable multiscale modelling.

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Thank you for your attention ! Any questions ?