Numerical simulation of Laser Ignition of Metallic Rods under Oxygen Pressure

PhD Thesis (2023-2026) - Samy TOUZOUIRT

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Outlines

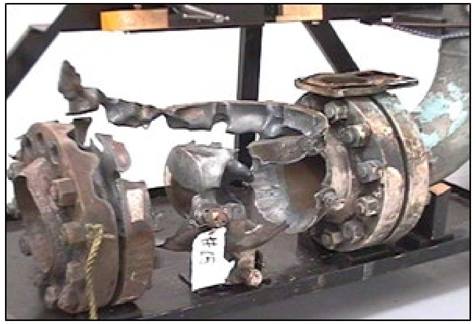
- Context of the study.
- Multiphysical Model.
- Primary results.
- Discussion.
- Conclusion and perspectives.

CONTEXT

- The ability of metals to sustain or not a self-sustaining combustion in a pure oxygen atmosphere is essential to the design of oxygen systems. In order to classify metals according to this ability, the **standard test method ASTM G124-18** has been developed and is widely used.

- The goal of this thesis is to first develop a multiphysical model to be used as a numerical equivalent for the standard ASTM test. A second part will include sensitivity calculations in order to determine which parameters controls the combustion process, these parameters will then be estimated using a dual experimental/numerical approach and implemented into the numerical model for its experimental validation.

Before



After

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MODEL

Heat transfer

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p(\vec{u}.\vec{\nabla}T) - \vec{\nabla}.(k\vec{\nabla}T) = (q_{abs} - q_{loss}).\delta + S$$

Hydrodynamics

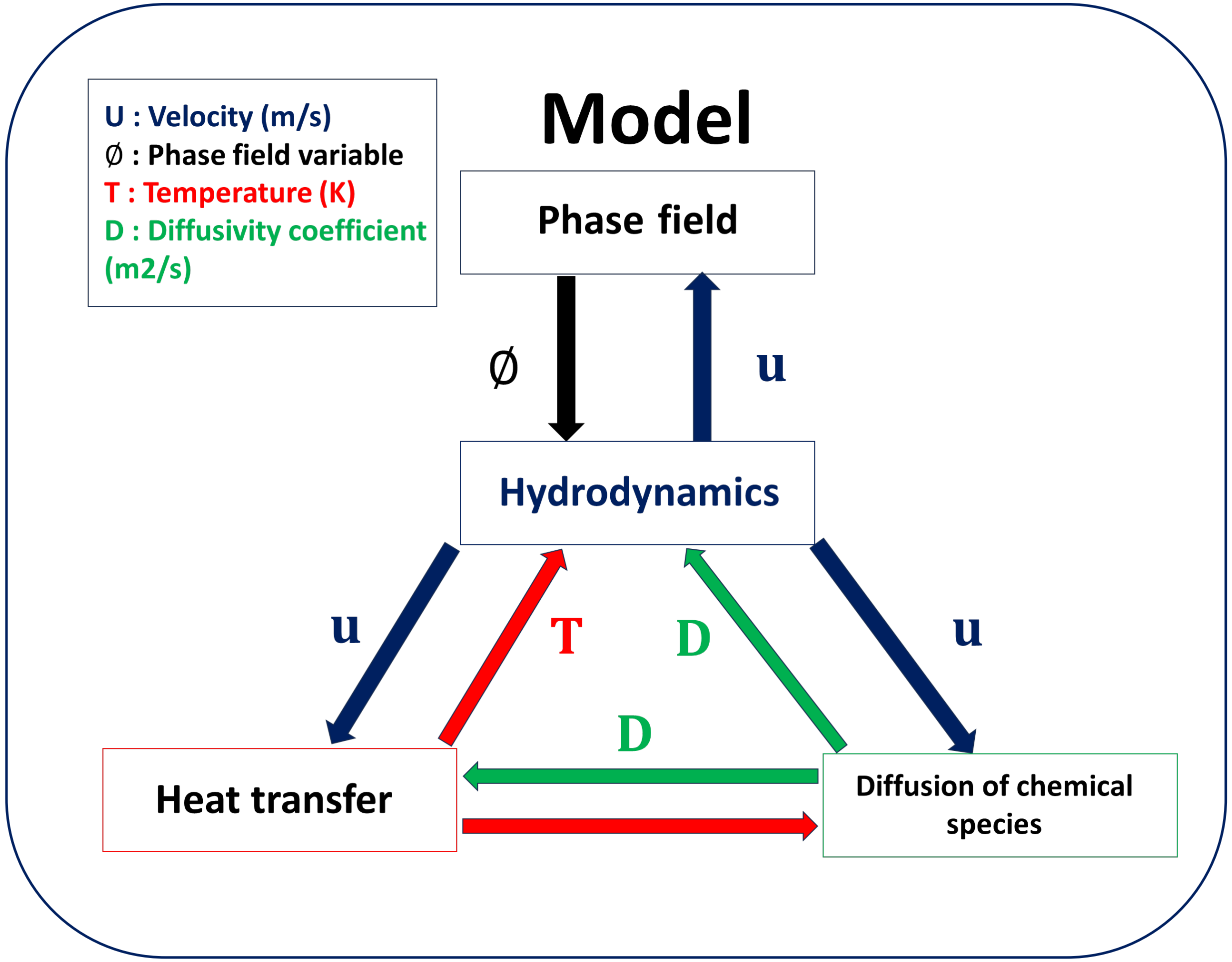
$$\rho\frac{\partial\vec{u}}{\partial t} + \rho(\vec{u}.\vec{\nabla})\vec{u} = \vec{\nabla}.(-p\bar{\bar{I}} + \bar{\bar{K}}) + \vec{F} + \rho\vec{g}\beta(T - T_{fus})$$

Diffusion of chemical species

$$\frac{\partial c}{\partial t} + \vec{\nabla}.\vec{j} + \vec{u}.\vec{\nabla}c = R$$

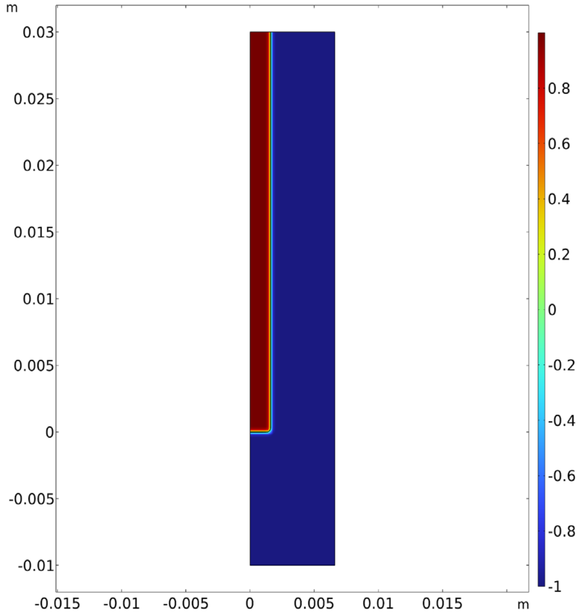
Phase-field

$$\begin{cases} \dfrac{\partial \emptyset}{\partial t} + \vec{u}.\vec{\nabla}\emptyset = \vec{\nabla}.\left(\dfrac{3}{2\sqrt{2}}\sigma\epsilon\chi\vec{\nabla\Psi}\right) \\ \psi = -\vec{\nabla}.(\epsilon^2\vec{\nabla}\emptyset) + (\emptyset^2 - 1)\emptyset \end{cases}$$

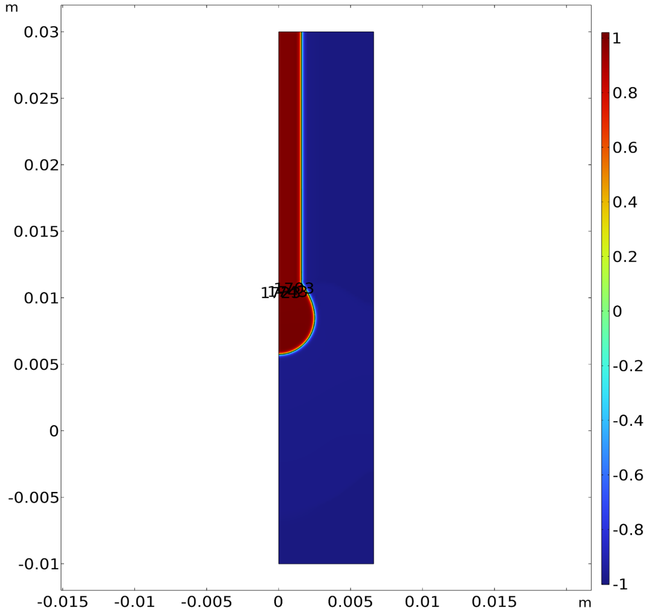


RESULTS

Model evolution

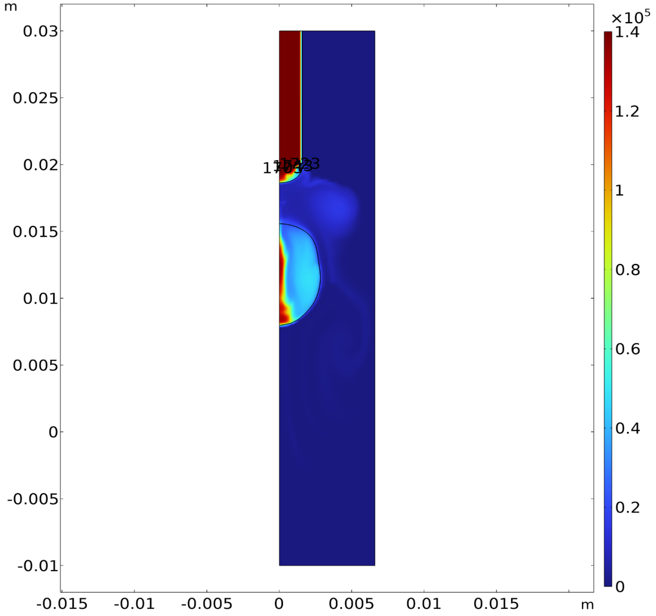


Phase Field + **Heat Transfer**



Phase Field + **Heat Transfer**

Fluid flow



Phase Field + **Heat Transfer**

Fluid flow

Oxydation

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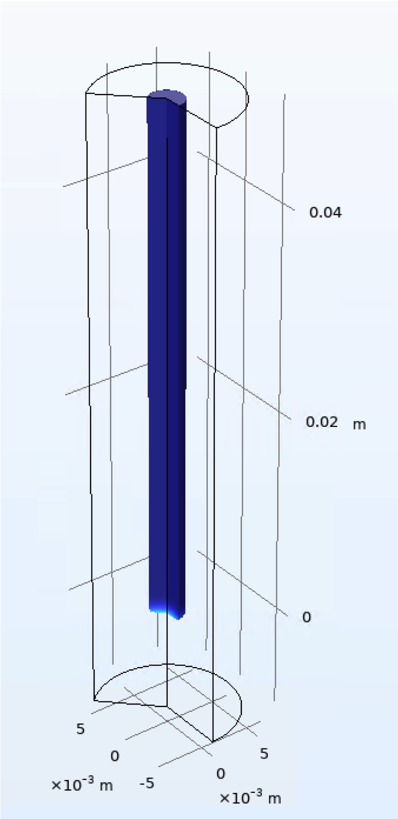
RESULTS

- **Simulation results for the rod combustion model**

❖ Accurate reproduction of the rod combustion process.

❖ Good management of the morphological changes of the interface, including the drop formation and detachment.

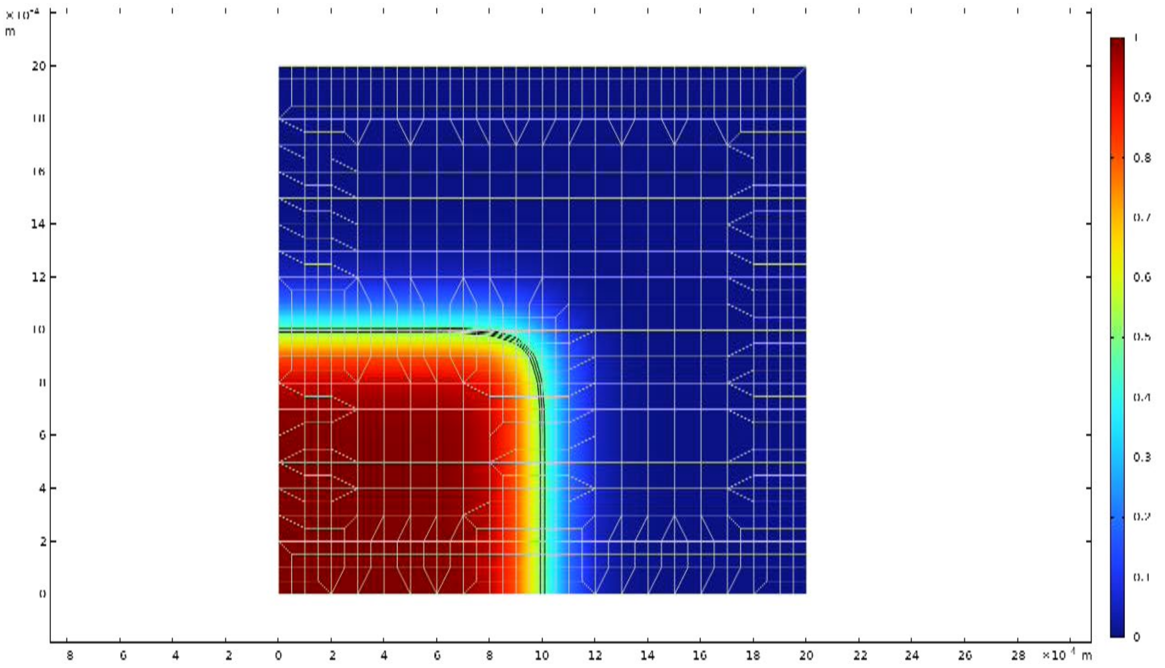


Numerical simulation of metallic rod combustion

RESULTS

Droplet model

- Low calculation Costs.
- Easily validated experimentally.
- Particularly useful for the characterization of oxidation and parameter estimation.



Numerical simulation of the droplet model

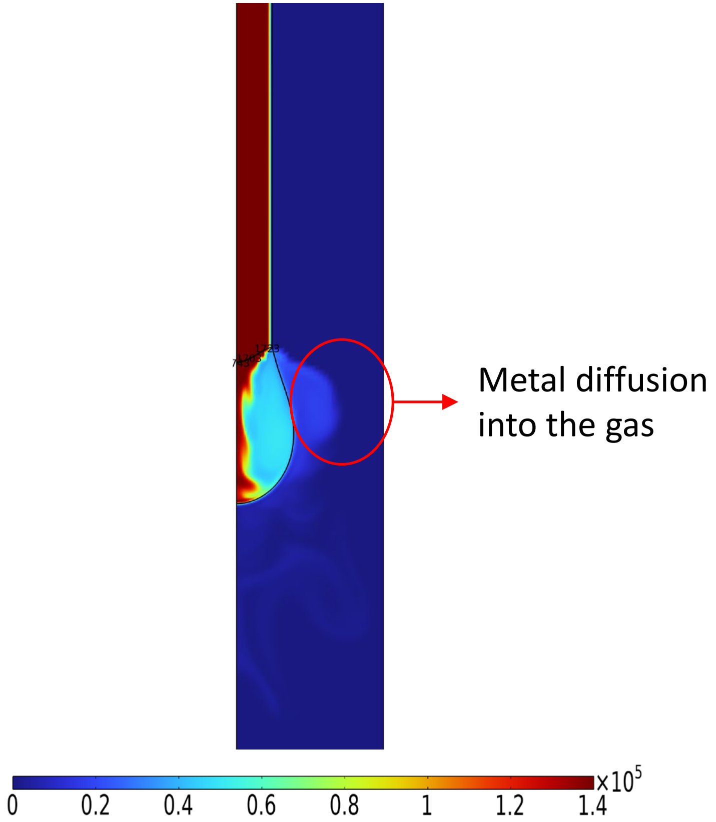
DISCUSSION

Non-physical diffusion of metal inside the gas

- Formulation of the diffusivity coefficients using phase indicators (pf.VF1 and pf.VF2)

$$D = (D_{metal} \cdot Pf.VF_1) + (D_{gas} \cdot Pf.VF_2)$$

- The use of numerical penalties to restrict the oxydation reaction to the metal only



Pure iron concentration field

CONCLUSION

Conclusion

- ❖ The Eulerian Phase-Field approach is well suited for our application as it reproduces accurately the rod combustion process.
- ❖ The process includes a high number of parameters and requires thus sensitivity calculations to determine which paremeters are of major interest.
- ❖ The droplet model is more suited for sensitivity calculation and parameter estimation.
- ❖ A more detailed formulation is needed for the diffusitivity coefficients to avoid non-physical diffusion.

Next Steps

- ❖ The development of a complete formulation for the diffusivitiy coefficients including the solubility and other oxydation kinetics.
- ❖ Implementation of a second conditionned phase field representative of the apparition of the oxyde.
- ❖ Carriyng out sensitivity calculations and parameter estimation using a dual numerical/experimental approach.
- ❖ Experimental validation of the numercial model using the estimated parameters.

THANK YOU FOR YOUR ATTENTION

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