Numerical modeling of impurities mass transfer in a wire wrapped fuel assembly under flowing lead bismuth eutectic

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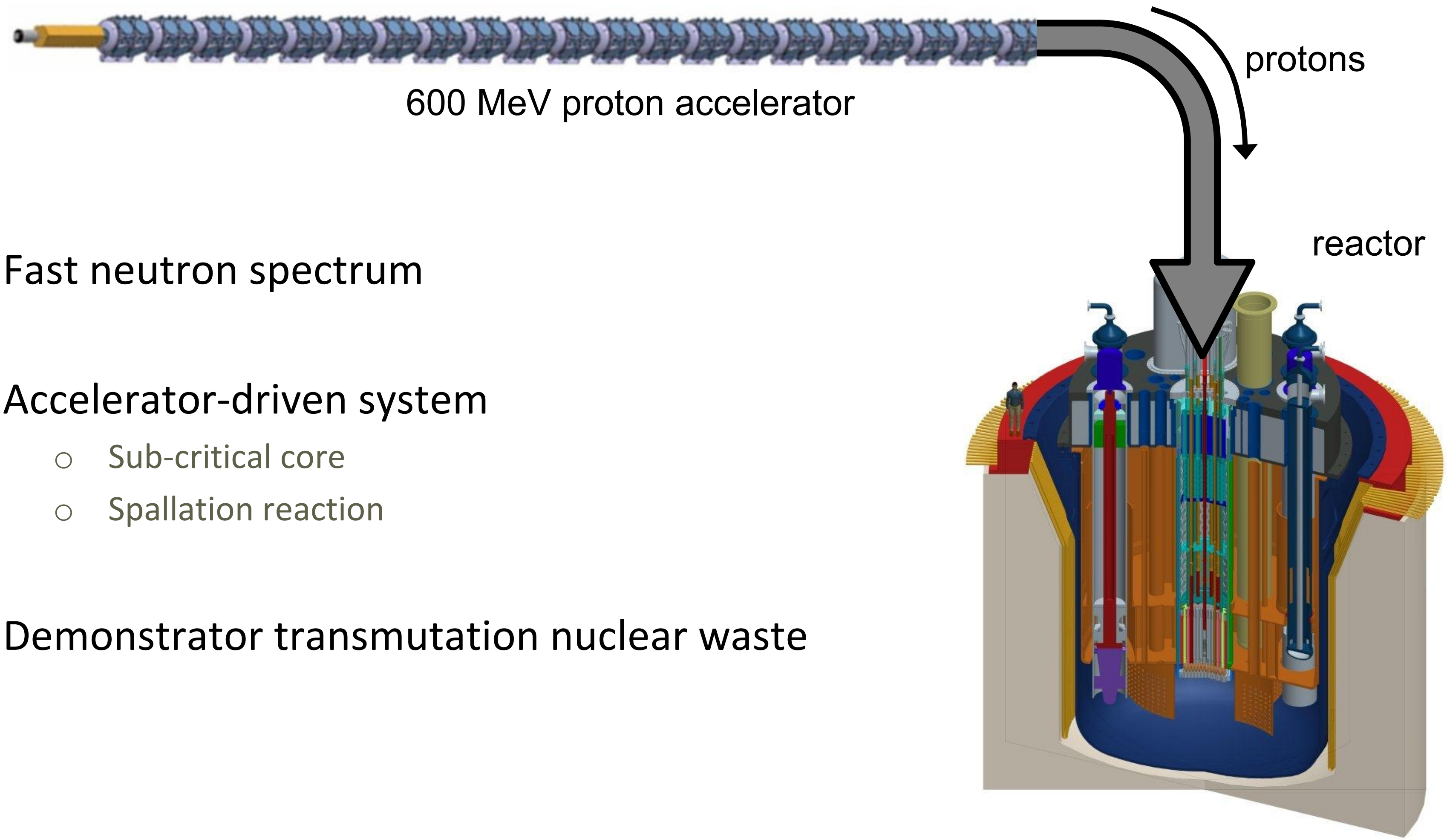
Introduction
The MYRRHA project



- Fast neutron spectrum
- Accelerator-driven system
  - Sub-critical core
  - Spallation reaction
- Demonstrator transmutation nuclear waste

Introduction

The MYRRHA project

- **Lead-bismuth eutectic (LBE)** is the spallation target and primary coolant of MYRRHA:

- Advantages:
  - Excellent neutron yield for spallation
  - Low neutron reaction cross sections
  - Low melting point
  - High boiling point
  - Excellent thermal properties

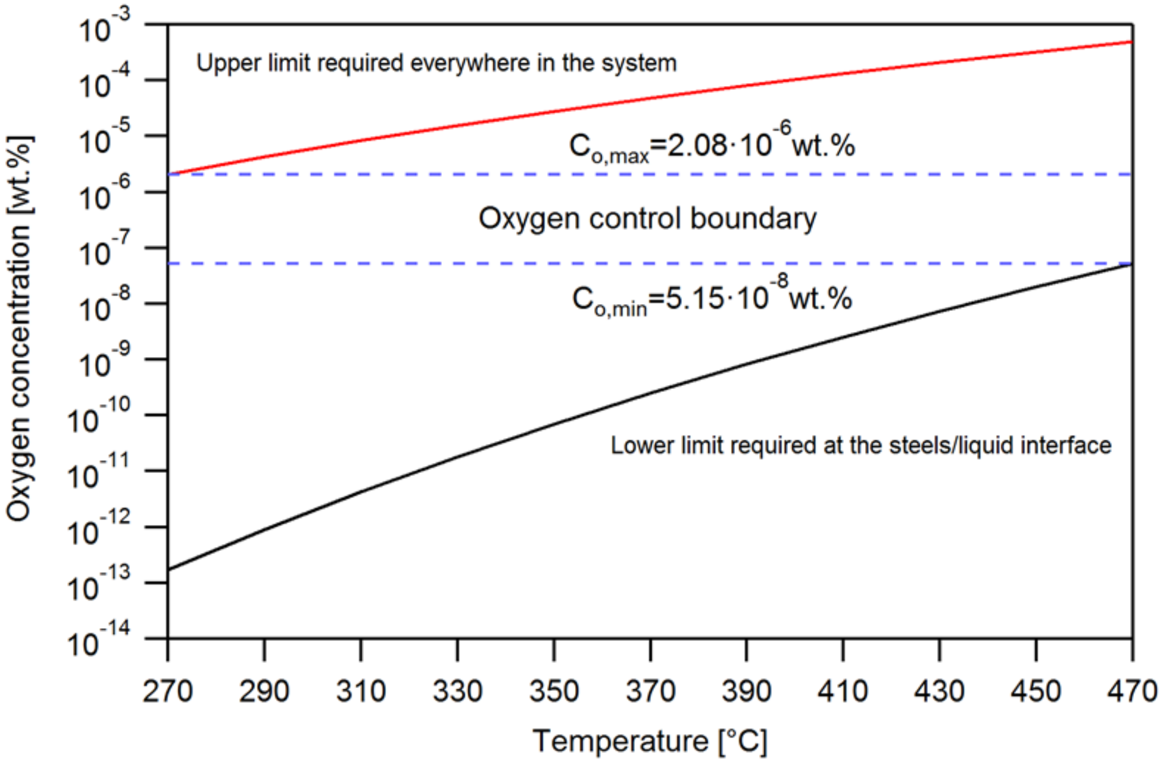
- Challenges:
  - Corrosive to steel
  - Chemistry control

Introduction

The role of oxygen

- Why oxygen is an important element?

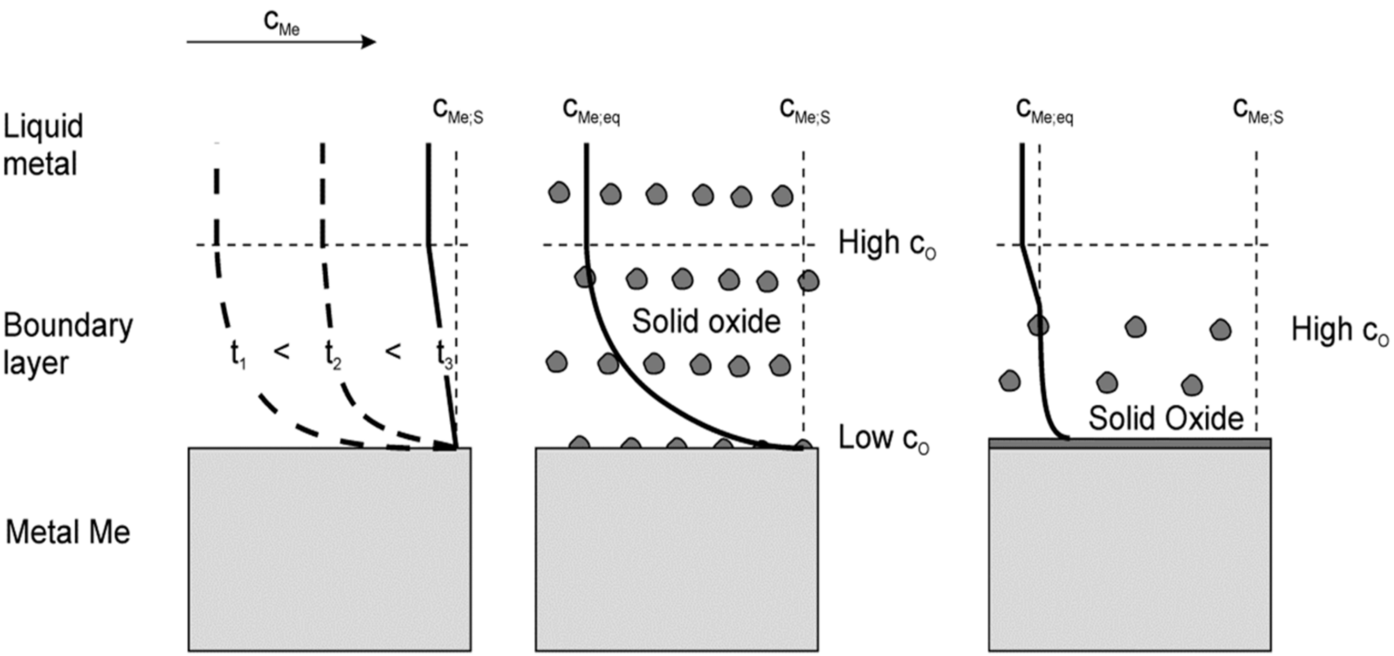
○ Mitigation of severe corrosion of steels in LBE



○ To prevent coolant oxidation

Introduction

The role of oxygen



No stable solid oxide.

Stable solid oxide, but insufficient replacement of oxygen consumed at the metal surface.

Formation of surface layer. Minimum solution of Me, determined by Me transfer from the oxide scale.

C.Schroer, Heavy liquid metal summer school, Mol 2015

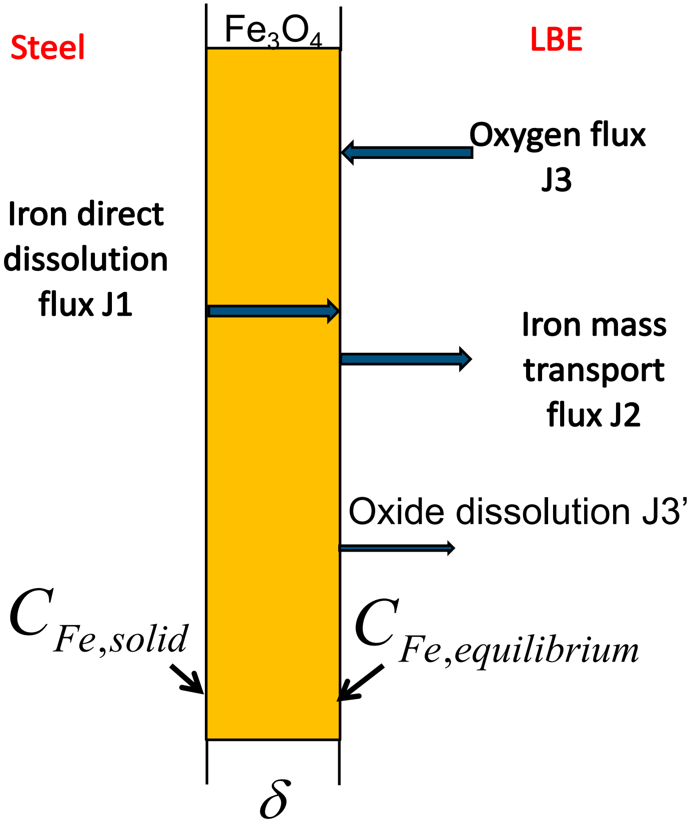
Outline

- Oxygen mass transfer modeling in the MYRRHA fuel assembly
  - Evaluate oxygen gradient at the interface of LBE and fuel cladding
  - Define required oxygen concentration in the bulk of LBE to provide enough oxygen at the interface
  - Provide insights and guidelines to establish representative experimental conditions for the corrosion program
- Corrosion products mass transfer in the MYRRHA fuel assembly
  - Modeling of mass transfer limited dissolution

Oxygen mass transfer modeling in the MYRRHA fuel assembly

Oxide growth model

- Simplified oxide growth model



Steel

Fe_3O_4

LBE

Oxygen flux J3

Iron direct dissolution flux J1

Iron mass transport flux J2

Oxide dissolution J3’

$C_{Fe,solid}$

$C_{Fe,equilibrium}$

δ

$$3[\mathrm{Fe}]_{surface} + 4[\mathrm{O}]_{in\ LBE} \rightarrow [\mathrm{Fe_3O_4}]_{surface}$$

$$\frac{d\delta}{dt} = \frac{(J1 - J2) + J3}{\rho_{FO}}$$

Which data do we need?

$$\delta(t,T)\begin{cases} J1 = \dfrac{D_{Fe}^{Ox}(C_{Fe}^{S} - C_{Fe}^{i})}{\delta} \\ J2 = K\dot{A}(C_{Fe}^{i} - C_{Fe}^{b}) \\ J3 = \dfrac{D_{o}^{Ox}(C_{o}^{i} - C_{o}^{b})}{\delta} \end{cases}$$

Oxygen mass transfer modeling in the MYRRHA fuel assembly

Modeling of steels oxidation

- If only Fe_3O_4 forms on the structural steels, the oxide growth rate will be determined by the mass flux of oxygen and iron into the oxide layer and can be expressed as follows:

$$\frac{d\delta}{dt} = \frac{(J1-J2)+J3}{\rho_{FO}} = (1 + \frac{3M_{Fe}}{4M_O}) \frac{J3}{\rho_{FO}}$$

where, ρ_{FO} is the density of Fe_3O_4, M is the atomic weight.

- $J3 = \left(A_{steel} \cdot \frac{d\delta}{dt} \cdot \rho_{FO}\right) / (1 + \frac{3M_{Fe}}{4M_O})$

- The oxygen mass flux into the oxide layer depends on the oxide growth rate of structural steels. If the oxide growth rate obeys the parabolic rate law, then we have:

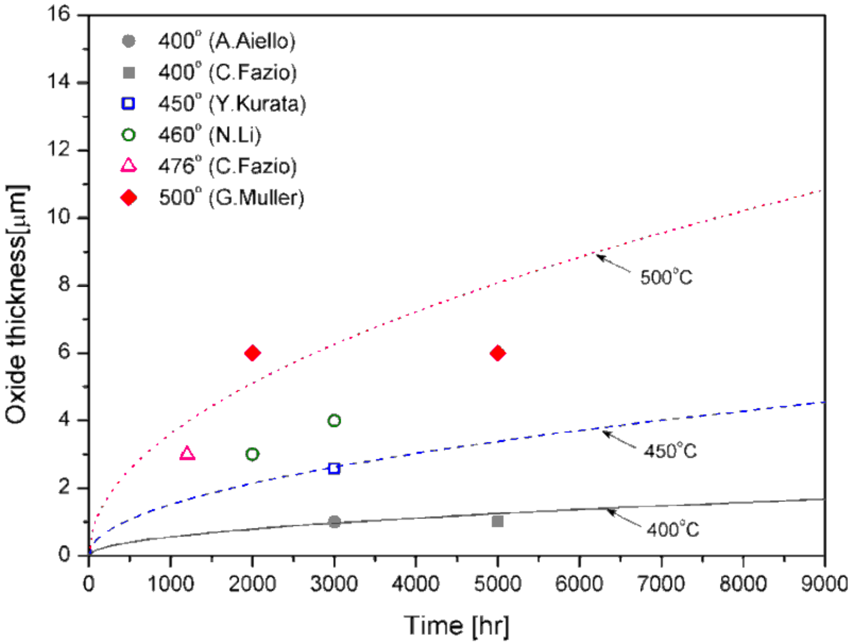
$$\frac{d\delta}{dt} = \frac{K(T)}{2\delta}$$

where, δ is the thickness of oxide layer and K(T) is parabolic growth rate constant of oxide layer

Oxygen mass transfer modeling in the MYRRHA fuel assembly

Oxidation kinetics

- $\delta(t) = [K(T)\bullet t]^{1/2}$, where $\delta(t)$ is the thickness of oxide in cm and t is time in second



$$K(T) = 3.027\times10^{-3}\exp\left(-\frac{161626}{RT}\right)\ \text{for AISI 316L}$$

Further data are needed to assess the dependance of K from the oxygen content

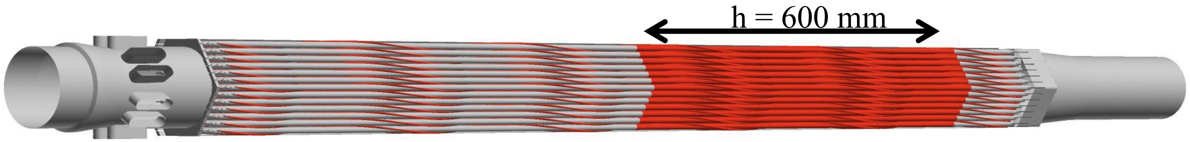
Il Soon Hwang, J. Lim, "Structural Developments for Lead-Bismuth Cooled Fast Reactors, PEACER and PASCAR", The 25th KAIF/KNS Annual Conference April 14-16, 2010.

Oxygen mass transfer modeling in the MYRRHA fuel assembly

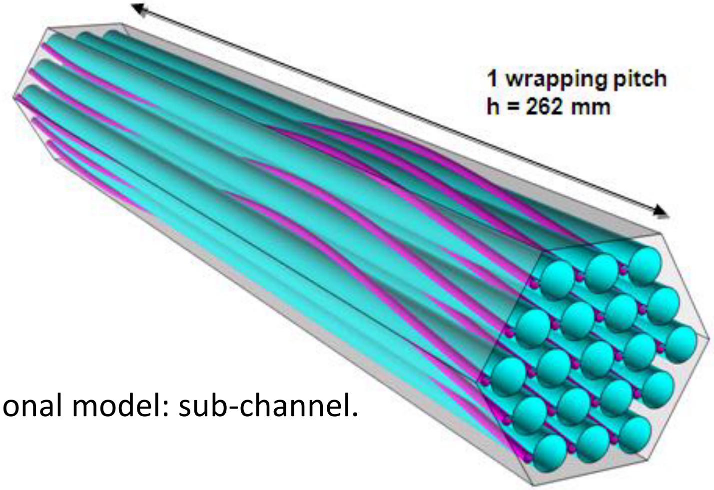
Simulation set up

- 19-pin scaled model of the MYRRHA bundle.
  - Axial power distribution and Reynolds number of the MYRRHA's hottest assembly.
  - Oxidation kinetics from experiemental data as boundary conditions at the walls.
  - Outlet variables of the first heated pitch used as inlet boundary conditions of the second.

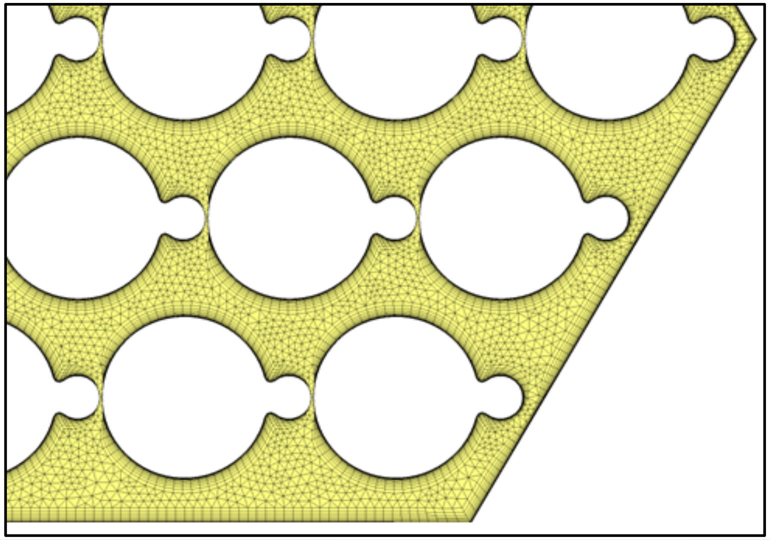
COMPLOT facility.



Full scale fuel bundle of MYRRHA reactor.



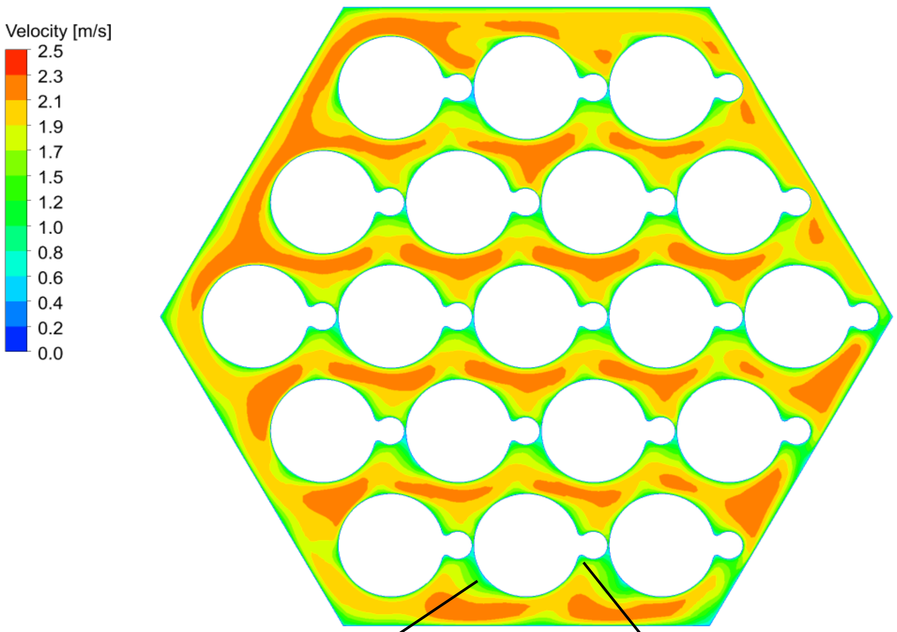
Computational model: sub-channel.



Oxygen mass transfer modeling in the MYRRHA fuel assembly

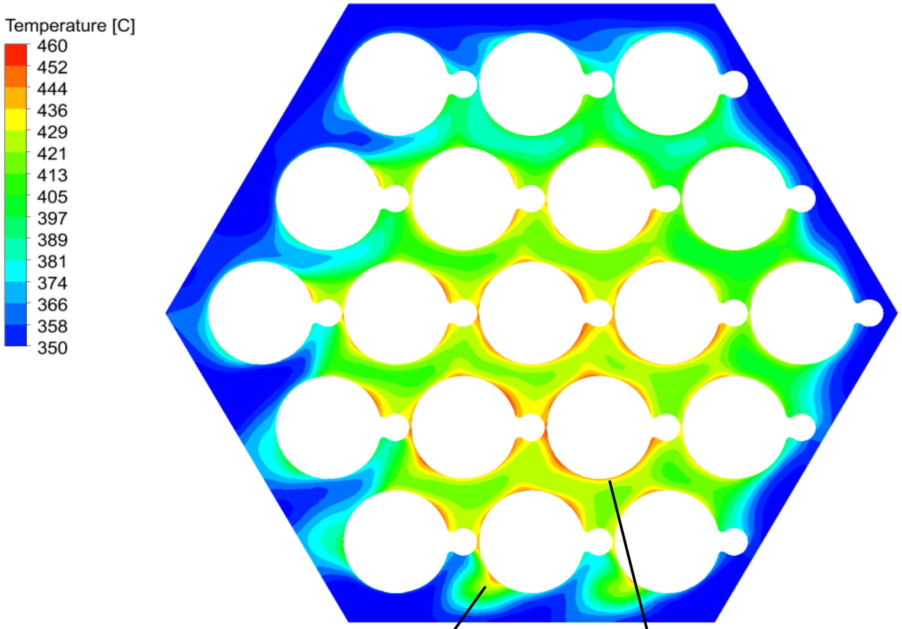
Velocity and temperature profiles

- Thermal hydraulic characterization of the fuel bundle.



Low velocity regions due to swirl

Thicker velocity boundary layer due to wire



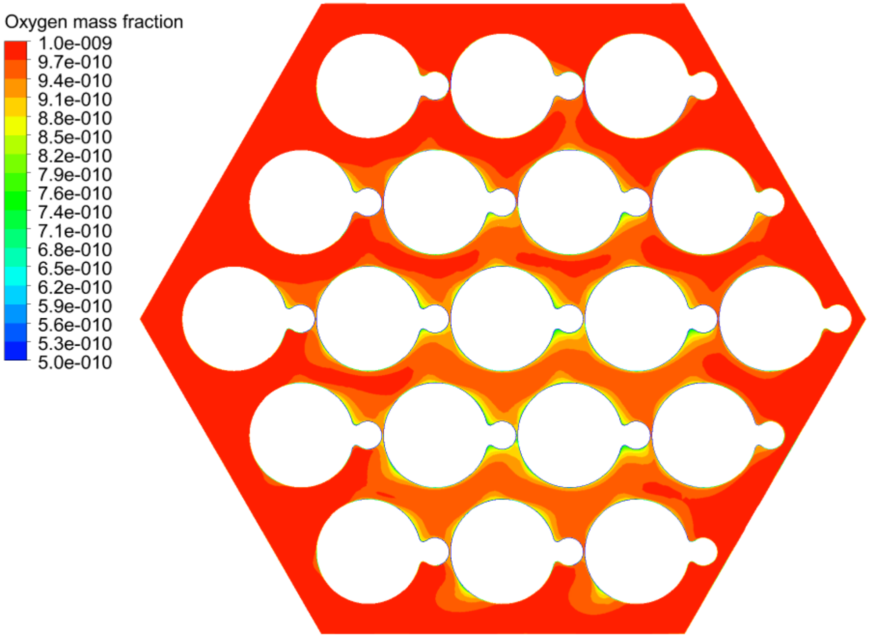
Hot spots due to swirl

Thick temperature boundary layer

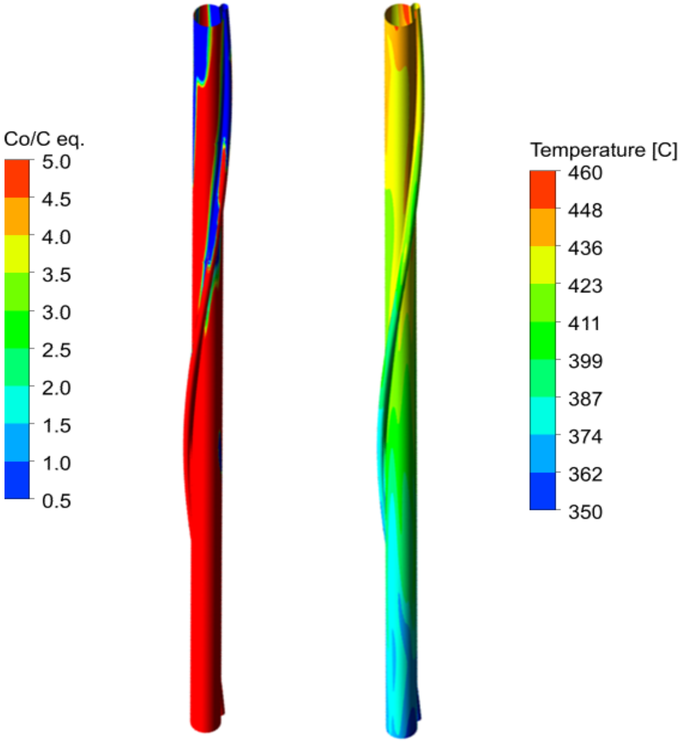
Oxygen mass transfer modeling in the MYRRHA fuel assembly

Oxygen profiles at the steels surface: case 1

- Oxygen mass transfer through the fuel bundle.



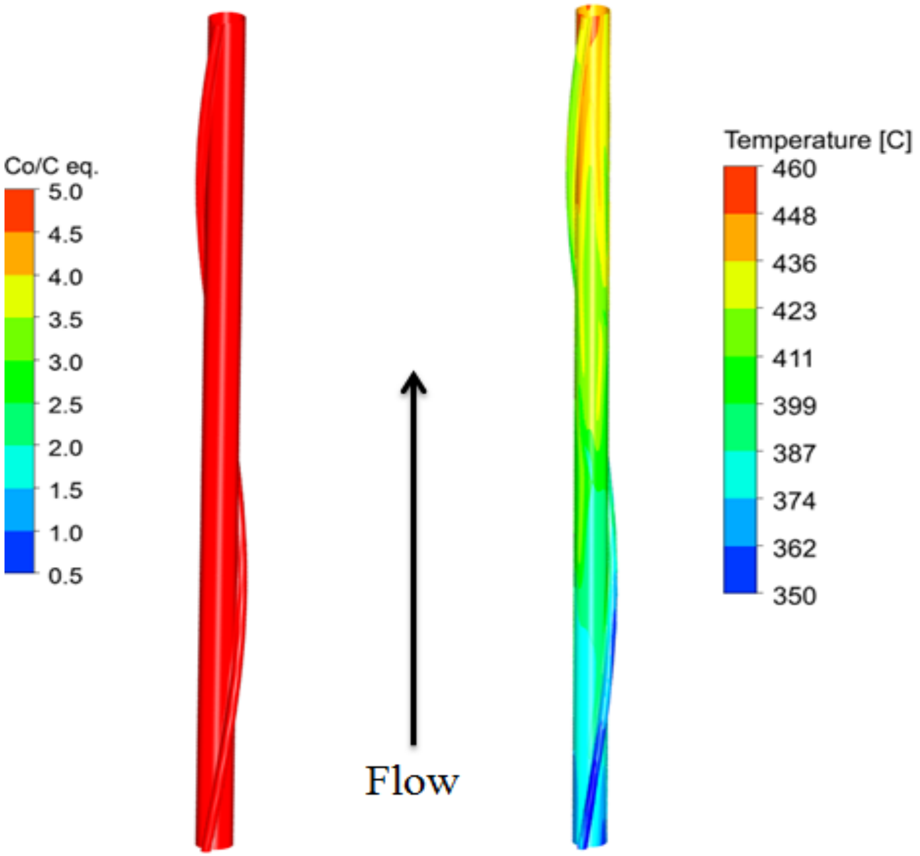
Oxygen concentration profiles. Maximum temperature 460 °C with 1 µm thick oxide layer on the cladding. Inlet bulk oxygen concentration 10^{-7} wt%.



Normalized oxygen concentration (left); temperature profile (right) for the central pin of the second pitch.

Oxygen mass transfer modeling in the MYRRHA fuel assembly

Oxygen profiles at the steels surface: case 2



Normalized oxygen concentration (left); temperature profile (right) for the central pin of the second pitch. Inlet bulk concentration 10^{-6} wt.%. Thickness of oxide layer 1 µm.

Oxygen mass transfer modeling in the MYRRHA fuel assembly

Oxygen profiles at the steels surface: case 3

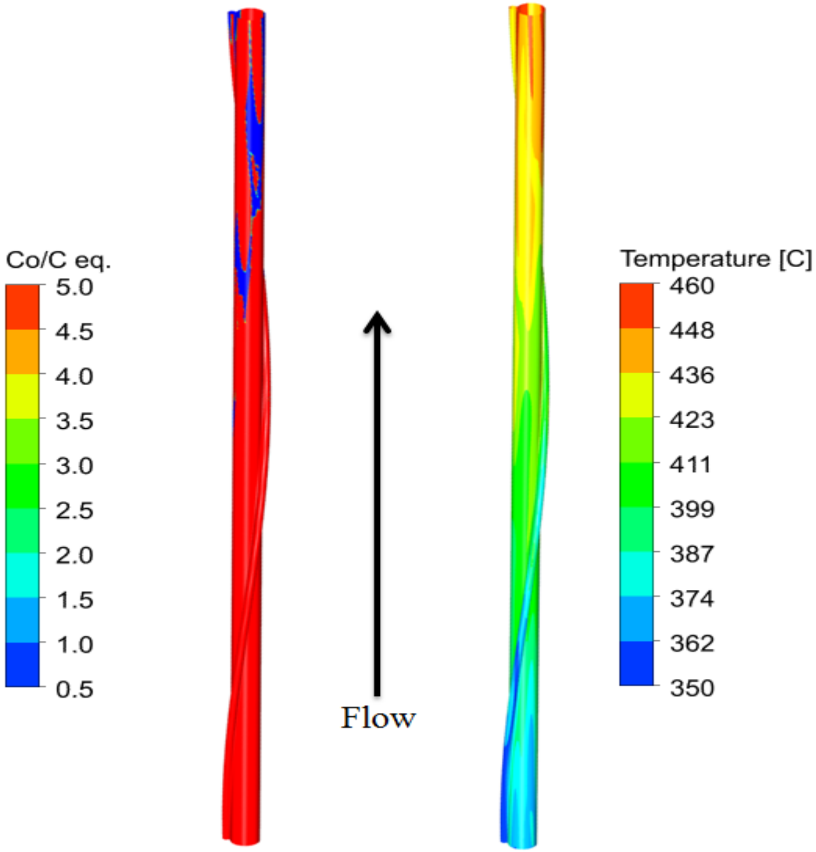
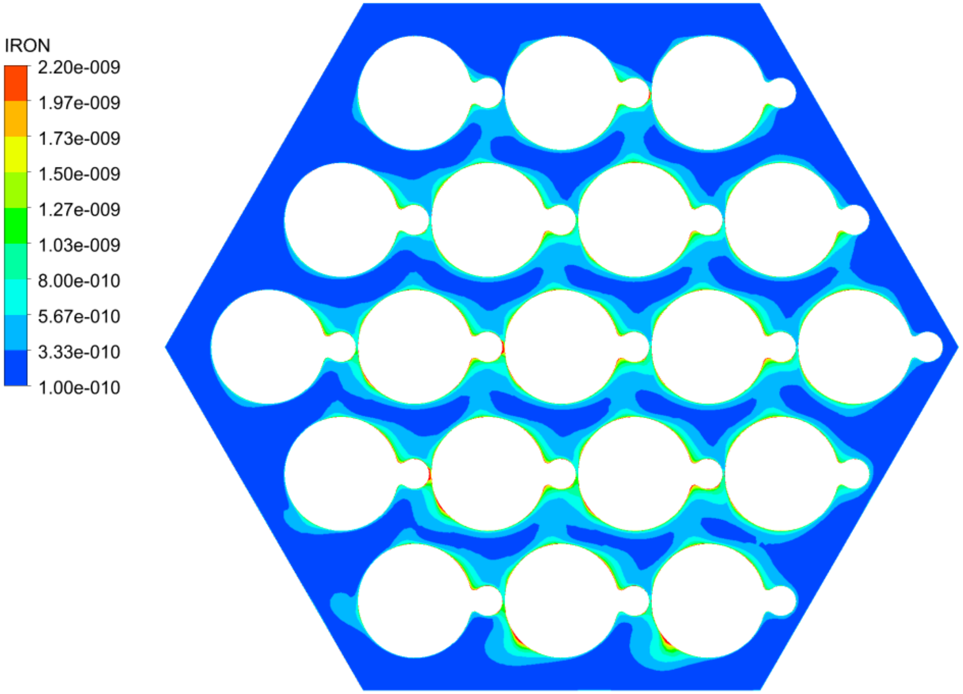


Figure 5.18. Normalized oxygen concentration (left); temperature profile (right) for the central pin of the second pitch. Inlet bulk concentration 10^{-6} wt. %. Thickness of oxide layer 100 nm.

Corrosion products mass transfer modeling in the MYRRHA fuel assembly

Iron release from structural steels



Iron mass fraction contour at the outlet of the second heated pitch

- ☐ Infinite fast dissolution reaction: mass transfer limited kinetics

T_{max}: 455 °C

Flow rate = 12.35 [kg/s]

Average Cin = $3.75 \cdot 10^{-10}$ m.f.

Cmax =$9.91 \cdot 10^{-7}$ m.f. (solubility T_{max})

Average Cout = $3.75 \cdot 10^{-10}$ m.f.

Average dissolution rate: 12 mg/h

Conclusions

- A model of oxygen mass transfer in LBE and oxidation reaction was developed to evaluate local oxygen concentration at the interface of LBE and fuel cladding.

- The maximum cladding temperature should be limited below 400 °C in case of a bulk concentration of 10^{-7}wt%. Pre oxidation at lower temperature might be required.

- In order to operate with a maximum cladding temperature above 450 °C, the required bulk oxygen concentration in LBE should be higher than 10^{-6} wt% and an appropriate pre-oxidation should be done on steels surface.

- In general, local effects such as hot spots, quasi stagnant areas and swirl, characterized the wire wrapped bundle. These regions are more inclined to corrosion due to depleted oxygen concentration.
- The simulations can be used to define representative experimental conditions for the corrosion programme.

Thank you for your attention

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