Modelisation and simulation of the thermo-hydrodynamique behavior of a mixture composed of supercritical water and molten salt

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1 Resumed

This thesis is part of an ANR project called HMS^2 which aims to synthesize stable Mn^{5+}-based oxides. In order to synthesize these oxides, a new solvent system has been discovered at ICMCB Laboratory called HyMoS (Hydrothermal Molten Salt). This new solvent system, composed of supercritical water and droplets of molten salt, appears to be a good way to synthesize the desired oxides. Nevertheless, despite it's good recycling properties (organic and inorganic) we lack information about this reaction medium. Therefore it is fundamental to understand the thermo-hydrodynamic in HyMoS. This is the objective of this thesis.

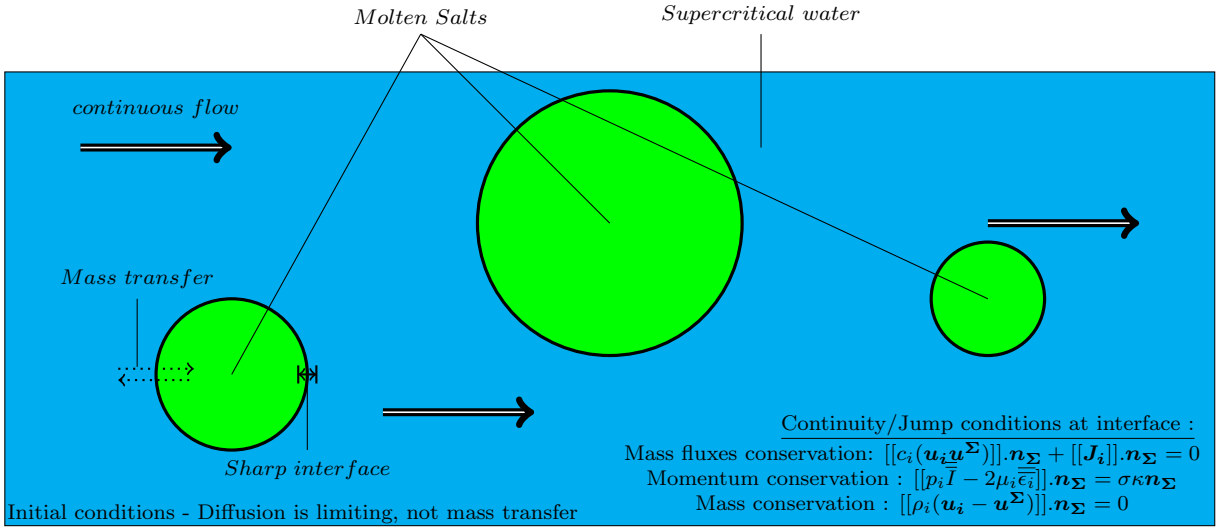

Figure 1: Schematic representation of HyMoS

Indeed, droplets of molten salts interact with the surrounding fluid of supercritical water through a phenomenon called mass transfer that will modify the thermo-hydrodynamic of this reaction medium (droplets size, composition) as shown in figure 1. So the objectives of this thesis is to numerically study the thermo-hydrodynamic behavior of this reaction medium. It require a full modelisation of the system :

- Take into account the different continuity and jump conditions across the interface.
- Model the mass transfer that occurs at the interface.
- Take into account the volume changes induced by mass transfer.

Then the characteristic times of the main mechanism will be study numerically (mass transfer through interface, thermodynamic equilibrium). Everything will be made in collaboration with the experiment realized at ICMCB. Especially the condition of the thermodynamic equilibrium needed to properly assign the value needed at the interface between these two phases.