# Contribution of the Numerical Simulations in the Development of the French HLLW Vitrification Processes – 15126

E. Sauvage, P. Brun, A. Bonnetier, J. Lacombe, C. Ladirat CEA Marcoule CEA-AREVA Joint Vitrification Lab BP 17171 - 30207 Bagnols-sur-Cèze Cedex, France

#### **ABSTRACT**

For many years, the CEA (Commissariat à l'Énergie Atomique et aux Énergies Alternatives) Marcoule France has developed various processes dedicated to radioactive waste confinement, especially vitrification processes for HLLW. For 10 years now, the numerical simulation has become an important tool for research and developement projects held in the CEA-AREVA Joint Vitrification Laboratory (LCV). Induction heating, fluid mechanics and thermal simulations take part of all new R&D projects. The apports of such simulations are, first, the enhancement of the working knowledge of existing process. Those data are very useful to define optimisation choices, for example upgrades made on the hot metallic melter used since the 90s at LaHague facility. Second, the simulations are, of course, also used at the conception stage of new processes as a tool allowing wide ranges parametric tests. This has been extensively used in the design of the cold crucible inductive melter (CCIM) commissioned in 2010 at La Hague plant. Finally, it is a powerful and relatively cheap tool for prospective studies for processes of the future. Whatever the purpose, the potential benefits are gains on the reliability, the output capacity and the life time.

#### INTRODUCTION

Vitrification of high-level liquid waste is the internationally recognized standard to both minimize the impact to the environment resulting from waste disposal and the volume of conditioned waste. In France, the vitrification of high-level liquid waste produced from nuclear fuel reprocessing has been successfully operating now for more than 25 years with three major objectives: durable containment of the long-lived fission products, minimization of the final waste volume and operability in an industrial context. As a result, CEA & AREVA have integrated a unique experience in the field of high level waste vitrification through the design and operation of facilities with high records of safety, reliability and product quality, in line with efficient reprocessing plants; continuous efforts to improve at the same time the technology (from hot to cold crucible) and the associated matrix formulations, with constant emphasis on quality and volume reduction, ended up with the design and qualification of the cold crucible melter (CCM) technology.

#### HISTORICAL OF NUMERICAL SIMULATION DEVELOPMENT

Numerical simulation has been used since the beginning of the process development in the 80s. At first it was mainly used for designing the induction generator, the induction coil and was quickly applied for the designing of the cold crucible itself. Thanks to these first tools, mainly based on strong analytical studies, various induction furnace (hot melter or cold crucible) were designed and then used to melt metals and various oxides. Then the need of thermal simulation has pointed out and was performed in coupling with induction simulation. But thermal repartition is greatly influenced by the fluid flow. At this time (90s), computation capacity was too weak to perform full 3D computation and the development of numerical simulation has slow down. The figure 1 shows typical results obtained in simulation of natural convection driven flow for a glass melt in cold crucible. Simulation were only 2D axisymetrical with a coulping between the velocity and temperature field due to the variation of the viscosity with the temperature.

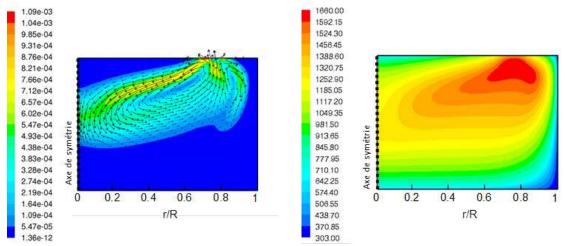


Fig 1. Simulated velocity and temperature field of a natural convection driven flow of a glass load melt in cold crucible. 2D simulation with Flux-Expert (1990).

In the early 2000s, commercials softwares specialized in induction and CFD become more efficient and thanks to the great increased of computation capacity, 3D simulations were successfully conducted. The coupling between 3D-CFD with 2D-induction has been done (Jacoutot 2006 [1]) followed with a 3D-CFD/3D-induction coupling (Sauvage 2009 [2]). Diphasic simulations of glass flow were added (Lima Da Silva 2014).

#### MODELISATION DESCRIPTION

In this section we will briefly described the simulation performed in our laboratory. Details will not be given here but are available in the cited reference [1,2,3]. Our tools are able to simulate induction heating from low to high frequency coupled to thermal simulation with the Joule power density in the metallic part of the process as well as in the molten glass itself. The flow simulation is also coupled and takes into account the mechanical stirring, gas injection and even Lorentz forces if necessary. The radiative heat transfer and the Marangoni convection are simulated as well. All these phenomena are computed on the full 3D real geometry of the furnace thanks to the use of supercomputing center as the TGCC (Très Grand Centre de Calcul) of the CEA. Software used was formerly academic software then commercial or open-source : Ansys® Fluent for CFD , Flux® (Cedrat) for induction, OpenFoam.

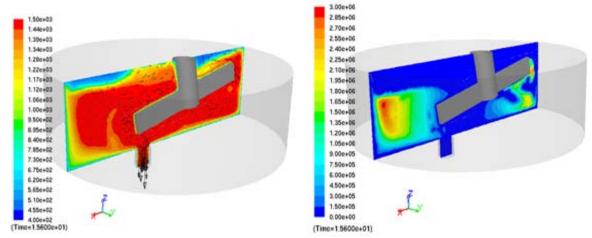


Fig. 2. 3D simulation of temperature on the left (K) and right Joule power density (W/m3) in CCIM

### EXAMPLES OF THE CONTRIBUTION OF NUMERICAL SIMULATION

Numerical simulation first objective is to help to understand physical phenomena within the molten glass. In fact, due to high temperature and high corrosive properties of the melt, accurate experimental data are very difficult to obtain. Thereafter, the simulation can help to optimize the design of structures or the high frequency power line distribution. But also, the simulation can give an evaluation of thermal and chemical homogeneity and the impact of the glass properties on this homogeneity. Here is a list of applications:

- optimization of internal water cooling of parts of the cold crucible melter
- optimization of glass mixing to assure a good thermal and chemical homogeneity
- studies to increase the throughput of glass production
- determination of residence time of material in the furnace.
- induction optimization of inductor design, melting pot
- simulation used in testing new concept of furnaces of higher capacity

The benefits are a higher power efficiency of the process, a longer life-time of optimized equipment, contribution to ensure the glass quality and of course conception of futur vitrification process.

### MAIN ISSUES OF SIMULATION OF VRITRIFICATION PROCESSES

Fluid flow simulation of glass has one major advantage in common fluid dynamics problems: it is only laminar flow. But in return, all the physical properties of the glass varies strongly with the temperature. Two problems arise: (i) a coupling between velocities, induced electrical current appears with temperature (ii) the law of the physical properties of the glass with the temperature are overriding.

The first point leads to develop numerical strategy to solve correctly the coupled physics especially

The first point leads to develop numerical strategy to solve correctly the coupled physics especially between the fluid flow simulation and the electromagnetic simulation which are two physics solve by two different software (most of the time) and even with different numerical scheme (Finite Element and Finite Volume). This coupling has been achieved quite early in two dimensional simulation but the coupling between two 3D software has been reached only in 2009 [3].

The second point is the acquisition of physical properties of the glass. In our laboratory, characterizing technique of glass have been extensively developed from the early beginning of vitrification (in the 80s) but for other purpose than numerical simulation feeding. As a consequence, a lot of data of this time are mostly unusable. For example, it was common to measure the viscosity of glass only at the temperature of elaboration which is inadequate to perform numerical simulation. So effort have been done to adapt the existing characterization method of glass for numerical simulation purpose or even to develop new characterization technique to measure new properties (surface tension and thermal conductivity for example).

## VALIDATION WORK

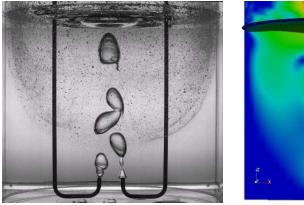
As the simulation is more and more often used in the development work, the need of validation of numerical results is very strong. Unfortunately, in-situ glass instrumentation at 1200°C is very limited. We perform a step by step validation of the simulation: (a) For the fluid flow simulation of glass we use the hydraulic similarity technique which consists in replacing the glass by oil with the same kinematic viscosity. As a result, the flow pattern of oil is similar to the glass one and instrumentation in oil is much easiest. This similarity technique allow us to perform quantitative comparison between CFD and experiment in the specific domain of highly viscous liquid which is not really widespread in the literature. (b) Electromagnetic simulation has been developed in the same time than cold crucible technology itself. The validation of such validation is made by magnetic field measurement in the air or Joule losses power measurement in the cooled metallic part of the furnace. The main limitation of this validation is the precision of experimental measurement due to the high frequency and high voltage of induction generator. (c) For the full coupled simulation (CFD+Induction+Thermal) experimental comparison can be done only by direct comparison with glass experiment. To do so, we used specific devices to measure the thermal power coming from the glass to a cooled device. Precision of this kind of probing is quite low

 $(\sim 10\%)$  and limit the validation of our simulation.

In order to optimize the effort of characterization enhancement, sensitivity analysis is performed with our simulation to target the physical properties having the most importance in the prediction of a specific result (wall heat flux, skull-melter thickness etc.). This kind of work may also be used as an uncertainty propagation method to determine the uncertainty of prediction of wall heat flux (for example) due to the uncertainty of physical properties due to the acquisition method.

#### MODELISATION DEVELOPMENT

As the simulation capability grows, the model is upgraded with new phenomena taken into account. The aim is to enhanced the prediction capability of simulation and widen the fields of its relevance. Different models are under development like a red-ox model to predict the fugacity of glass or an elaboration model for the glass from his raw materials inspired from **Hrma** *et al.* [4]. The figure 3 shows new developments in the simulation of bubbling in viscous liquid with the Vloume Of Fluid (VOF) method compared to an experimental visualization of the same flow with oil.



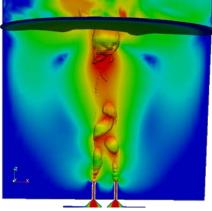


Fig. 3. Diphasic simulation of the interaction of two bubble columns in a viscous fluid representative of molten glass. Left, experimental view of oil, right CFD with Openfoam)

#### **CONCLUSIONS**

The numerical simulation of vitrification furnaces has started in the same time of the first development of the process in the 80s. Thanks to the software and hardware development, the simulation takes a more and more important part in the current projects. Contributions of the simulation become valuable but simulation itself is not so easy. Physical properties measurement and data acquisition for validation are essential and specific development to feed the simulations are required. Also, even if commercial software becomes quite easy-to-use, the savoir-faire remains very important.

#### REFERENCES

- [1] Jacoutot, L.; Fautrelle, Y.; Gagnoud, A.; Brun, P. & Lacombe, J. Numerical modeling of coupled phenomena in a mechanically stirred molten-glass bath heated by induction Chemical Engineering Science, 2008, 63, 2391 2401
- [2] Sauvage, E.; Gagnoud, A.; Fautrelle, Y.; Brun, P. & Lacombe, J. Thermoconvective flow of molten glass heated by direct induction in a cold crucible Magnetohydrodynamics, 2009, 45, 535-542
- [3] Sauvage, E.; Bonnetier, A.; Gautheron, D.; Brun, P. & Lacombe, J. Numerical Simulation of Vitrification Processes: Glass Homogeneity by Gas Bubbling Study Procedia Chemistry, 2012, 7, 593 59

# WM2015 Conference, March 15 – 19, 2015, Phoenix, Arizona, USA

[4] R. Pokorny and P.R. Hrma. Mathematical model of cold cap - preliminary one-dimensional model development. Technical Report PNNL-20278, Pacific Northwest National Laboratory for the U.S. DOE, Richland Washinton 99352, march 2011.