

# Transient Model of a Fluorine Electrolysis Cell

J. Vukasin<sup>1</sup>, I. Crassous<sup>2</sup>, B. Morel<sup>2</sup>, J. Sanchez-Marcano<sup>3</sup>, P. Namy<sup>4</sup>

<sup>1</sup>HRP, AREVA NC and Institut Européen des Membranes - CNRS, France

<sup>2</sup>HRP, AREVA NC, France

<sup>3</sup>Institut Européen des Membranes - CNRS, France

<sup>4</sup>Simtec, France

## Abstract

In the nuclear fuel cycle, fluorine is produced by the electrolysis of the molten salt KF-2HF according to the following equation:



Fluorine is then added to UF<sub>4</sub> to obtain UF<sub>6</sub>. This electrolysis is a complex process to study since hydrofluoric acid and fluorine are hazardous and highly corrosive. Also it must be performed under anhydrous conditions. The process is exothermic and a heat exchanger using cool water is placed inside the cell to maintain the electrolyte at the operating temperature. For more than 50 years, many studies have been done to improve the electrolysis but some phenomena are still not understood.

Since 2005, COMSOL Multiphysics® has been of great use at AREVA to increase our understanding of this process. Indeed, modeling the electrolysis involves strong coupling between different physics. After validation, modeling gives access to data that are difficult to obtain, such as the hydrodynamics of the system or the local HF concentration.

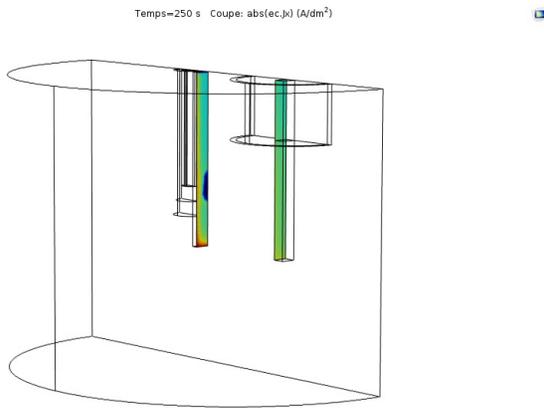
More recently, a 3D-model of a lab-scale electrolysis cell has been developed. Five COMSOL physics interfaces were used: "Electric current", "Heat transfer in fluids", "Bubbly flow", "Transport of concentrated species" and "Turbulent flow" to simulate the flow of cooling water inside the heat exchanger placed inside the cell. This model, in which the former modules are all coupled, enables us to study the impact of various parameters of the industrial process.

One particular feature of this model is to take into account the solidification of the electrolyte that occurs when the temperature and/or the HF concentration drops. The heat capacity method has been used to model the phase change. Since very few studies on KF-2HF had been published, only data for liquid KF-2HF were available. The diffusion coefficient of HF was derived from molecular dynamics. Some key parameters for the solid phase were missing, such as heat capacity, density or thermal conductivity. The first two were determined using a theoretical approach. To get the last crucial parameter, heat fluxes of a reactor filled with solid KF-2HF were measured, allowing us to determine the value of the thermal conductivity of this

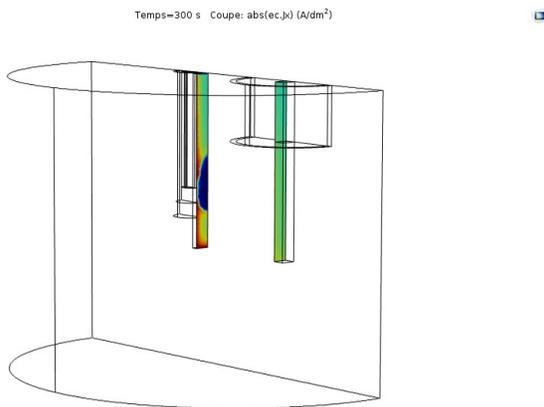
solid.

Transient studies of 300 seconds were carried out, using a segregated solver with a mesh composed of 487000 elements. Since phase change at the electrodes depends on the HF concentration and the temperature at the interface between the electrodes and the electrolyte, the electrolysis was simulated for different HF concentrations and for different current densities at the anode. The impact of the cooling system on the electrolysis was also studied. The solid fraction and the current densities at the electrodes at different times are shown in the different figures. Results will be discussed in this poster.

## Figures used in the abstract

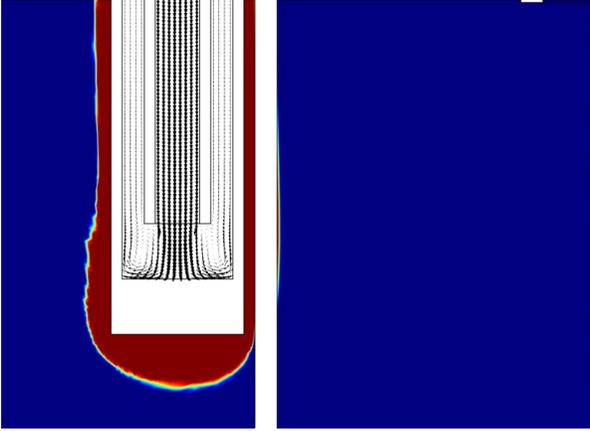


**Figure 1:** Current density at the electrodes after 250 seconds.



**Figure 2:** Current density at the electrodes after 300 seconds. The growth of the solid phase at one electrode changes the current density at the interface.

Temps=300 s Surface: Indicateur de phase, phase 1 (1) Flèches sur surface: Champ de vitesse  
Flèches sur surface: Champ de vitesse, phase liquide



**Figure 3:** Solid fraction around the cooling system and at the cathode.

---

**Figure 4**