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Thermal Simulation of an Evaporation Reactor

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Abstract: In this article we present simulations results of an evaporation reactor for optical layer applications.

The thermal simulation concern the source of the evaporated material. An experimental problem is related to the shape of the material powder surface: due to the evaporation rate, the surface don't keep his flat initial shape and this has a strong effect on the local evaporation rate. In this process there is a strong coupling between thermal effects and the position of the surface of the powder. The simulation aim is to take in account heat transfer by conduction and radiation as well as evaporation direct and non direct effects on thermal transfer. The presented simulation are a coupled solving of thermal transfer including heat of state change of the material, and ALE model to follow the powder surface change during evaporation.

Keywords: Evaporation,Change of state, Deposition process, Thermics.

1. Introduction

In this article we present simulations results of an evaporation reactor in order to predict surface shape of the evaporated material. The shapes are note the real one and the results are shown in normalized scale but the modeling procedure and models are exactly the same than the models of the real industrial study. The methodology used for these modeling is a coupling of heat transfers and deforming mesh instead of equivalent heat capacity method. The advantage is that, in case of pure material, we find this method more precise. The disadvantage is that we have to deal with topological problem during deformation of the mesh. We present here some results of this method for evaporation modeling but also use it for solidification.

2. Geometry and mesh

The evaporated material is a powder inside a cylindrical crucible. The crucible is heated by a resistor inside ceramic holder. All other part of the reactor are not cylindrical but we also assume axi-symmetry for radiative heat transfer on the cold parts of the reactor.

All other cooled parts of the reactor are not modeled because there are assumed at constant temperature.

The crucible and heater will be deformed as well as powder in order to keep the topology of the geometry. Then the top of the crucible and the heater will be expended during transient calculation, and the bottom will be contracted. The mesh is refined in the top parts of crucible and heater to be able to follow this deformation.

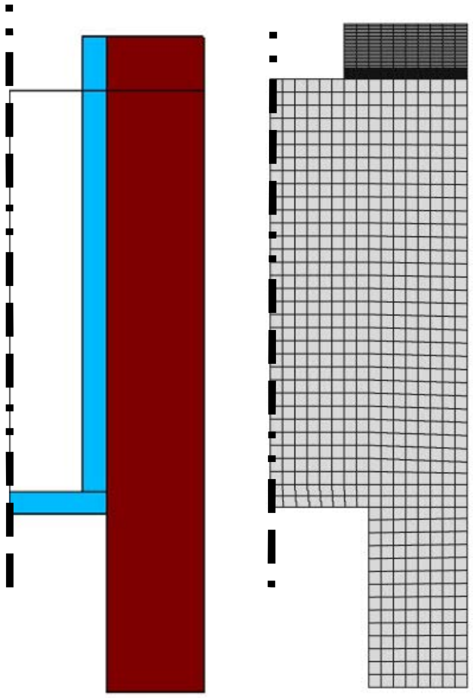

Figure 1. Cylindrical geometry of the crucible (blue) the powder (white), and the ceramic holder (red) with the heater, and mesh (right) before evaporation.

3. Models and Boundary Conditions

We solved thermal transfers by conduction in solids and radiation coupled with ALE to describe surface move during evaporation. Due to low pressure, we didn't solve transfer by conduction or convection in "vacuum". The latent heat is taken in account as a surface source term at evaporation surface. The evaporation rate is assumed linear versus temperature. The local evaporation rate is wedged to fit the global experimental rate.

The model is the following:

- Heat transfer by conduction / radiation with the following heat source on evaporation surface

- $Q_s[W/m2]=v_{evap}*rho_{htgh}*L_{evap}$ (1)

- $v_{evap}[m/s]=\alpha*v_{\exp}/rho_{htgh}$ (2)

and α is wedged to fit experimental global rate.

The boundary conditions are the following for heat transfers:

- Powder surface: radiation on other part of reactor, mainly the crucible, with an “ambient temperature” equal to cold part's temperature (293K),
- Outside of heater and inside of insulators: radiation to insulators and same ambient temperature,
- Outside insulators: radiation to ambient temperature equal to cold part's temperature (293K),

ALE model is solved only in powder crucible and heater by free displacement. The boundary conditions are the following:

- Powder surface: vertical velocity equal to v_{evap} (see equation 2), no horizontal displacement velocity,
- Top and bottom of crucible and heater: no displacement,
- Vertical boundaries of crucible and heater: no horizontal displacement, free vertical displacement,
- Horizontal line in crucible and heater at powder level: same vertical displacement than surface powder on crucible contact. This is done using coupling variable by extrusion.

This method use crucible and heater deformation but don't use re meshing. Some other method are possible but have to deals with topology of the powder surface during evaporation and mesh quality.

3. Results

The first result is the wedge local rate in order to fit the global rate: the local rate of the mass evaporate per unit surface and second is faster than the global rate. The figure 2 shows a comparison of modeled and measured global evaporation rates.

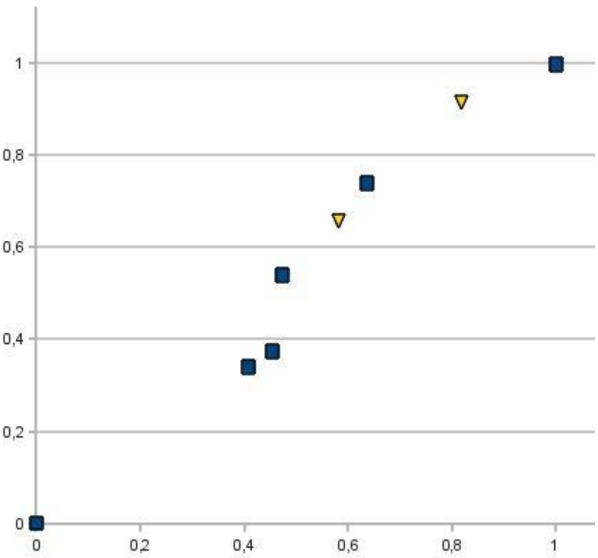

Figure 2. Measured (blue) and modeled (yellow) global evaporation rates

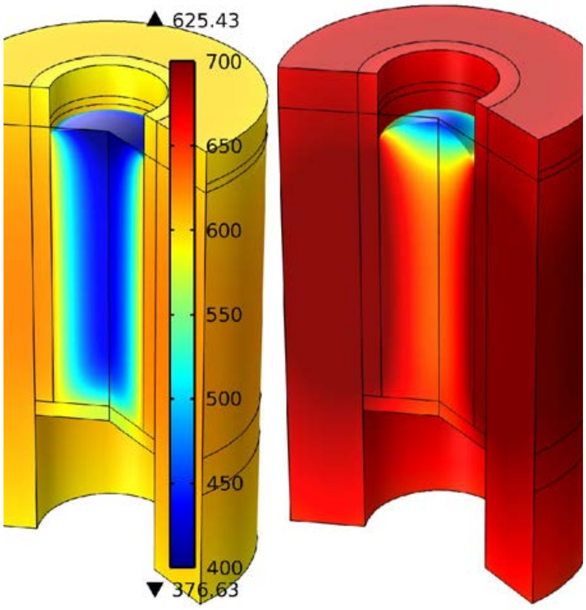

Figure 3. Temperature in crucible and powder during heating (left) and beginning of evaporation (right)

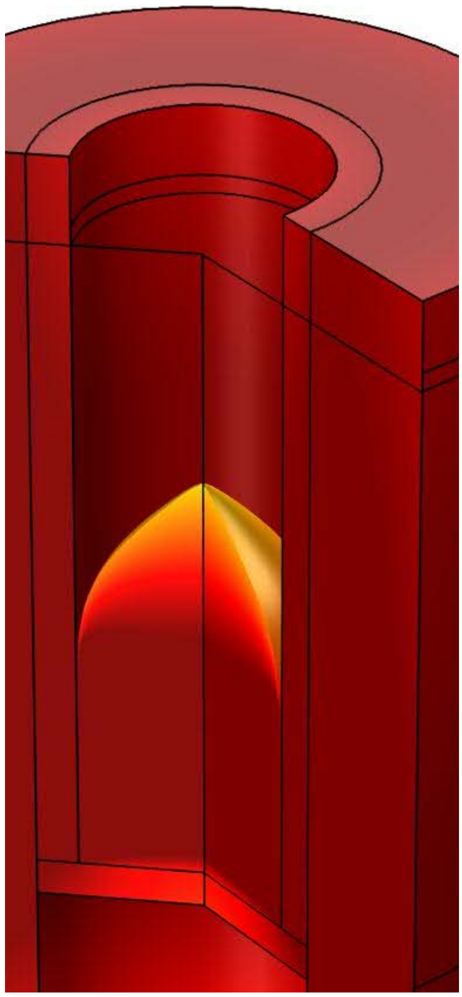

Figure 4. Temperature in crucible and powder after few hours of evaporation

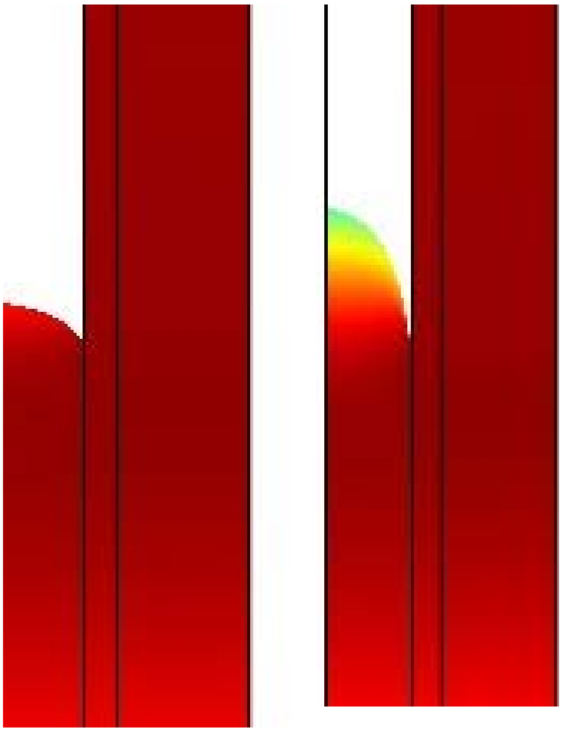

Figure 4. Shape of the surface with high powder conductivity (left) and ten time lower conductivity (right) at same time.

The wedged local rate allow to fit the global evaporation rate and the sensibility of this rate on temperature. The second important result is that the shape of the surface is no longer flat: the evaporation is faster close to the crucible wall mainly because the center is colder. The shape of the surface obtain by the model fit well the experimental results (Figure 3).

The last result is that the shape of the surface depends strongly on the powder thermal conductivity: when the conductivity decrease the heterogeneity of the evaporation rate increase and the shape is less and less flat (Figure 4).

4. Conclusions

An evaporation process has been simulated. The local evaporation rate was wedged in order to fit the experimental global rate. Then the model is able to predict the shape of the surface of the evaporated material. The sensibility of the shape on powder characteristic is also shown.

Some similar modeling are under progress, in 2D but also 3D, for evaporation or solidification.