High temperature process simulation

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Abstract: The purpose of this article is to show a simplified way of modeling for high temperature processes. For all processes of this type (crystal growth, heat treatment, deposition…) radiation is the most effective heat transfer way, but the three ways of heat transfer are non negligible, and they are coupled with some other phenomenon. These other phenomenon may be in electromagnetism field (for inductive heating), in chemistry field (for heating by combustion, diffusion of contaminant, reactive gaseous, or reaction product), multi phase flow, phase change (melting, solidification, condensation) … The main aim of our studies is usually to provide a thermal description to the researchers, to help their interpretation works of measurements and modeling works, or process engineers to improve the hardness of their design or adaptation of equipment and help them in investment decisions. So the procedure we follow and describe here is a simplified thermal modeling using comparison with measurement to increase precision of final results.

Keywords: high temperature thermal modeling, radiation.

1. Introduction

Two of the main technological problems of industry using high temperature processes are the knowledge of heat gradients (for example in case of solidification, crystal growth…), or temperature prediction in all parts of an equipment (for example for design purpose). In both cases the simplest way is an analytical estimation, but usually with precision lack. In the opposite side, numerical simulations tacking in account all physical and chemical phenomenon may be more precise but is still a research topics, and still needs very large computers and long calculations. The very general procedure we follow in order to propose concrete and efficient studies is a mixed approach of a predictive use of validated models and sensitivity studies on the uncertain models and parameters. Comparison with known temperatures are performed to improve precision an decrease sensitivity studies effort.

This procedure has been used in many field, for example in microwave simulation [1], and for high temperature process simulation. The example presented in this article deals with crystal growth in a reactor heated by hydrogen combustion.

2. Models

2.1 Methodology and models

As mentioned in introduction the goal of this study isn't combustion or solidification modeling, but "only" a thermal characterization of the reactor, with some precision on the crystal during it's growth. In this example, combustion is the most important phenomena for thermal analysis, because it is the heat source, but what we need to help industrial applications is only the heat source itself, not a precise combustion model. This is possible because our industrial collaboration allow us to improve and validate the complete model by comparison to experimental datas of three types:
- Phase change temperature (solidification temperature in this example),
- Process conditions (flow rates and crystal growth velocity),
- Temperature measurements when and where it's possible (external parts of the reactor in our case).

Following this simplified approach the solved models are:
- Mass conservation,
- Momentum conservation,
- Energy conservation taking in account heat transfer by conduction, gaseous convection, and radiation,

- Conservation of the reactive gaseous and product of the hydrogen combustion, resolved for water vapor and oxygen.

The combustion should be laminar, so we use the standard equations from COMSOL MULTIPHYSICS "weakly compressible Navier stockes (chns)", "General heat transfer (htgh)" and two "convection and diffusion (chcd)" for the water and oxygen mass fractions. The diffusion coefficients are estimated from the gaseous kinetic theory [2]. The source terms of each gaseous depends on the kinetics of the combustion which is chosen as an Arrhenius law with low activation energy. The rate is adapted in order to obtain the known flame temperature of 2810°C.

A solid powder of the deposited material is injected in the gas flow, melted, and then deposited on the crystal. The powder effect on the flow is not modeled (as a multiphase flow) because it is mass negligible. It's thermal effect is not negligible because the powder thermal radiation is much higher than the flame radiation. This radiation effect is taken in account by an arbitrary and constant thermal flux added to the radiation flux received by the crystal and reactor faces around the flame. This flux is chosen in order to obtain the fusion temperature on the crystal surface. To be conservative, the energy of this heat flux is subtracted to the heat source in the flame. In a similar way, the heat for powder melting is subtracted in the flame, and added to the crystal surface where th liquid is solidified.

2. 2 Geometry, mesh, and BC

The reactor is cylindrical then we use the 2D axi-symmetrical form of the models. Some detail which didn't follow this symmetry were not meshed. Their effect will be discussed or simulated in further parts of this study.

In all figures the axis of the reactor is on the left, the gaseous inlets are on the top of the figures, and the crystal is the cylinder on the axis. The reactor walls, on the right are made of different kind of insulators.

The mesh is made of quadrangle for more precision in the flow region, and also quadrangle but much larger in the outside part of the reactor. Triangle are use between both.

The boundary conditions are the oxygen and hydrogen flow rate on the inlets, atmospheric pressure at the bottom of the reactor, measured temperature on the external reactor walls.
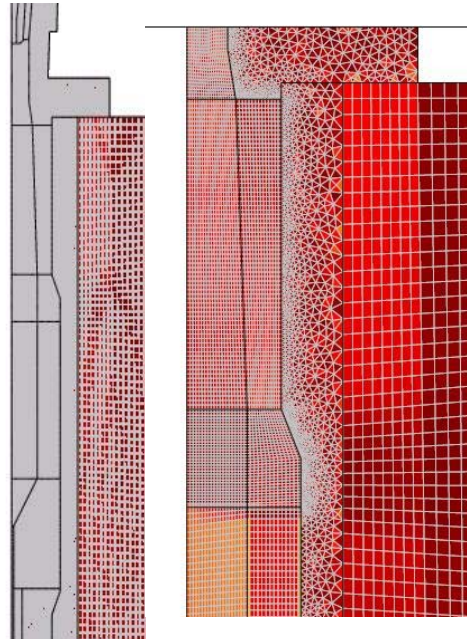

Figure 1. Geometry and mesh (left), and mesh detail (right)

3. Results

Du to the chemistry, and to radiative transfer at high temperature, the solved system is highly non linear. The convergence strategy is the following: we start the resolution by flow computation at room temperature, then we include diffusion and reactivity, and slowly increase heat source. At the end we include the flux modeling the powder radiation. The figure 2 shows flow velocity and temperature obtain during the increase of heat source.

When convergence is completed, the kinetic rate is adapted to obtain the real flame temperature, and the heat flux from powder radiation is chosen to obtain crystal temperature.

The velocity field shows the flow speed around the crystal, with the stagnation point on the crystal center and the horizontal flow shape going against the reactor insulator. This explain the wear of the insulator. The temperature field, after convergence, provide some data about insulators temperatures and possible improvement: best insulators may not be able to

be used at highest temperature, so they have to be chosen and designed following the prediction of temperature.
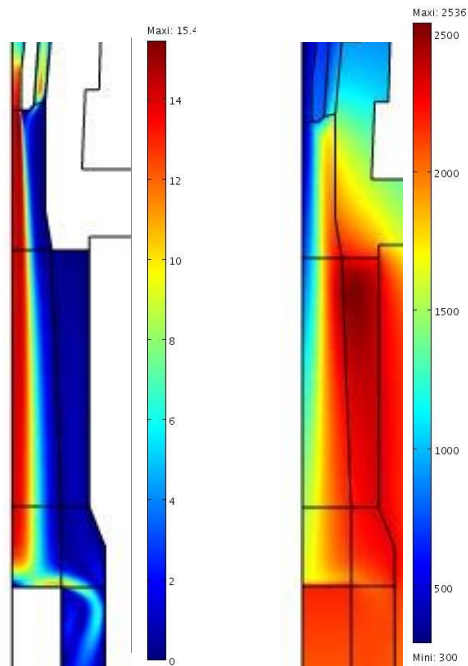

Figure 2. Intermediate results for gaseous velocity (m/s) on the left, and temperature on the right.
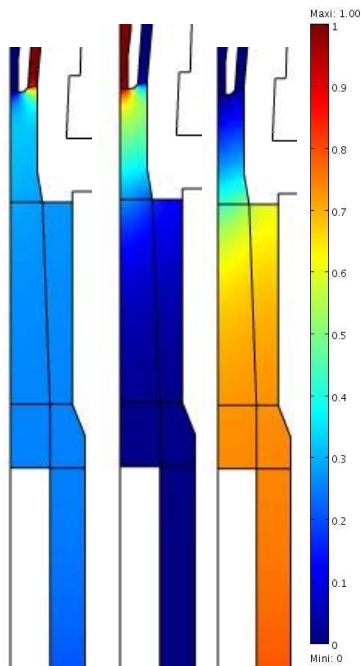

Figure 3. Mass fraction of hydrogen, oxygen and water vapor from left to right.

The gas mixture composition is given on figure 3: the oxygen and hydrogen composition decrease in the flame region to form water vapor.

The precision of this procedure is checked in two ways:
- Sensitivities to the worst known parameters are checked: emissivities, powder radiation, kinetics, and diffusions.
- Sensitivities to process conditions are also checked and compare to real results: flow rates, flow rate sensitivity to geometrical modifications.

These sensitivity studies show that the results are mainly sensitive to the diffusion, but this does not affect a lot the final results: The exact reactive concentration and gradient depends on kinetics and diffusivities, but they don't change if the heat source has the good place, and if the main temperatures (crystal, flame) are the good one. In other words, the flame length change with some parameters of the model. But when the flame length is the good one, the temperature field in the crystal and the reactor are unchanged even by changing these parameters.

The sensitivity work on process conditions and geometrical modifications allow to check the model precision. The precision is good for gradient prediction in the crystal but may be increased by 3D effect modeling for temperature prediction of the reactor and crystal surface. Another conclusion is that the temperature gradients are highly sensitive to reactor dimensions.

The final results, and most interesting for industrial application is the thermal flux in the crystal, which is an image of temperature gradients. The figure 4 and 5 show respectively the radial and vertical components of the thermal flux. The high values near the corner (figure 4) are a radiation effect, the highest value isn't significant. The radial flux vanished far from the surface. The vertical flux is high around the crystal corner and also at the bottom.

Figure 4. Thermal flux, radial component, in the top part of the crystal, during growth.
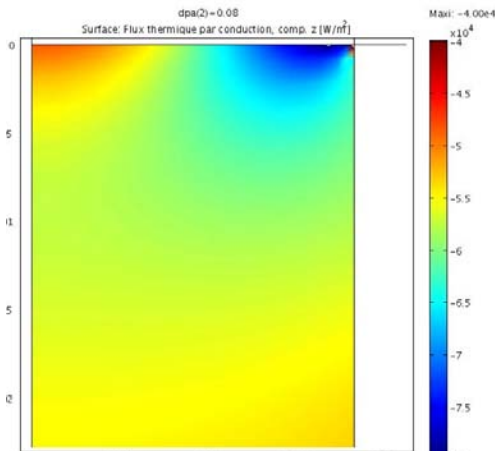
Figure 5. Thermal flux, vertical component (K/m) in the top part of the crystal, during growth.

4. Conclusions

The crystal growth industry usually use high temperature process. To improve production efficiency, as well as research team interpretation and modeling capacities, a good knowledge of thermal effects is necessary. We show in this article a methodology to get reliable data by mixing simplified models, sensitivity studies and parameters adjustments. This allow to improve knowledge and design capacities without too complex models, and to decrease experimental plan size by predictively modeling well known phenomenon. The precision is improved by increasing comparison with experimental measurements. We show some results in high temperature crystal growth, but also use such approach for thermal treatment process

simulation heated by induction, deposition process (COMSOL conference 2006), or microwave simulation (COMSOL conference 2007).

5. References

1. H. Rouch, O. geoffroy, "3D EM Simulation for microwave plasma coupling", *COMSOL Conference 2007*.
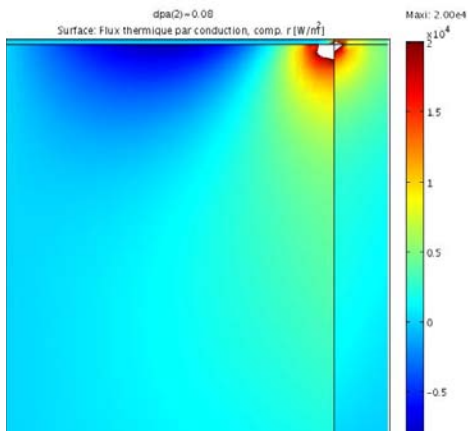2. R.Bird, W. Stewart, E. Lightfoot, "Transport Phenomena" John Wyley and Son NY (2002)