

Modelling of pellets in a sintering furnace using COMSOL Multiphysics®

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Abstract

In the nuclear fuel industry, sintering process is employed to transform ceramic pellets into dense, solid structures. The natural sintering occurring in the furnace operates through controlled heating and atmosphere, below the melting point and without external forces. This sintering furnace involves coupled physical phenomena and hosts a uranium oxide conversion reaction taking place upstream in the pre-sintering region. Modeling this process with COMSOL Multiphysics® offers valuable support for optimizing industrial performance and improves the quality of the final products.

Ceramics pellets are loaded in boats conveyed thanks to a walking beam through the furnace. The model focuses on the journey of a boat filled with pellets along the process, where heat transfer, chemical reaction, densification and mechanical stress occur. In the pre-sintering zone, the uranium sesquioxide present in a small fraction reacts to become uranium dioxide. The uranium dioxide pellets enter in a zone where the sintering process takes place. After initially focusing on a single isolated boat, the thermal analysis is refined by incorporating adjacent boats and the walking beam, allowing radiative view factors, setpoint temperature heterogeneity, and heat transfer from surrounding components to be considered. For the chemistry study, the exothermic nature of the reaction is studied as well as the mechanical stresses generated by the change of stoichiometry during the transformation. Then, the influence of humidity on densification during sintering is investigated to optimize operating conditions. To test different configurations on geometry or operating conditions, a user interface has been developed using COMSOL Server™ which provides remote access to the model over a secure HTTPS connection.

The developed model provides detailed access to key outputs, including temperature distribution, reaction extent, and stress fields. These results enable a quantitative comparison of the different configurations tested along with a better understanding of the interaction between the various physical phenomena occurring within the furnace. All these features are integrated into the user interface, enabling efficient sensitivity analysis of the most influential parameters.

Keywords: Sintering furnace, heat transfer, chemical reaction, densification, structural mechanics, user interface.

1. Introduction

Numerical simulation represents an increasingly valuable tool for understanding and optimizing the complex physical phenomena involved in the industrial production of nuclear fuel pellets. Among the different manufacturing steps, the sintering furnace combines heat transfer, chemical reactions, densification and mechanical effects that strongly influence the quality of the final product. To overcome the lack of literature on this specific process, a coupled thermal, chemical, and mechanical model was recently developed using COMSOL Multiphysics®[1], focusing on the journey of an isolated pellet-filled boat through the furnace.

As a direct extension of that initial study [1], this work extends the simulation capabilities to better represent the industrial furnace and to investigate additional coupled phenomena involved during the process. The thermal model has been enhanced by accounting for the influence of neighboring boats and the walking beam, providing a more realistic description of radiative and conductive heat transfer. Furthermore, the uranium oxide conversion reaction occurring in the pre-sintering zone is investigated through its thermal and mechanical effects, while the influence of humidity on densification during sintering is assessed to optimize operating conditions. Finally, the model has been integrated into a user interface based on COMSOL Server™, enabling rapid evaluation of different operating conditions and geometrical configurations.

Following an overview of the updated model configuration, these new multiphysics results are discussed.

2. Experimental Set Up

The sintering furnace is used to produce dense uranium oxide pellets through a combination of chemical conversion and thermal treatment. Pellets are placed in boats that are continuously conveyed through the furnace, which is divided into three successive sections: pre-sintering, sintering and cooling.

The uranium oxide conversion takes place in the pre-sintering zone, where the residual uranium sesquioxide reacts with injected dihydrogen to form uranium dioxide. This reaction is considered complete before the pellets reach the sintering zone. During this stage, the additives initially contained in the powder are also removed, leaving only uranium dioxide.

The thermal and gaseous environment is controlled by heating elements and gas injectors distributed along the furnace. Temperature, hydrogen concentration and water vapor profiles are prescribed throughout the process to define the local conditions surrounding each boat.

The boats are transported by a walking beam through the furnace. As they enter the sintering zone, the temperature rises to activate the densification process. The pellets are then progressively cooled in the final section before leaving the furnace.

3. Numerical Models

The following studies have been conducted independently, based on the model presented in a previous article [1].

3.1 Geometry

The study is performed at the boat scale using the geometry introduced in our previous work [1]. Both 2D and 3D models are employed depending on the investigated physics, with symmetry used to reduce the computational cost. The complete description of the geometry and modelling assumptions is available in [1].

To improve the thermal model, elements surrounding the boat have been added to the geometry and are presented Figure 1. These new

elements are only considered in the heat transfer model refinement, while the other studies are based on the previous geometry and results.

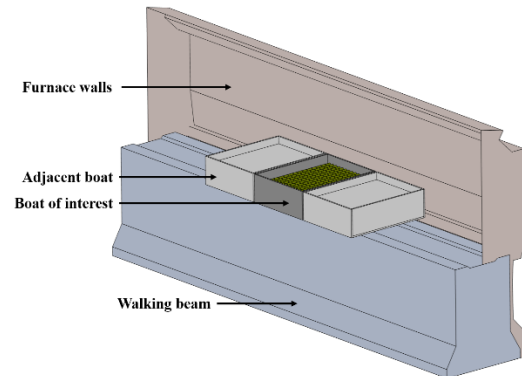


Figure 1: 3D geometry used for the new thermal model. Only half of the furnace walls are represented.

3.2 Heat transfer model refinement

The heat equation detailed in the previous article [1] is solved in all solids (three boats, pellets and the walking beam). For the two adjacent boats, the pellets/gas inside are represented as an equivalent block where each property is calculated as an equivalent property to the pellet/gas mixture. The *Surface-to-ambient radiation* boundary condition is now replaced by a *Surface-to-Surface Radiation* physics interface. All solid surfaces adjacent to the gas radiate energy to one another. Now, the temperature of the furnace walls depends on their relative position to the specific boat. In each section of the furnace, the temperature of the walls is still homogenous. A symmetry condition (normal boundary flux =0) is applied to each extremity of the beam.

3.3 Consideration of the exothermic nature of the chemical reaction

A chemical reaction occurs in the pre-sintering zone. The pellets originally made of U_3O_8 (considered as $UO_{8/3}$) and UO_2 transforms into pure UO_2 pellets thanks to H_2 and heat.

The chemical reaction studied is exothermic: heat is released during the transformation from U_3O_8 to UO_2 . To evaluate if this phenomenon is negligible, a study considering this exothermic behavior has been conducted. Numerically this study adds a coupling from chemistry to thermal physics, which was previously neglected.

The enthalpy of the reaction is taken into account in heat transfer physics by adding a heat source equal to:

$$\Phi_{chemistry} = -r_{UO_{8/3}} * \Delta_r H \quad [W/m^3]$$

With $r_{UO_{8/3}}$ the reaction rate detailed in the previous article [1], and $\Delta_r H$ the enthalpy of the reaction. Locally, the temperature may increase which may accelerate the reaction.

3.4 Effect of the chemical transformation on mechanical stresses

The chemical transformation induces a change of stoichiometry. The molar volume of $UO_{8/3}$ is higher than the one of UO_2 . To account for this densification, the molar concentration of the two species during the reaction needs to be extracted from the 2D-chemical model (detail in [1]) to be used in the 3D-mechanical model.

After computing the 2D-chemical simulation, the 2D molar concentration fields are extracted and extruded in the direction of the length of the pellet (missing direction in the 2D cut plane) thanks to *General Extrusions*. The concentrations are then considered homogeneous in the length direction and are now available in the 3D component.

These concentrations are used in the expression of the volumetric deformation dL :

$$dL = \sqrt[3]{\frac{[c_{UO_{8/3}} * M_{UO_{8/3}} + c_{UO_2} * M_{UO_2}]}{\rho_{app}}} - 1$$

With c_i the molar concentration of species i , M_i the molar mass of species i and ρ_{app} the apparent relative density assumed to be constant in the pre-sintering zone. The mechanical approach using this deformation is detailed in the previous article [1].

3.5 Effect of humidity during sintering

To study the densification process during sintering, a macroscopic data-based model has been developed and detailed in the previous work [1].

The densification law currently in use assumes a dry atmosphere. The same law is derived from data obtained in a humid atmosphere (Figure 2). Linear interpolation and extrapolation between the dry and humid laws are performed to obtain a global law that accounts for humidity dependence. This main law can be refined if additional experimental data becomes available in the future.

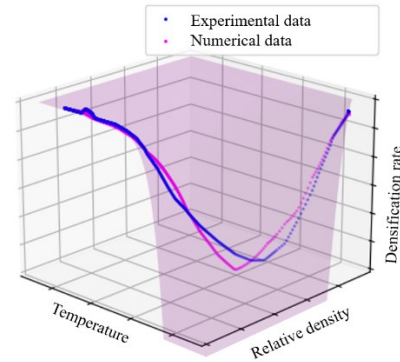


Figure 2: Numerical law under humid atmosphere linking densification rate, relative density and temperature based on experimental results.

To feed the enriched densification law, the local amount of water present in the pellets needs to be accessible. The local molar fraction is already available in 2D for the pre-sintering zone thanks to the 2D-chemical study [1]. For the rest of the process, the H_2O molar fraction is calculated with a pure diffusion model as an extension of the 2D-chemical model, initializing with its last results to assure continuation.

$$\frac{\partial c_{H_2O}}{\partial t} - \nabla \cdot (D_{H_2O/i} \nabla c_{H_2O}) = 0$$

where c_{H_2O} is the molar concentration of H_2O [mol/m³], and $D_{H_2O/i}$ is the H_2O diffusion coefficient in medium i (gas or pellet) [cm²/s]. This equation is implemented using the *Transport of Diluted Species* physics interface.

A gaseous sky imposing a H_2O molar fraction on top of the pellet stack is considered while no chemical reaction is assumed to occur after the chemical reaction study.

Using a *General Extrusion* operator, the 2D H_2O volume fraction is mapped along the longitudinal direction, making the local H_2O content available to the 3D densification model and the subsequent mechanical analysis [1].

3.6 Numerical aspects

The meshing strategy and solver settings are based on those presented in our previous work [1]. The new 3D geometry mesh is built around the boat of interest (Figure 3) and still exploits the symmetry. For this boat, a swept mesh is employed for the 3D model, while a finer 2D mesh is used for the chemistry calculations to accurately capture diffusion and reaction fronts. All studies are time-dependent except for the quasi-static mechanical analysis, and

iterative and segregated solvers are used to efficiently handle the coupled multiphysics problem.

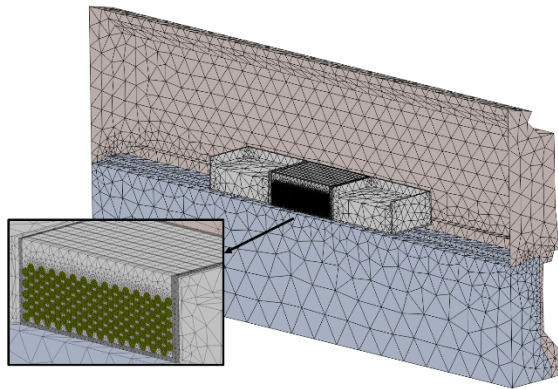


Figure 3: 3D-model mesh view

4. Results and Discussion

New heat transfer results:

The temperature field visible in Figure 4 verifies that the heat comes from the front of the furnace during heating. To interpret this new approach and the consequences on the whole process, heat flux as well as thermal gradients have been studied.

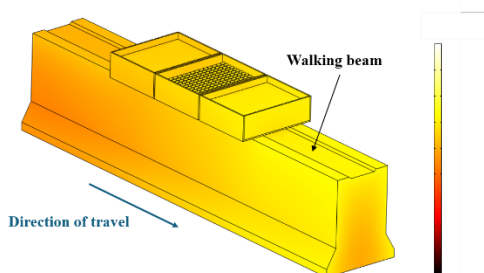


Figure 4: Snapshot of temperature in half the geometry during heating.

Figure 5 reveals a heterogeneous radiation pattern within the furnace, leading to an uneven distribution of thermal energy. Unlike the previous homogeneous heating, heat losses are observed at the rear while additional heat is received at the front during the heating, resulting in asymmetric thermal behavior and modified thermal gradients. Consequences of these new results on the mechanical model have been studied although it is not detailed in this paper.

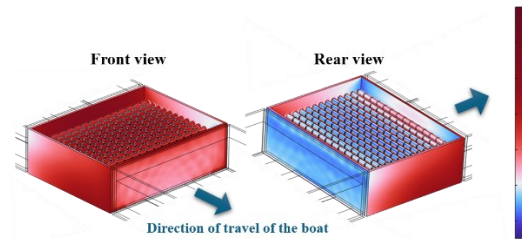


Figure 5: Snapshot of radiating flux received (red) and emitted (blue) by the boat and pellets during heating.

Effect of the exothermic nature of the reaction:

Including the exothermic nature of the transformation makes it possible to evaluate the heat released by the reaction (Figure 6). As expected, the heat generation is highest at the reaction front and decreases behind it, following the reaction rate.

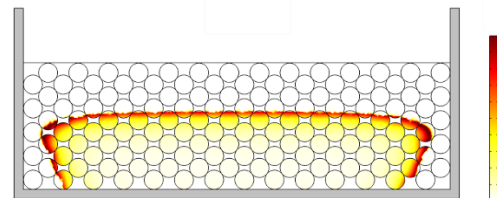


Figure 6: Snapshot of the heat flux generated by the chemical transformation.

Mechanical stresses induced by chemical reaction:

The reaction front is visible in Figure 7 where the von Mises stresses on a selected pellet are represented. The highest mechanical stresses are concentrated at the reaction front, where the deformation is directly induced by the local concentration changes associated with the chemical transformation.

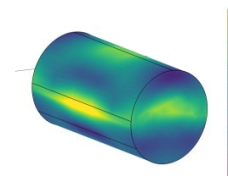


Figure 7: Snapshot of the von Mises stresses generated by the chemical reaction.

These stresses have been compared to those generated by sintering to evaluate if they can be assumed negligible or not.

Effect of humidity during sintering:

The humidity study provides access to the evolution of water content within the pellets throughout the process (Figure 8). Water originates both from the uranium oxide conversion reaction and from the controlled humidity of the furnace atmosphere.

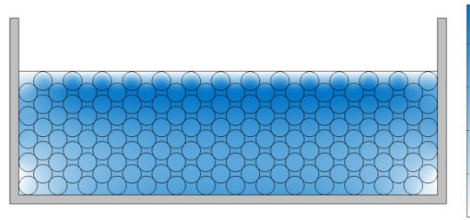


Figure 8: Snapshot of the H_2O volume fraction

This approach makes it possible to assess the influence of water content on the densification kinetics during sintering (Figure 9), as well as on the mechanical stresses generated within the pellets.

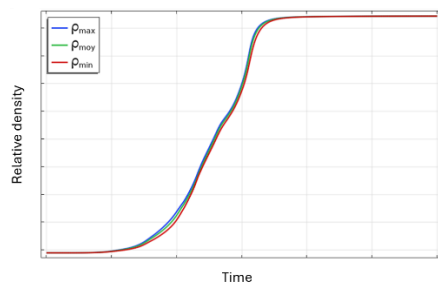


Figure 9: Evolution of the maximum, average and minimum relative density of a selected pellet over time under a humid atmosphere.

These results provide valuable insights for optimizing the furnace atmosphere humidity in order to improve the quality of the final product.

5. User interface

The interface was developed by SIMTEC with the COMSOL Application Builder. This application is used by Framatome through COMSOL Server™, which provides secure remote access over HTTPS to the model hosted at SIMTEC.

The application is divided into three sections. The input section enables users to modify geometry, operating conditions, and material properties. Setpoint curves can be defined through editable tables, and predefined configurations can be selected from a drop-down menu. The button section provides controls to update the geometry and launch the different studies depending on the physics considered. The results section includes the available post-processing tools, with results exportable as images or as .txt files for plotted curves. A glimpse of the interface in presented Figure 10.

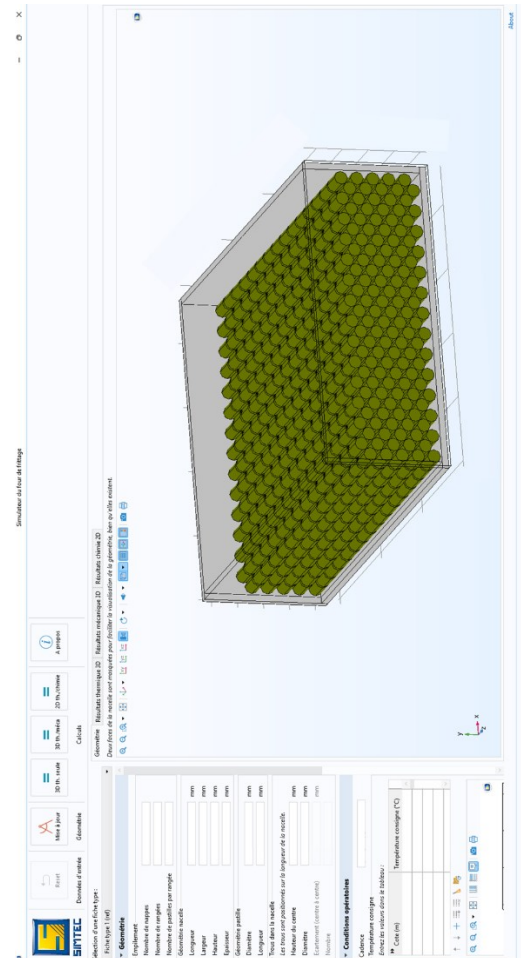


Figure 10: View of the executable COMSOL app interface

6. Conclusions

This work extends the previously developed COMSOL Multiphysics® model of the sintering furnace by improving the description of heat transfer and introducing additional chemical, mechanical and humidity-related couplings. The model provides deeper insight into the interactions between the different phenomena occurring during the process and offers an efficient tool for evaluating operating conditions through the developed COMSOL Server™ application. Future work will focus on validating the model against experimental data and performing sensitivity analyses to identify the most influential process parameters.

References

- [1] J. Pérard, G. Raveu, F. Viry, P. Namy and J. Bischoff, "Modelling of a sintering furnace using COMSOL Multiphysics®," in *COMSOL Conference*, Amsterdam, 2025.

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