

Modelling of a dry conversion furnace using COMSOL Multiphysics®

J. Pérard¹, C. Nicollet², A. Marie², P. Namy¹, J. Bischoff²

¹ SIMTEC, Grenoble (France)

² FRAMATOME, Romans-sur-Isère (France)

Abstract

In nuclear fuel manufacturing, dry conversion is a key step used to produce UO_2 powder from crystalline UF_6 for subsequent pellet fabrication. The properties of the final material are highly sensitive to operating conditions, which makes a thorough understanding of the process crucial for maintaining both safety and supply reliability. These processes involve materials that are challenging to handle and require high-temperature operation. In this context, numerical modeling and simulation provide valuable support for process analysis and optimization.

The dry conversion step is a continuous chemical sequence combining a reactor and a furnace. Once treated in the reactor, the powder is transferred into a heated tubular furnace where it is transported along its length. During this stage, UO_2F_2 is gradually converted into UO_2 through successive gas–solid reactions, involving both exothermic and endothermic mechanisms, with gases flowing in counter-current to the powder.

The furnace has been modelled using COMSOL Multiphysics®. A one-dimensional approach is employed to model the thermochemistry along the furnace, enabling the determination of reaction locations, temperature profiles within the equipment, and the composition of the produced powder. To evaluate the level of temperature heterogeneity on transversal section, a two-dimensional-thermal model is developed in different cut planes along the furnace. Then, the grains dynamics is modelled in a two-dimensional approach to estimate the proportion of powder above and in the powder likely to react with the gas. A user interface has been developed to enable easy adjustment of operating conditions. COMSOL Server™ provides remote access to the model over a secure HTTPS connection.

These models provide a deeper understanding of the chemical reactions occurring within the furnace, the temperature field, and how the furnace rotation impacts powder distribution. Sensitivity studies on operating conditions can be conducted using the user interface to optimize parameters and thereby enhance the quality, efficiency and productivity of the process.

Keywords: Dry conversion, Rotating furnace, Thermochemistry, Heat transfer, Temperature heterogeneity, Particle dynamics, Gas–solid interaction

1 Introduction

The dry conversion of uranium is a critical stage in nuclear fuel manufacturing, during which enriched UF_6 is transformed into UO_2 powder before pellet fabrication. The process consists of a reactor followed by a rotating tubular furnace, where the powder undergoes successive gas–solid reactions while being transported through a high-temperature environment. Numerical models have been developed for both the reactor and the furnace; however, the present work focuses exclusively on the furnace.

The furnace involves strongly coupled phenomena, including chemical reactions, heat transfer, gas flow,

and powder motion. The one-dimensional thermochemical model previously developed for the furnace is refined by developing a two-dimensional thermal model to account for temperature heterogeneities across the tube cross-section. In addition, a two-dimensional model of powder dynamics is developed to investigate the influence of tube rotation on powder distribution and gas–solid contact. These complementary models are implemented in COMSOL Multiphysics® and coupled with a dedicated user interface, enabling operating conditions to be easily modified and sensitivity analyses to be performed. This approach provides an improved framework for understanding and optimizing furnace operation.

2 Process Description

The furnace consists of a slightly inclined rotating tube through which the powder is transported. The tube is maintained at high temperature, while a mixture of H_2 and H_2O flows counter-currently to the powder. Within the furnace, the UO_2F_2 powder undergoes a sequence of gas–solid reactions leading to its progressive conversion into UO_2 . First, UO_2F_2 reacts with H_2O to form UO_3 and HF . UO_3 then decomposes into U_3O_8 , releasing O_2 , before U_3O_8 is finally reduced by H_2 to produce UO_2 and H_2O .

The counter-current gas flow is directed back towards the reactor, while the remaining gases leave the process through filters designed to prevent uranium powder losses. In the long term, powder deposition on the tube walls and filters can lead to clogging, requiring maintenance operations and reducing the overall process productivity.

3 Numerical Models

The model is split into four models: a gas flow model in 3D which is not detailed in this article (see [1]), a 1D-thermochemistry model, a 2D-thermal model and a 2D-grain dynamics model.

3.1 Thermochemical Model

A one-dimensional thermochemical model is used to describe reactive transport along the rotating tube. This model is detailed in the previous article [1]. The uranium conversion is represented by four heterogeneous and homogeneous reactions involving the successive transformation of UO_2F_2 , UO_3 , U_3O_8 and UO_2 . Solid species are described by convection–reaction equations, whereas gaseous species are modeled in two interacting domains: the gas region above the powder bed and the porous powder bed, using coupled convection–diffusion–reaction equations. Mass exchange between these two domains is represented by an interphase transfer term proportional to the concentration difference. Reaction rates depend on the local temperature, gas composition, and the fraction of powder present in each domain.

The thermal model simultaneously describes the temperatures of four elements: the gas, powder bed, tube, and pyrometric cane through coupled one-dimensional energy balance equations. These equations account for axial convection and conduction, heat released or consumed by chemical reactions, heat exchanges between the different media (forced convection and radiation), and heat

exchanges with the external environment. Because the model is one dimensional, the temperature is assumed to be homogeneous in the perpendicular cut plane. The complete thermo-chemical model is solved at steady state.

3.2 2D Thermal Model

The main goal of this model is to estimate temperature variations in six cross-sections perpendicular to the length of the furnace and their effects on the chemical reactions.

The heating elements heat uniformly (in yellow) to maintain the temperature of the control thermocouple at its setpoint (pink dots). Heat is transferred to the rest of the cross-section by conduction (dark blue arrows) or radiation (green arrows), while the rotation of the tube is accounted for by convection, without any rotation of the geometry (orange arrow). The tube is defined as a fluid with a specific velocity field. Natural convection in air (purple arrows) and forced convection in gas (red arrow) are accounted for by enhanced thermal conductivity.

The outer surface of the bricks is maintained at a certain temperature (light blue arrows) to dissipate heat toward the workshop.

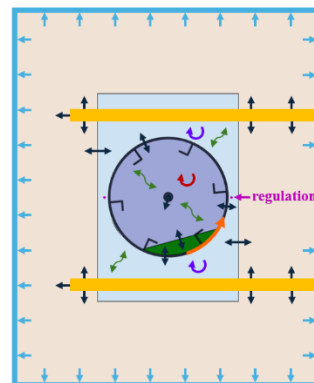


Figure 1: Drawing of the boundary conditions of the 2D-cut plane thermal model

The average temperature of the elements of the 1D thermochemical model (powder, gas, pyrometric cane, and tube) is maintained at the temperature predicted by the 1D model. This allows for out-of-plane conduction and convection, as well as the effect of chemical reactions, to be considered. For each element and each cut plane, the temperature from the thermochemical study is used in a *Heat source*:

$$q_i = 10^9 * \left(T_i^{1D} - \frac{\iint T_i^{2D}(x,y) dS}{S_i} \right)$$

Where i refers to powder, gas, pyrometric cane or tube, T_i^{1D} is the temperature of element i from the 1D study, $\frac{\iint T_i^{2D}(x,y) dS}{S_i}$ is the average temperature of element i .

The 2D-thermal model is solved at steady state for each cross section thanks to an *Auxiliary sweep*, with a direct and fully coupled solver.

3.3 Grain Dynamics Model

The rotating tube, equipped with lifters, suspends a fraction of the powder bed. The amount of powder in suspension may be a key parameter governing the overall reaction kinetics within the tube. The aim of this work is to improve the estimation of the suspended powder fraction through numerical modeling of powder dynamics in a cross-sectional plane of the tube, considering gravity, particle packing, and gas-particle drag.

This study uses the *Particle Tracing Module* and assumes a particular approach: each grain position is modeled. The grains are supposed to be spherical. The modeling is based on a number N of grains with a specific diameter Φ and density ρ depending on operating conditions. For each particle, the second Newton's law of motion is solved:

$$m \cdot \vec{a} = \vec{F}_g + \vec{F}_c + \vec{F}_d$$

With m the mass of the particle, $\vec{a}$ the acceleration vector, $\vec{F}_g = m \cdot \vec{g}$ the gravitational force, $\vec{F}_c$ the contact force and $\vec{F}_d$ the drag force.

Drag force:

To account for the aerodynamic drag acting on particles during their fall, the Schiller-Naumann law is used [2].

$$\vec{F}_d = m \cdot \frac{3\mu_{\text{gas}} Re_r}{4\rho\Phi^2} \cdot C_D \cdot (\vec{u}_{\text{gas}} - \vec{v})$$

With μ_{gas} the gas viscosity, Re_r the relative Reynolds number, ρ the particle density, Φ the particle diameter, C_D the drag coefficient, $\vec{u}_{\text{gas}}$ the gas velocity, and $\vec{v}$ the particle velocity. The gas is assumed to be static on the cut-plane.

Contact force:

The contact force is made of a spring and a damping contribution [3]. Both forces are applied to each particle and follow the same methodology. The global force applied is the sum of all particle contributions on particle i . For example, for the global spring force:

$$\vec{F}_{s_i} = \sum_{\substack{j=1 \\ j \neq i}}^N \vec{F}_{s_{j/i}}$$

The force of one particle j on particle i is expressed as follows:

$$\vec{F}_{s_{j/i}} = -k \cdot (d(t) - d_t) \cdot \vec{n}_i$$

With k the contact stiffness, $d(t)$ the distance between center of the two particles, $d_t = R_i + R_j$ the threshold distance (distance between the two centers at the impact), and $\vec{n}_i$ the vector tangent to the two centers alignment, pointing at the opposite direction of the impact.

For the damping force, only the force of particle j on particle i changes:

$$\vec{F}_{d_{j/i}} = -\mu \cdot [(\vec{v}_i - \vec{v}_j) \cdot \vec{n}_i] \cdot \vec{n}_i$$

Where μ is the contact damping.

The two forces $F_{s_{j/i}}$ and $F_{d_{j/i}}$ only apply if the two particles are interpenetrating, i.e., when the distance between the two centers is smaller than the distance of the centers at the impact.

This contact model depends on two parameters: k and μ which can be set by evaluating the contact duration or the restitution coefficient [3].

Particles are released in a specified area within the cut plane.

To allow the walls to rotate, the walls' edges are made of specific particles undergoing a rotating force. This makes it possible to model damped rebounds of free particles on the moving walls.

The grain dynamics model is solved with a time dependent study to complete a full rotation of the tube. The mesh used for this study is visible Figure 2:

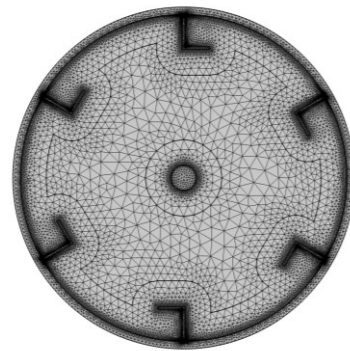


Figure 2: Grain dynamics mesh view.

4 Results and Discussion

2D-thermal and new 1D-thermochemical results:

The newly developed two-dimensional thermal model provides access to the temperature distribution within the different cross-sectional planes of the tube. This temperature field is used to calculate the local rates of the four reactions in both the gas phase and the powder bed (Figure 3). For each cross-sectional plane and each reaction, the spatial average reaction rate is calculated separately in the gas phase and in the powder bed. These average rates are then compared with the corresponding rates predicted by the one-dimensional thermochemical model.

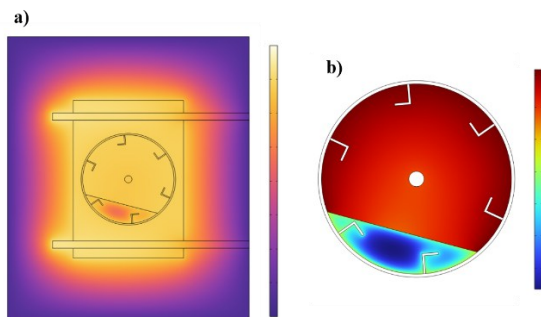


Figure 3: a) Temperature field and b) reaction rate of one of the four reactions, of a selected cut plane.

A significant difference between the two predictions indicates that temperature heterogeneities within the cross-section cannot be neglected. To refine the one-dimensional thermochemical model and indirectly account for these heterogeneities, the ratio between the two-dimensional and one-dimensional reaction rates is applied as a correction factor to the reaction rates predicted by the one-dimensional model. This correction is applied for each cross-sectional plane, each reaction, and each domain, namely the gas phase and the powder bed. Results of this refinement are visible Figure 4.

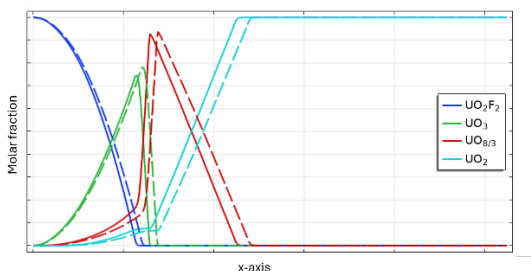


Figure 4: Solid species distribution along the furnace before and after applying 1D/2D reaction rate ratio (solid or dashed curves).

Grain dynamics results:

The particle dynamics model is used to simulate the motion of a given number of particles. Increasing the number of particles improves the representativeness of the simulation but also increases the computational cost and simulation time. The model provides insight into particle behavior during furnace rotation and their spatial distribution within a cross-sectional plane (Figure 5). In particular, it enables a more accurate estimation of the fraction of powder in flight over time.

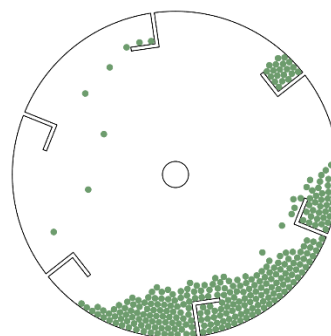


Figure 5: Grains dynamics modelling in a dry conversion rotating furnace

5 User interface

A dedicated user interface was developed by SIMTEC using the COMSOL Application Builder. The application is deployed on COMSOL Server™, enabling Framatome users to securely access the model remotely via HTTPS while it remains hosted by SIMTEC.

The application is divided into four sections, representing the four available models (left side). The input section enables users to modify operating conditions while results are accessible after the computation. The post-treatments are exportable as images or as .txt files for plotted curves. A glimpse of the interface in presented Figure 6.

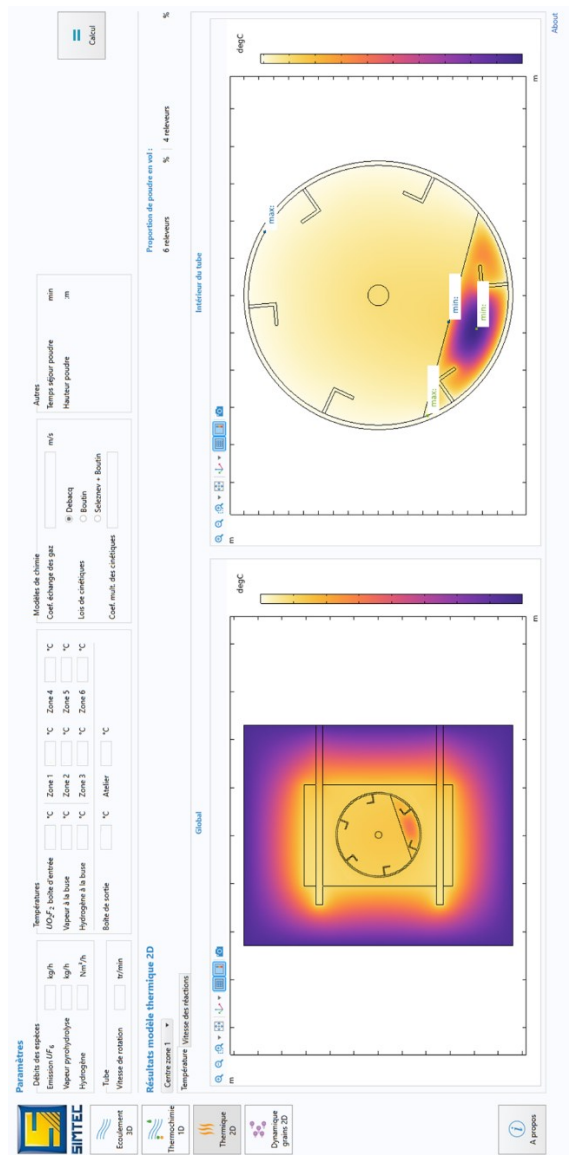


Figure 6: View of the executable COMSOL app interface

6 Conclusions

This work presents complementary models developed to improve the understanding of the dry conversion furnace. A two-dimensional thermal model was used to quantify temperature heterogeneities across the furnace cross-section and to refine the previously developed one-dimensional thermochemical model. In addition, a two-dimensional particle dynamics model was developed to investigate powder motion during tube rotation and improve the estimation of the fraction of powder in flight.

The models were integrated into a dedicated COMSOL application, providing a practical tool for

investigating the influence of operating conditions on furnace behavior. This framework offers new insight into the coupled thermal, chemical, and powder dynamics phenomena governing the conversion process.

The next step will be to validate the models through comparison with experimental measurements and to use the resulting framework to evaluate the effects of potential process modifications.

References

- [1] F. Viry, C. Nicollet, A. Marie, P. Namy and J. Bischoff, "Modeling the Dry Conversion Process with COMSOL Multiphysics®," in *COMSOL Conference*, Amsterdam, 2025.
- [2] *COMSOL 6p2 Particle Tracing User's Guide*, p. 273.
- [3] R. L. Rangel, "DEM Contact Force Models," 2021.

Acknowledgements

This work has been funded by Framatome and made in a fruitful collaboration between Framatome and SIMTEC.