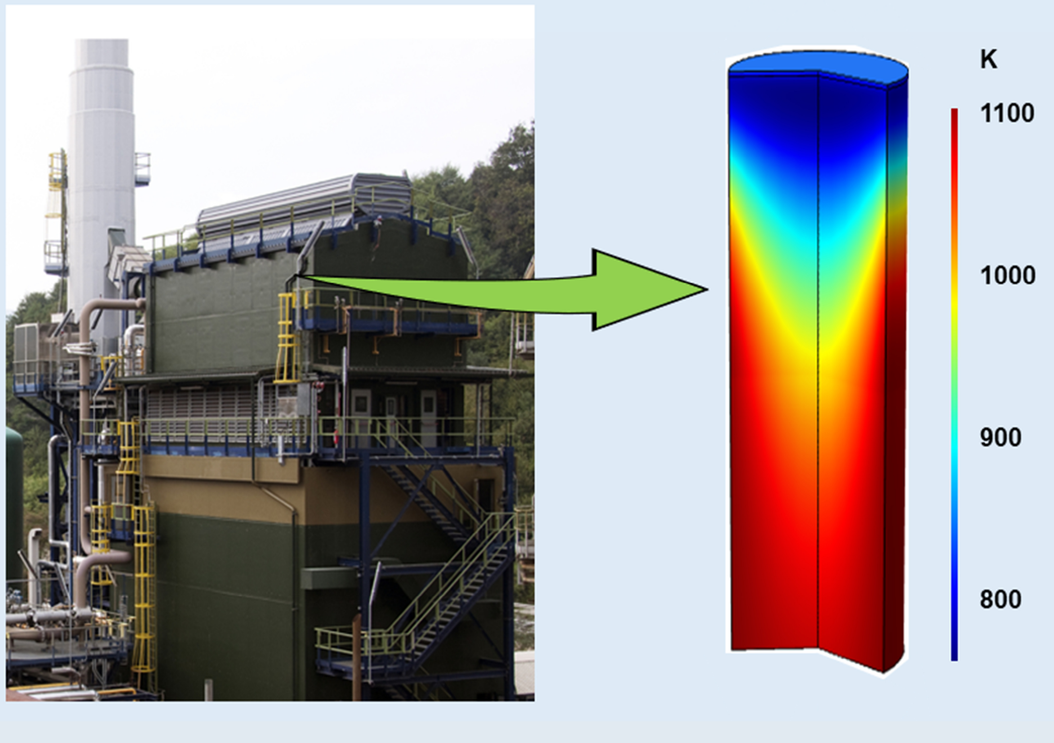


# COMSOL Multiphysics® Model of an Industrial Top-Fired Steam Methane Reforming Reactor

Steam methane reforming (SMR) chemical reactors are an established technology for hydrogen production. Multi-physics simulation is developed, and its predictive capability demonstrated.

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## Abstract

A first-principle fully-coupled multi-scale model is developed for a typical top-fired, packed-bed multi-tubular SMR reactor. The tubes contain two adjacent catalytic sections, filled with NiO supported on calcium aluminate commercial catalysts, with cylindrical-quadrilobe shape. All tubes are supposed to be identical and operated in identical conditions, and therefore only one tube is simulated. The predictive capability of the model is assessed through validation against previous literature results, as well as multiple sets of experimental data obtained from a full-scale industrial SMR reactor. The model makes it possible to account for the effects of the catalyst features, on the one hand, and the operating conditions of the furnace, on the other. The model provides a detailed study of the phenomena occurring inside the steam methane reforming reactor, paving the way for further detailed investigations such as for example coke deposition.

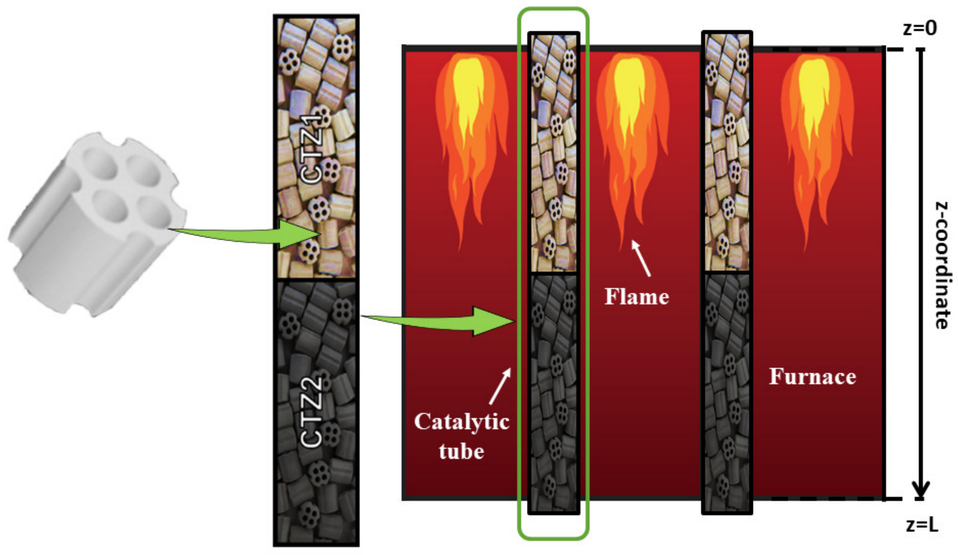


FIGURE 1. Left: Catalytic pellet. Middle: Detail of a catalytic tube. Right: Scheme of the furnace with the catalytic tubes.

## Methodology

At the microscopic scale, mass transport and reaction inside the catalyst pellets are simulated through a 1-dimensional model. At the intermediate (mesoscopic) scale, the catalytic tube model is based on local mass, energy, and momentum balances, coupled to a local reaction kinetics embedding the catalyst pellets model. The equations are written and solved in 2-dimensional cylindrical symmetry. At the macroscopic level, the tube simulation is then coupled to the furnace simulation. For the latter, a 1-dimensional model is proposed, based on local mass and energy balances, coupled to linear combustion kinetics. Overall, the model contains only one adjustable parameter i.e., $L_f$, the length of the flame in the furnace. The model equations are integrated through a finite element method in COMSOL Multiphysics®.

## Results

An exothermal combustion occurs in the furnace, and an endothermal SMR process inside the tube. This triggers heat transfer. Heat passes through the thickness of the tube wall by conduction and is subsequently transferred through the catalytic bed towards the center. Consequently, the process-gas temperature is higher close to the wall than at the tube axis, as reported in Figure 2. Figure 2 also shows the associated concentration profiles. At the inner tube wall, where the temperature is higher, the SMR reaction rate is faster and larger hydrogen production and methane consumption are predicted. All results show a clear deviation from ideal plug-flow behavior, reinforcing the need for a detailed non-ideal model for SMR reactors.

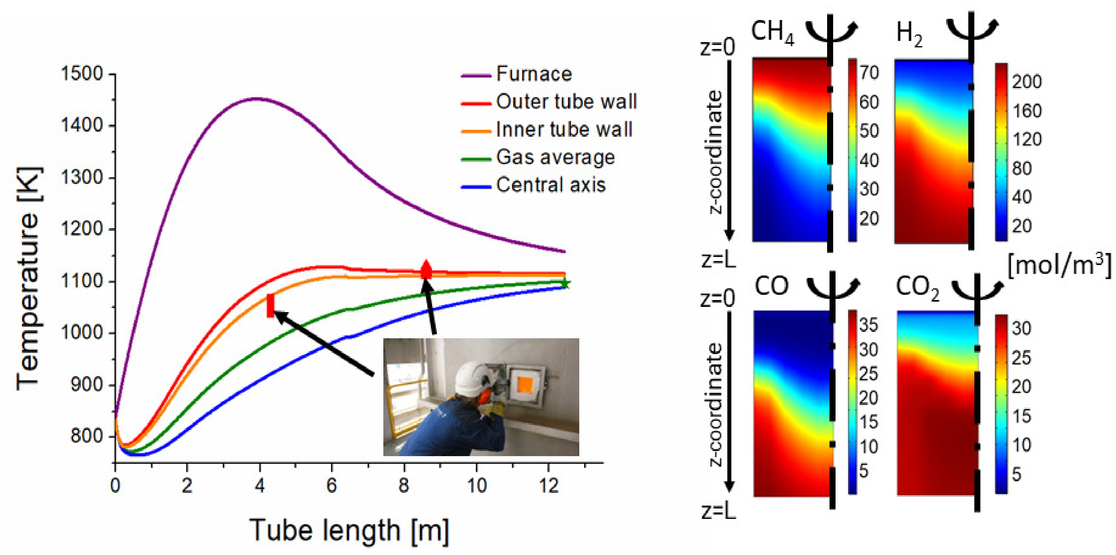


Figure 2. Left: temperature distribution along the furnace and the catalytic tube. Lines: simulation. Symbols: experimental data. Right: Concentration of chemical species along the tube.

## REFERENCES

V. Tacchino, P. Costamagna, S. Rosellini, V. Mantelli, A. Servida, "Multi-scale model of a top-fired steam methane reforming reactor and validation with industrial experimental data", *Chemical Engineering Journal*, vol. 428, Article number 131492, pp. 1-26, January 2022.

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