11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

PARAMETRIC AND MODEL UNCERTAINTY PROPAGATION IN CATALYTIC PARTIAL OXIDATION

Jorge E. P. Navalho*,[1], José M. C. Pereira[2] and José C. F. Pereira[3]

Universidade de Lisboa, Instituto Superior Técnico, Mechanical Engineering Department, LASEF, Av. Rovisco Pais 1, 1049-001, Lisbon, Portugal
E-mails: [1]jorge.navalho@ist.utl.pt, [2]jose.chaves@ist.utl.pt, [3]jcfpereira@ist.utl.pt

Key words: *Catalytic Partial Oxidation, Uncertainty Quantification, Foam Monolith, Synthesis Gas, Methane.*

The application of uncertainty quantification methods is a valuable procedure to gain insight on the impact of specific random parameters or uncertain model assumptions on the stochastic model solution. Several statistical methods have been employed in the literature to propagate uncertainty through a deterministic model. In particular, Monte Carlo methods are very robust techniques but at the same time are extremely demanding strategies due to the large number of deterministic simulations required to construct the stochastic solution. On the other hand, spectral projection methods based on polynomial chaos (PC) expansion are more efficient techniques [1]. In particular, non-intrusive spectral projection (NISP) methods based on polynomial chaos expansion have been widely used in the literature [2, 3]. NISP methods do not require the reformulation of the deterministic model and can be employed alongside with the deterministic model.
In this work the NISP method is employed to evaluate the parametric and model uncertainty in the autothermal catalytic partial oxidation of methane performed within a 80 ppi Al_2O_3 foam monolith reactor. The deterministic formulation to describe the catalytic partial oxidation of methane to synthesis gas is based on a 1D two-phase mathematical model that accounts for proper surface kinetic steps, external transport coefficients through suitable Nusselt and Sherwood correlations and radiative heat transfer. The current mathematical model was extensively validated in the past over a large range of operating conditions [4, 5].
The results of the application of the NISP method show the sources for the error bars of the relevant model solution variables. In particular, the uncertainty range prescribed for the porosity, the specific surface area and the ratio between catalytic and geometric surface area is the main responsible for the error bars observed in the stochastic output model solution for temperatures and product distribution along the reactor.

REFERENCES

[1] Dongbin Xiu and George Em Karniadakis. Modeling uncertainty in flow simulations via generalized polynomial chaos. *Journal of Computational Physics*, Vol. **187**, 137–167, 2003.

[2] M. T. Reagan and H. N. Najm and B. J. Debusschere and O. P. Le Maître and O. M. Knio and R. G. Ghanem. Spectral stochastic uncertainty quantification in chemical systems. *Combustion Theory and Modelling*, Vol. **8**, 607–632, 2004.

[3] M. A. A. Mendes and J. M. C. Pereira and J. C. F. Pereira. Calculation of premixed combustion within inert porous media with model parametric uncertainty quantification. *Combustion and Flame*, Vol. **158**, 466–476, 2011.

[4] J. E. P. Navalho, I. Frenzel, A. Loukou, J. M. C. Pereira, D. Trimis and J. C. F. Pereira. Catalytic partial oxidation of methane rich mixtures in non-adiabatic monolith reactors. *International Journal of Hydrogen Energy* , Vol. **38**, 6889–7006, 2013.

[5] J. E. P. Navalho, J. M. C. Pereira and J. C. F. Pereira. Conical-shaped foam reactors for catalytic partial oxidation applications. Accepted for publication in the *International Journal of Hydrogen Energy* , DOI:10.1016/j.ijhydene.2013.12.107.