COLLABORATIVE SIMULATIONS AND EXPERIMENTS FOR A NOVEL YIELD MODEL OF COAL DEVOLATILIZATION IN OXY-COAL COMBUSTION CONDITIONS

S. Iavarone[1,1], S.T. Smith[2], P.J. Smith[2] and A. Parente[1]

[1]*Universite´ Libre de Bruxelles, Ecole Polytechnique de Bruxelles, Aero-Thermo-Mechanics Laboratory, Bruxelles, Belgium*

[2]*University of Utah, Department of Chemical Engineering, Salt Lake City, UT, 84112, USA*

Introduction

Fossil fuels are expected to continue supplying much of the energy used worldwide. Among them, coal shows the most important growth in demand and it will still account for 30% of the overall electricity generated in 2030 [1]. To reduce the environmental concerns linked to the use of coal, oxy-combustion technologies are of intense industrial interest. The use of simulation tools such as computational fluid dynamics (CFD) appears necessary to allow the development of cost-effective oxy-coal technologies at a scale sufficient to augment existing energy options. CFD calculations can be applied directly at the industrial scale of interest, thus avoiding scaling-up the results from lab-scale experiments. Despite the improvements in the computational capability, the coupling of detailed chemistry models and CFD simulation can still be prohibitive for real combustors, which require large computational grids. In these cases, the development of scale-bridging models, namely reduced physics model with quantified model-form uncertainty to bridge scales from a more complex physics model, is necessary. Comprehensive CFD codes for the study and optimization of coal combustion in lab, pilot and industrial scale plants, demand a proper devolatilization model, being that devolatilization is the first step in thermochemical processes involving solid fuels that influences the overall subsequent reactions [2]. Devolatilization processes can be viewed from a kinetic or thermodynamic perspective. A comprehensive devolatilization model must be capable of capturing thermodynamic characteristic, i.e. the ultimate volatile yield of the coal, and the kinetics of how the coal reaches its ultimate yield. In industrial applications, kinetics occurs with very low time scales and within a minimal region of the whole domain: the amount of material transferred to the gas phase is judged to be more influential within the application than the rate at which this occurs. Hence, for this type of applications, thermodynamic effect must be deeply investigated. Devolatilization modeling has focused mostly on kinetics, providing significant uncertainty in the yield model functional form and parameters. In some cases, the dependency of ultimate-yield models on physical constraints and operating conditions is poorly modeled and the consistency with experimental data is not achieved. The ultimate/steady-state/equilibrium yield can always be obtained from a kinetic model, but obtaining accurate yields requires resolution of all time scales in the kinetic mechanism. An explicit equilibrium-yield model avoids the need to accurately integrate through these fast time scales and is thus highly desirable for a CFD application. For these reasons, the development of a yield model, derived through useful information gathered from collaborative experiments and numerical simulations, is required. This work presents a methodology for coal devolatilization modeling in the presence of uncertainty: an engineering approach, based on dataset consistency evaluation [3], and a Bayesian approach, based on Gaussian Process for Regression (GPR) [4], are involved for the development of a novel yield model for coal devolatilization. Requiring the joint analysis of experimental data and CFD simulations of an oxy-coal entrained flow reactor (EFR), the two approaches lead to a valuable evaluation of uncertainty in the data, in the model form and in the model parameters.

Conclusions

Two methodologies based on joint experimental and numerical investigations of coal devolatilization were used to propose a new yield model, for application in large-scale CFD simulations. The approach was demonstrated for the devolatilization of Sebuku bituminous coal in oxy-coal conditions, in the IFRF's entrained flow reactor. Preliminary CFD simulations using phenomenological (CPD) [5] and empirical (Biagini and Tognotti) [6] models were performed to identify the limitations of existing approaches in the prediction of coal conversion for conditions where equilibrium is reached.

A reduced physics model for the coal devolatilization yield has been proposed,

$$X_f = 0.5\left[1 + erf\left(\frac{T_p - T_1}{\sqrt{2}T_2}\right)\right], \qquad (1)$$

based on the particle temperature T_p and on only two parameters, T_1 and T_2, which we calibrated using a consistency analysis against the selected quantity of interest of the problem, i.e. the conversion or yield X_f. This model form was chosen because its codomain is

[1] Corresponding author: Salvatore.Iavarone@ulb.ac.be

equal to the interval [0,1], namely all the possible values of coal conversion. This function was embedded in the Single First Order Reaction (SFOR) model, which is the simplest and most used kinetic approach, easily included in CFD codes, and considers devolatilization occurring in a single step according to a first order law

$$\frac{dX}{dt} = A\exp\left(-\frac{E}{RT_p}\right)(X_f - X), \qquad (2)$$

where X is the coal yield (or conversion), t is the time, R is the ideal gas constant and T_p is the absolute temperature of the particle.

The results of the consistency analysis are shown in Figure 1.

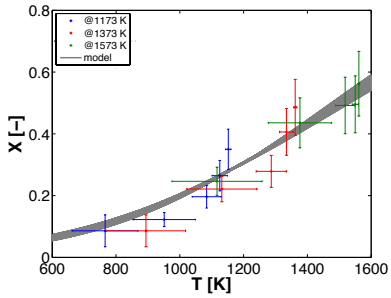

Figure 1. Experimental data with 18% relative error on conversion values and yield curve predicted by the new yield model (Equation 1) with the consistent values of T_1 and T_2. The data provided by the same test are grouped with the same color. Horizontal bars represent the particle temperature interval at each sampling point.

A Gaussian-Process Regression was performed, to improve the understanding of the uncertainty associated to the coal devolatilization process, based on the available experimental measurements. The novel yield model shown in Equation (1), with consistent parameters found through the methodology described in [3], fits the posterior model form outlined by the GPR approach (see Figure 2 and 3).

Once the model form and experimental uncertainties had been quantified with the two methods, CFD simulations were carried out using the novel ultimate yield model with first-order kinetics. Results show promising agreement between predicted and experimental conversion for all the examined cases.

The methodology developed in the present paper can be simply applied to alternative coal types, to derive scale-bridging models that describe both kinetic and thermodynamic aspects. This work shows an innovative methodology that joins experiments and simulations to assess the model-form uncertainty regarding the ultimate yield and that can be simply applied to alternative coal types, to derive scale-bridging models describing both kinetic and thermodynamic aspects. The process has the potential for continuous refinement, e.g. the inclusion of experimental data provided at temperature higher than 1600 K could greatly reduce the uncertainty in the model form for higher temperature applications, as it has been illustrated through the GPR approach.

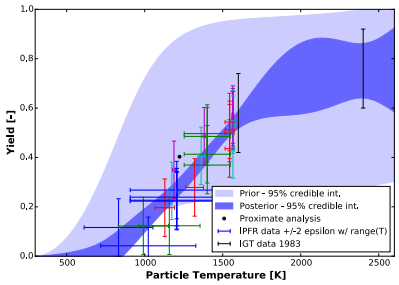

Figure 2. Prior credible interval, 95% (light shaded area), posterior credible interval, 95% (dark shaded area), for yield and experimental data (horizontal bars, range of particle temperatures & vertical bars, experimental noise ±2ε) from IPFR and IGT [7].

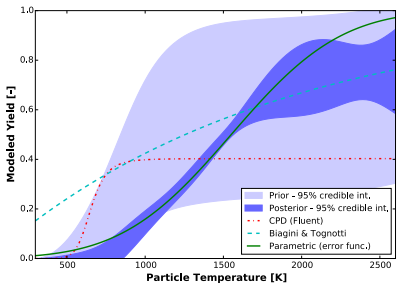

Figure 3. The empirical posterior credible interval, 95%, of the yield (dark shaded area), yield curve implied by the CPD model (dot-dashed curve), yield curve explicitly provided by the BT model (dashed curve), and a proposed yield curve (solid line).

Acknowledgements

This material is based upon work supported by the Department of Energy, National Nuclear Security Administration, under Award Number(s) DE-NA0002375.

References

[1] Smeets, E. M. and Faaij, A. P. and Lewandowski, I. M. and Turkenburg, W. C., Prog. Energy Combust. Sci., 56-106 (2007)

[2] Alvarez, L. and Gharebaghi, M. and Jones, J. M. and Pourkashanian, M. and Williams, A. and Riaza, A., "", Appl. Energy, 653-665 (2013)

[3] Feeley, R. and Seiler, P. and Packard, A. and Frenklach, M., J. Phys. Chem. A, 9573-9583 (2004)

[4] Gelman, A. and Carlin, J. B. and Stern, H. S. and Dunson, D. B. and Vehtari, A. and Rubin, D. B., Bayesian Data Analysis, Third Edition, Chapman & Hall/CRC Texts in Statistical Science (2014)

[5] Fletcher, T. H. and Kerstein, A. R. and Pugmire, R. J. and Solum, M. S. and Grant, D. M., Energy Fuels, 414-431 (1992)

[6] Biagini, E. and Tognotti, L., "", *Fuel Process. Technol.*, 513-520 (2014)

[7] Talwalker, A. T., A Topical Report on Coal Pyrolysis, Institute of Gas Technology (1983)