Optimal Particle Parameters for CLC and CLR Processes – Predictions by Intra-Particle Transport Models and Experimental Validation

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ABSTRACT

Validated models for predicting oxidation and reduction kinetics of multi-component porous particles in chemical looping combustion (CLC) and chemical looping combustion (CLC) processes are of key importance to identify the rate limiting in these processes. Since particle properties (i.e., their composition, porosity, pore size, grain size, etc.) can be adjusted by modern synthesis techniques, there is an open question on the optimal set of these properties that would lead to the most economic process.

In this study we present an overview of recent developments [1,2] in the field of continuum and shrinking-core-type intra-particle models. We then introduce a general open-source simulation environment, called *ParScale*, that can be used to simulate models relevant for CLC and CLR processes. Most important, *ParScale* features a generalized one-dimensional spherical discretization which enables the user to predict an arbitrary number of reactions within non-isothermal porous particles consisting of multiple solid (reactive or inert) species. We perform an optimization study (constrained by typical process requirements like maximum oxidation time, or minimum particle size) based on an analytical (for isothermal) and numerical (for non-isothermal) solution of the governing equations.

Finally, materials consisting of active nanoparticles embedded in a matrix of a different composition are synthesized and tested in a lab scale reactor under CLR conditions. Pre and post analysis of the materials by X-ray diffraction and scanning electron microscopy are performed to confirm the predicted reactions under the given conditions.

REFERENCES

[1] T. Melchiori and P. Canu, “Improving the Quantitative Description of Reacting Porous Solids: Critical Analysis of the Shrinking Core Model by Comparison to the Generalized Grain Model”, *Ind. Eng. Chem. Res.*, 53, 8980−8995 (2014).

[2] S. L. Singer, *Gasification and Combustion Modeling for Porous Char Particles*, PhD Thesis, Massachusetts Institute of Technology (2012).