Proceedings of CHT-15
ICHMT International Symposium on Advances in Computational Heat Transfer
May 25–29, 2015, Rutgers University, Piscataway, USA
CHT-15-163

ADVANCES IN COMPUTATIONAL THERMAL TRANSPORT FOR SOLAR THERMOCHEMICAL APPLICATIONS

Wojciech Lipiński[*,§]
[*]Research School of Engineering, The Australian National University, Canberra, ACT 2601, Australia
[§]Correspondence author. Tel: +61 2 612 57896. E-mail: wojciech.lipinski@anu.edu.au

ABSTRACT

High-temperature solar thermochemical systems are designed for maximum solar-to-chemical energy conversion efficiency and fast process rates. High temperatures are achieved by exposing solar reactors to high-flux irradiation from concentrating solar collectors. The reactors typically feature solid–gas heterogeneous media at temperatures exceeding several hundred degrees Celsius, and in some applications reaching more than 2000ºC. In directly-irradiated reactors, radiation is predominantly absorbed by a solid that provides surface to a chemical reaction. In indirectly-irradiated reactors, radiation is absorbed by an inert solid and then transferred to a chemical reaction by conduction, convection, and/or radiation through an intermediate heat transfer medium (solid, fluid, or multiphase medium) (Lipiński et al. [2012], Modest [2013]).

Thermal transport processes have been extensively studied at discrete spatial levels varying from nano- to micro- to macro-scale. Accurate characterization and simulation techniques connecting highly disparate spatial and temporary scales of solar thermochemical systems require significant advancements to become computationally effective. Such techniques are desired for direct design and optimization of reactors featuring prescribed materials of unknown continuum characteristics. Advancements in materials and computational sciences have also enabled a less explored approach of materials-by-design, in which materials of prescribed continuum characteristics indicated by predictive reactor-level models are inversely engineered by targeted identification of suitable composition and morphology. Both the direct and materials-by-design approaches are useful for understanding and optimizing the complex thermal transport processes and, consequently, for minimizing irreversibilities and achieving high solar energy conversion efficiency.

The basic approach to modelling coupled heat and mass transfer in reacting media of high-temperature solar thermochemical systems involves simultaneous solutions of the radiative transfer equation (RTE) along with the mass, momentum, and energy conservation equations. The interactions between thermal radiation and chemical kinetics are of special interest. Transient variation of radiative properties typical for such systems requires determination of the radiative contribution to the energy equation at any instant of the solution, leading to high computational cost. The complexity of solution further increases for systems for which gas radiation effects cannot be neglected, requiring application of accurate but computationally expensive spectral methods.

In this presentation, advances in computational thermal transport pertinent to modelling solar thermochemical systems are reviewed. Examples of computational studies of heat and mass transfer in solar reactors, reactive media and media features such as individual reacting particles are discussed together with recent developments in direct numerical predictions of thermal transport and optical properties of heterogeneous materials, from nano- to micro- to macro-structures.

REFERENCES

Lipiński, W., Davidson, J.H., Haussener, S., Klausner, J.F., Mehdizadeh, A.M., Petrasch, J., Steinfeld, A., and Venstrom, L. [2013], Review of heat transfer research for solar thermochemical applications, *Journal of Thermal Science and Engineering Applications*, Vol. 5, No. 2, pp. 021005-1–14.

Modest, M.F. [2013], *Radiative Heat Transfer*, third edition, Academic Press, New York.