Reduced-order modeling of nanoparticle dynamics in flame synthesis using reactor networks

S. Dübal[1,2*], L.L. Berkel[2], T. Faravelli[3], C. Hasse[2], H. Nicolai[2], S. Hartl[1]
*lead presenter: soeren.duebal@hs-esslingen.de
1 University of Applied Sciences Esslingen, Kanalstraße 33, 73728 Esslingen, Germany
2 Technical University of Darmstadt, Otto-Berndt-Straße 2, 64287 Darmstadt, Germany
3 Politecnico di Milano, Piazza Leonardo Da Vinci 32, Milan, 20133, Italy

Nanoparticle formation and growth play a crucial role in a wide range of technical applications. While the controlled production of functional nanomaterials with tailored properties in spray flame synthesis is explicitly desired [1], nanoparticle formation in metal dust flames poses a challenge for large-scale application and needs to be mitigated [2]. Computational fluid dynamics (CFD) simulations provide comprehensive insights into the characteristics of turbulent flames. However, the number of equations involving detailed kinetic mechanisms combined with a population balance-based modeling approach to describe nanoparticle dynamics results in expensive computational effort, especially for studies on a variety of parameters. Complementing this, reduced-order modeling simplifies the flow field, thereby enabling the integration of detailed models for gaseous and particulate pollutant formation while maintaining computational efficiency. In this regard, chemical reactor network (CRN) modeling is a promising approach. The resulting reduction in computational time allows for the integration of detailed physical sub-models for nanoparticle dynamics.
This work presents the integration of nanoparticle dynamics in a multi-phase CRN framework. A sectional method including nucleation and growth of polydisperse nanoparticles is seamlessly coupled to a detailed mechanism for gas phase combustion within ideal reactors. To assess the viability of the approach, experiments and simulations from spray flame synthesis serve as validation. As an initial step, profiles of gaseous precursor species and nanoparticle properties within laminar flames are compared to literature [3]. Subsequently, the CRN approach is applied to a large scale combustion device [4]. First, the initial design of the CRN is based on averaged flow and temperature fields from experiments and a three-dimensional CFD simulation. Based on this network configuration, the formation of nano-oxides with respect to the different model complexities is investigated. Finally, the sensitivities of nanoparticle dynamics based on reactor conditions and model assumptions, are discussed.
Potentials, as well as limitations describing the complex physics of nanoparticle dynamics using the CRN approach, are discussed. The advancement of CRN modeling presented in this work paves the way for the simulation-aided design of technical combustors with the objective of an efficient description of nanoparticle dynamics.

References

[1] J. M. Bergthorson et al., "Direct combustion of recyclable metal fuels for zero-carbon heat and power," Applied Energy, vol. 160, pp. 368–382, 2015.
[2] W. Y. Teoh, R. Amal, and L. Mädler, "Flame spray pyrolysis: An enabling technology for nanoparticles design and fabrication," *Nanoscale*, vol. 2, no. 8, pp. 1324–1347, 2010, doi: 10.1039/c0nr00017e.
[3] I. Wlokas et al., "Mechanism of Iron Oxide Formation from Iron Pentacarbonyl-Doped Low-Pressure Hydrogen/Oxygen Flames," Int J of Chemical Kinetics, vol. 45, no. 8, pp. 487–498, 2013.
[4] O. M. Feroughi et al., "Laser-based in situ measurement and simulation of gas-phase temperature and iron atom concentration in a pilot-plant nanoparticle synthesis reactor," Proceedings of the Combustion Institute, vol. 35, no. 2, pp. 2299–2306, 2015.