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Numerical modelling the reaction propagation in Al based thermites

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Reactive materials or nanothermites are composites or physical mixtures that demonstrate self-sustaining exothermic reactions upon receiving an initial energy input. This category of materials is distinctive within the realm of energetic materials, differing from explosives in the manner in which reaction fronts propagate subsonically and rely on atomic diffusion or other physical transport mechanisms. A range of studies have explored the numerical modeling of reaction propagation in Al-based thermites. Kim [1] and Tichtchenko [2] both focused on the self-propagation of combustion waves in nanoscale thermite composites, with Kim's model predicting wave speed and Tichtchenko's model analyzing the reaction front progression rate. Lahiner [3] proposed a diffusion-reaction scheme for predicting ignition and reaction dynamics in Al/CuO multilayered thin films, considering the decomposition of CuO and the diffusion of released oxygen. Tichtchenko [4] developed a model for predicting gas generation during the reaction of aluminum-based thermites, with a focus on pressure generation and its components. These studies contributed to the understanding of combustion of Al-based thermites, but do not consider coupled gas-condensed phased processes. In nano-sized materials especially, the combustion processes include thermal conduction, phase change, mass diffusion etc., which happen simultaneously and play an important role [5]. However, models considering coupling of thermo-mechanical-chemical physics are still absent. In this talk, I will present a novel one-dimensional deflagration model that describes the dynamics of the reaction front propagation in Al/CuO powdered thermite considering the reacting flow combined with heat transfer, chemistry and fluid flow. Separate mass, momentum and energy transport equations for the three phases, namely Al, CuO particles and gas mixture, are written in the frame of N-Euler approach for multiphase reactive flows. These equations are coupled by modeled interphase transfer terms.

[1] Kim, K., *Computational Modeling of Combustion Wave in Nanoscale Thermite Reaction.* World Academy of Science, Engineering and Technology, *International Journal of Chemical, Molecular, Nuclear, Materials and Metallurgical Engineering* 8 (2014): 679-682.

[2] Tichtchenko, E., Estève, A. and Rossi, C., *Modeling the self-propagation reaction in heterogeneous and dense media: Application to Al/CuO thermite.* *Combustion and Flame*, 228 (2021): 173-183

[3] Lahiner, G., Nicollet A., Zapata J., Marín L., Richard N., Djafari Rouhani M., Rossi C. and Estève A., *A diffusion-reaction scheme for modeling ignition and self-propagating reactions in Al/CuO multilayered thin films.* *Journal of Applied Physics* 122 (2017): 155105.

[4] Tichtchenko, E., Folliet, V., Simonin, O., Bédard, B., Glavier, L., Estève, A., Rossi, C. *Combustion model for thermite materials integrating explicit and coupled treatment of condensed and gas phase kinetics* *Proceedings of the Combustion Institute* 39 (3) (2023): 3637-3645.

[5] Wang, H., Baptiste J., Kline, D.J., Alibay, Z., Rehwoldt, M.C., Rossi C. and Zachariah, M.R., *Probing the Reaction Zone of Nanolaminates at $\sim\mu\text{s}$ Time and $\sim\mu\text{m}$ Spatial Resolution.* *Journal of Physical Chemistry C* 124 (2020): 13679-13687.