



HAL
open science

Toward a computational tool to simulate for the flame propagation in thermites powders

Emilian Tichtchenko, Pillemont Léa, Benoît Bédât, Olivier Simonin, Ludovic Glavier, Alain Esteve, Carole Rossi

► To cite this version:

Emilian Tichtchenko, Pillemont Léa, Benoît Bédât, Olivier Simonin, Ludovic Glavier, et al.. Toward a computational tool to simulate for the flame propagation in thermites powders. Europyro 2023, Af3P (Association Française de Pyrotechnie); GTPS (Groupe de Travail de Pyrotechnie), Sep 2023, Saint Malo, France. hal-03922512

HAL Id: hal-03922512

<https://laas.hal.science/hal-03922512>

Submitted on 17 Oct 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Toward a computational tool to simulate for the flame propagation in thermites powders

Emilian Tichtchenko^{a,c}, Pillemont Léa^a, Benoit Bedat^b, Olivier Simonin^b, Ludovic Glavier^c,
Alain Esteve^a, Carole Rossi^a

^aLAAS, University of Toulouse, CNRS-UPR 8001, France

^bIMFT, University of Toulouse, CNRS-UMR 5502, France

^cArianeGroup SAS, 66 Route de Verneuil, 78130 Les Mureaux, France

Mixtures of metal/metal-oxide, commonly known as thermite, can burn in a self-sustained reaction with an ultra-high energy density [1-2]. The high combustion temperature, safety, and tunability of thermites make it possible to produce totally novel pyrotechnical devices for in-space maneuvers (stage separation, pulse power generation for extended space missions, ...) [3-4]. However, the effective transfer of thermites from research laboratories to industrial products faces a core challenge, which is the lack of realistic deflagration models to guide the system design. Thus, the customization of a thermite mixture is still guided more or less by empirical considerations mostly from observations in flame tube experiments or using the empirical “Edisonian” approach, based on trial-and-error. Both approaches are totally inadequate to explore the large number of possible metals and oxides, in which not only the chemistry but also the microscopic (particle scale) and mesoscopic properties (systems of particles) influence the macroscopic combustion. This paper presents a one-dimensional (1D) model that simulates Al reaction propagation when in contact with a strong oxidizer in a cylindrical tube. CuO was chosen as it is the widest used metallic oxidizer that decomposes below the reaction temperature. In addition to condensed phase theory [5], representations of the gas phase combustion at the different scale is implemented using a computational fluid dynamics scheme enabling to model multiphase physics and combined physico-chemical mechanisms [6] taking place during the thermite reaction which are all extremely important factors to account for.

The model is designed as a combustion tube as used for flame speed measurements, i.e. with rigid walls filled with homogenous mixture of Al and CuO particles. The Al particle richness, the powder density, the particles diameters, and stoichiometric ratio and heat loss through the wall define the main parameters of the system. The 1D heat flow equation is coupled with mass and momentum equations and both diffusion and advection are considered. The calculated values of flame velocity show a reasonable compatibility with the experimental data.

Reference:

- (1) Pantoya, M. L.; Granier, J. J. Combustion Behavior of Highly Energetic Thermites: Nano versus Micron Composites. *Propellants, Explosives, Pyrotechnics* **2005**, 30 (1), 53–62.
- (1) Zapata, J.; Nicollet, A.; Julien, B.; Lahiner, G.; Esteve, A.; Rossi, C. Self-Propagating Combustion of Sputter-Deposited Al/CuO Nanolaminates. *Combustion and Flame* **2019**, 205, 389–396.
- (3) Rossi, C.; Larangot, B.; Pham, P. Q.; Briand, D.; de Rooij, N. F. ; Puig-Vidal, M.; Samitier, J. Solid propellant microthrusters on silicon: Design, modeling, fabrication, and testing, *J Microelectromech S*, **2006**, 15 (6), 1805-1815
- (4) Finazzi, A.; Maggi, F.; Paravan, C.; Galfetti, L.; Dossi, S.; Murgia, A.; Lips, T. ; Smet, G. Thermite-for-Demise (T4D): Concept Definition for Exothermic Reaction-Aided Spacecraft Demise during Re-entry, *EUCASS 22, 9TH European Conference for Aeronautics and Space Science, Lille, France, 27 June-1 July 2022*
- (5) Larangot, B.; Rossi, C.; Camps, T. ; Berthold, A.; Pham, P.; Briand, D.; Puig-Vidal, M.; Miribel, P.; Esteve, D.; Rooij, N. D.; Montanes, E.; Macias, G.; Samitier, J. Solid Propellant Micro Rockets - Towards a New Type of Power MEMS, *NanoTech 2002 - "At the Edge of Revolution" Houston, Texas, 9-12 September 2002*

- (5) Lahiner, G.; Nicollet, A.; Zapata, J.; Marín, L.; Richard, N.; Rouhani, M. D.; Rossi, C.; Estève, A. A Diffusion–Reaction Scheme for Modeling Ignition and Self-Propagating Reactions in Al/CuO Multilayered Thin Films. *Journal of Applied Physics* **2017**, *122* (15), 155105.
- (6) Tichtchenko, E.; Folliet, V.; Simonin, O.; Bedat, B.; Glavier, L.; Esteve, A.; Rossi, C. Combustion model for thermite materials integrating explicit and coupled treatment of condensed and gas phase kinetics, *Proc. Combust. Inst.*, **2022**, *1-9*.