



HAL
open science

Direct Numerical Simulation of the combustion of an aluminium particle in a reacting oxidizing flow

Lea Pillemont, Alain Estève, Benoît Bédard, Olivier Simonin, Carole Rossi

► **To cite this version:**

Lea Pillemont, Alain Estève, Benoît Bédard, Olivier Simonin, Carole Rossi. Direct Numerical Simulation of the combustion of an aluminium particle in a reacting oxidizing flow. 12th International Conference on Multi-phase Flow, ICMF, May 2025, Toulouse, France. <hal-05014600>

HAL Id: hal-05014600

<https://hal.science/hal-05014600v1>

Submitted on 1 Apr 2025

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.



HAL Authorization

Direct Numerical Simulation of the combustion of an aluminium particle in a reacting oxidizing flow

L. Pillemont^{1,2}, A. Esteve¹, B. Bédard², O. Simonin², C. Rossi¹

¹ LAAS-CNRS, University of Toulouse, 7 Avenue du Colonel Roche, Toulouse 31400, France

² IMFT, University of Toulouse, CNRS, 2 Allée du Pr. Camille Soula, 31400 Toulouse, France

Abstract:

A 3-dimensional Direct Numerical Simulations (DNS) of an isolated aluminum (*Al*) particle combustion in air is presented. The focus is placed on three elements: 1) developing an accurate and robust numerical scheme for understanding the physiochemical processes involved in the *Al* combustion, 2) quantifying the impact of sub-oxides condensation onto the burning droplet and subsequent heterogeneous surface reactions on the *Al* vaporization processes, and finally, 3) evaluating existing vaporization laws (burn rate) which are applicable to macroscopic combustion models.

Keywords: CFD-DNS, Aluminium combustion, Reactive Flow, Surface Kinetics, Vaporization rate, OpenFOAM.

Introduction:

Aluminum particles are attractive fuel candidates for various propulsion and energy-conversion applications [1]. Consequently, for four decades, research on *Al* combustion has been an ongoing effort both experimentally and theoretically. The burning behavior of micron-sized *Al* particles in an oxidizing environment can be divided into two stages. First, the particle undergoes steady and symmetric combustion in the vapor phase. Then the alumina decomposes and releases gaseous sub-oxides. Their condensation and subsequent dissolution in the liquid droplet mark the onset of the second stage, characterized by unsteady and asymmetric combustion forming liquid aluminum oxide. The multiphase mechanisms and chemical reactions leading to the production of liquid aluminum oxide from aluminum sub-oxides condensation onto the burning droplet remain elusive, negatively impacting the accuracy of current combustion models [2-3]. In this study, we employ a DNS approach to model accurately the combustion of a single *Al* particle in flowing air. This approach is based on a single-phase formalism of the Navier–Stokes equations. Our aim is to gain a deeper understanding of the gas-particle flow physics and to obtain quantitative data on the vaporization rate (burn rate) to support upper-level model development.

Numerical method:

A fixed spherical *Al* particle (100 μm in diameter) is immobilized in a hot oxidizing gas (1 mm^3 of air). We use a body-fitted (BF) method, meaning the *Al* particle is modeled as a non-deformable boundary condition. The conservations of mass, momentum, energy and species mass fractions are solved by DNS using *reactingFoam* solver in OpenFOAM, coupled with chemical kinetics in both condensed and gas phase. Four levels of mesh with successive refinements were implemented, resulting in 2.395.524 elements. The initial gas temperature is set at 2500 K , above the *Al* vaporization and alumina melting temperatures. Ambient air at temperature T_a can flow at a fixed velocity ($0.1 < Re < 100$) through the *Al* particle. The boundary conditions at the *Al* particle surface (mass flux, species mass flux and heat flux) are given through a *Al* vaporization rate ($\dot{\omega}_{vap}$), calculated as an equilibrium between the desorption flux ($\dot{\omega}_{desorp}$) and the condensation flux ($\dot{\omega}_{cond}$) at the *Al* particle surface.

$$\dot{\omega}_{desorp} = W_{Al} \frac{N_s}{N_A} T_s \exp\left(-\frac{E_a}{RT_s}\right) \quad (1)$$

$$\dot{\omega}_{cond} = W_{Al} \frac{\gamma}{1 - \gamma/2} \frac{P_{Al}}{\sqrt{2\pi W_{Al} RT_s}} \quad (2)$$

T_s is the *Al* surface temperature, γ is the sticking coefficient, N_s is the number of *Al* atoms per surface unit. For their part, P_{Al} and W_{Al} are respectively the *Al* partial pressure and *Al* molar mass.

The implemented mechanism for vapor-phase *Al* combustion was developed accordingly with the Swihart and Catoire's scheme [4], but also contains sub-mechanisms for nitrogen-containing species. This leads to 12 homogeneous gaseous reactions with 11 gas-phase species. Finally the condensation of aluminium sub-oxides on the particle is based on reactions and mechanisms reported in [5], containing 11 reactions for 7 condensed species.

Results and discussion:

The behavior of the proposed combustion model is presented in comparison with other reference models. Calculations provide results on the vaporization rate, surface temperature, temperature sensitivity and species profiles as a function of initial temperature and air flow rate ($0.1 < Re < 100$) (Fig.1). This enables us to better understand the role of non-equilibrium evaporation/condensation mechanisms, heterogeneous reactions at the burning particle surface on the flame structure and vaporization rate. In addition to the new understanding provided by these simulations, the resultant DNS data can be used to evaluate existing *Al* vaporization laws (burn rate) which are applicable to macroscopic combustion models.

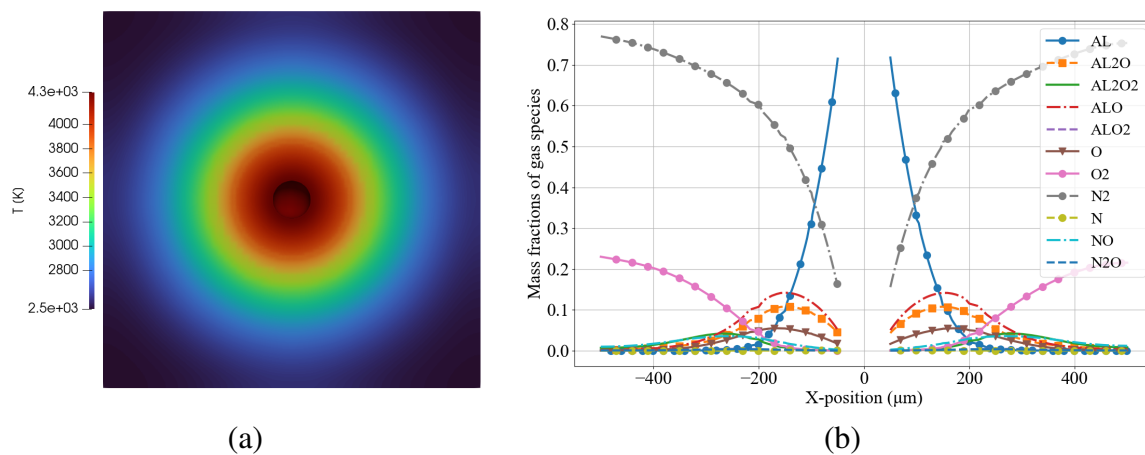


Figure 1: (a) Temperature field on a plane passing through the particle center and (b) radial profiles of species mass fractions for a single *Al* burning particle in a flow at $Re = 0.1$ and $t = 20 \mu s$.

Conclusion:

The combustion of an isolated aluminium particle in a reactive flow ($0.1 < Re < 100$) was studied by DNS on OpenFOAM coupling gaseous and surface chemical reactions with heat, mass and momentum transfer. This work enabled to analyse the surface and gas-phase kinetics impact on combustion modes, to have a depth-understanding of the physics involved and extract macroscopic models to accurately represent it.

Acknowledgments:

The authors acknowledge the French Defense Agency for funding L.P.'s scholarship and CALMIP supercomputing centre in Toulouse for providing us computational resources.

References

- [1] RA Yetter & RA Grant & SF Son *Metal particle combustion and nanotechnology*, Proceedings of the Combustion Institute, **32**, 2, 1819-1838 (2009)
- [2] MW Beckstead & Y Liang & KV Pudduppakkam *Numerical Simulation of Single Aluminum Particle Combustion (Review)*, Combustion, Explosion, and Shock Waves, **41**, 6, 622-638 (2005)
- [3] R Bhatia & WA Sirignano *Convective burning of a droplet containing a single metal particle*, Combust. Flame, **93**, 3, 215-229 (1993)
- [4] MT Swihart & L Catoire *Thermochemistry of aluminium species for combustion modelling from Ab Initio molecular orbital calculations*, Combustion and Flame. **121(1-2)**, 210-222 (2000).
- [5] J Glorian & S Gallier & L Catoire *On the role of heterogeneous reactions in aluminium combustion*, Combustion and Flame. **168**, 378-392 (2016).