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Aluminum combustion in a solid rocket motor environment

Merrill K. King *

Software and Engineering Associates, Inc., Carson City, NV 89701, USA

Abstract

A model for prediction of particle radius and oxide cap size/shape versus time for an aluminum particle tracking a stream-tube through a solid rocket motor port has been developed. Following preliminary calculations leading to a postulated flame structure, a quasi-steady model to predict instantaneous consumption of aluminum and generation of condensed oxide (both as a cap on the aluminum particle and as smoke) as a function of instantaneous particle size, ambient conditions, and cumulative amount of oxide in the cap was developed. Finally, this model was imbedded into a framework tracking evolution of particle size, oxide cap size, and ambient conditions, which change as the particle travels along a stream-tube consuming oxidizer and releasing heat. Qualitative agreement was found between predictions and limited observations.

Keywords: Metal combustion; Aluminum; Solid rocket motors

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1. Introduction/preliminary calculations

In 1995, Brooks and Beckstead [1] published a paper in which the state-of-the-art regarding aluminum particle combustion modeling and data was well reviewed. Subsequent papers by Babuk [2], DesJardin [3], Fabignon [4], and Bazyn [5] added further information in this area. Due to word limitations, these papers will not be discussed in detail. The model development presented in the next section drew on all of these papers as well as on the following preliminary calculations.

(1) Aluminum partial pressure adjacent to the particle surface was determined as a function of surface temperature from $K_P = P_{Al.g}$ (atm) $= \exp(-\Delta G^0/RT_s)$ where ΔG^0 is the change in free energy accompanying vaporization as tabulated in the JANAF Thermochemical Tables [6].

(2) This relationship was combined with a simplified B-Number analysis (as described in Turns' textbook [7]) to estimate the surface temperature: this calculation indicates that the surface temperature is far below the boiling point of aluminum at normal motor operating pressures, counter to assumptions made in some previous models.

(3) From several sets of thermochemistry calculations, it was concluded that the predominant Al_xO_y specie would be Al_2O_3 liquid at any place in the flame structure where the oxygen/aluminum atomic ratio is high enough to take it there.

(4) Further free energy calculations indicated that Babuk's [2] claim that $4Al(l) + Al_2O_3$ (l) will convert to 3 Al_2O (g) at the oxide-aluminum interface in the oxide cap region is unlikely.

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* Address: 9524 Daniel Lewis Lane, Vienna, VA 22181, USA. Fax: +1 202 358 3091.
E-mail addresses: mking9524@verizon.net, merrill.king@nasa.gov

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(5) Additional thermochemistry calculations indicated that likely reactions at the aluminum surface are Al vaporization and $4AlO \rightarrow Al_2O_3$ (l) + Al_2O (g).

(6) Still more thermochemistry calculations indicate that if the principal oxidizers are CO_2 and H_2O (typical in an aluminized solid rocket motor) the likely reaction sequence is $Al(g) + CO_2 \rightarrow AlO/1/2Al_2O_2 + CO$ and $Al(g) + H_2O \rightarrow AlO/1/2Al_2O_2 + H_2$ at a primary flame sheet followed by further oxidation to Al_2O_3 (l) + CO + H_2 at an outer condensation sheet.

(7) Finally, thermochemistry calculations were used to estimate the fraction of Al_xO_x which will appear as monomer rather than dimer as a function of flame-sheet temperature: these calculations yielded mass fraction monomer = 0.122 + 0.000577 (T-3500).

2. Model development

A sketch of the postulated quasi-steady combustion model is presented as Fig. 1. (As will be discussed later, this model is imbedded in another code in which the progressions of boundary conditions as the particle travels along a given stream-tube are updated.) As shown, the structure is composed of three zones (inner, middle, and outer) bounded by the droplet surface, an infinitesimally thin flame sheet where primary oxidation occurs, and another infinitesimally thin zone where final oxidation to Al_2O_3 and oxide condensation occur. It is postulated that, in addition to vaporization of aluminum from the particle surface, AlO diffusing back to the surface from the primary flame sheet undergoes collision-limited reaction with the surface to form Al_2O_3 liquid, which is added to the cap, and Al_2O(g) (via $4AlO \rightarrow Al_2O_3(l) + Al_2O(g)$), with the aluminum vapor and Al_2O then traveling outward toward the primary flame sheet. At this flame sheet, it is assumed that the aluminum vapor reacts instantaneously with CO_2 and H_2O (coming from the outer regions) to form a mixture of AlO and Al_2O_2, with the ratio of monomer to dimer being determined by the flame zone temperature, as discussed earlier. Based on the preliminary calculations, it is assumed that the Al_2O does not react here but instead travels outward along with the AlO/Al_2O_2 mixture to the condensation sheet where the suboxides react with additional carbon dioxide and water vapor to produce Al_2O_3(l), hydrogen, and carbon monoxide. It is further assumed (flame sheet approximation) that there are no gas phase reactions occurring in the three zones permitting standard development of algebraic equations describing the transport of species and enthalpy across the three zones. Fick's first law, with "effective" binary diffusion coefficients calculated at the midpoint temperature of each zone and with Lewis number = 1 is used in the development of these equations.

Total enthalpy (chemical plus sensible) is assumed to be constant across each zone (no reactions) with the values of the total enthalpy in each zone being determined by energy balances at the surface, at the primary flame sheet, and at the condensation sheet, accounting for source/sink terms associated with reactions at those locations. In addition, the outer boundary conditions, which would normally be specified at an infinite radius, are instead applied at a radius specified by the spacing of the particles relative to one another in the stream-tube flow. An "inert" specie, representing all the free-stream species other than CO_2, H_2O, CO, and H_2 is included as part of the overall gas composition. Obviously, for a quasi-steady analysis (no accumulation terms) its flux through each zone will be zero, as will fluxes of CO and H_2O in the inner zone, where diffusion and convection of these species are required to cancel out. The aluminum oxide smoke produced at the condensation zone as a 'sink" term is assumed to disappear from the system though its thermal effects must be included. For solution of this problem, the condensation temperature has to be a model input, based on the previously discussed thermochemistry considerations.

Boundary conditions for solution of these equations describing the aluminum burning rate, deposition of oxide at the surface (as characterized by oxide cap size) and production of oxide smoke at the condensation "sink" region are brought into the single particle analysis from the wrap-around code in which this analysis is imbedded. These conditions include free-stream temperature (T_{AMB}), free-stream mass fractions of CO_2, H_2O, CO, H_2, and "inert" ($Y_{j,AMB}$), instantaneous particle radius (r_{surf}), fraction of surface coated by oxide (β), pressure (P), amount of aluminum still unburned (M_{Al}), and mass of oxide accumulated in the cap (M_{OX}).

In line with the assumption of infinitesimally thin reaction/condensation sheets, it is assumed that the mass fractions of Al(g), H_2O, and CO_2 at the flame sheet are zero as are the mass fractions of Al_2O and Al_xO_x at the condensation sheet. In addition, the ratio of AlO to Al_2O_2 is assumed to be frozen at the flame-sheet radius value elsewhere. The remaining unknowns after application of these assumptions/approximations are mass fractions of species and mass fluxes through the three zones

At $r = r_{surf}$: $Y_{Al,S}, Y_{AlO,S}, Y_{CO,S}, Y_{H2,S}, Y_{Inert,S}$

At $r = r_{FZ}$: $Y_{AlO,FZ}, Y_{Al2O2,FZ}, Y_{Al2O,FZ}, Y_{CO,FZ}, Y_{H2,FZ}, Y_{Inert,FZ}$

At $r = r_{CZ}$: $Y_{H2,CZ}, Y_{CO,CZ}, Y_{CO2,CZ}, Y_{H2O,CZ}, Y_{Inert,CZ}$

Inner zone ($r_s < r < r_{FZ}$):

$\dot{m}_{Al,Inner}, \dot{m}_{Al_xO_x,Inner}, \dot{m}_{Al_2O,Inner}, \dot{m}_{Net,Inner}$