

Simulation of Fe₂O₃/Al Combustion: Sensitivity Analysis

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Abstract

The self-propagating high temperature reactions, as the Fe₂O₃/Al thermite combustion, are hard to follow by experimentation due to the extreme conditions that characterize them. Hence, theoretical prediction of these processes represents a valuable guideline for experimental work.

The availability of experimental results of radial combustion on disk shaped samples (Durães et al., 2006a) has stimulated the derivation of a one-dimensional model to describe the Fe₂O₃/Al combustion radial propagation (Durães et al., 2006b). This model considers non-steady combustion propagation on thin circular samples of Fe₂O₃/Al mixtures, zero order kinetics and conductive/radiative heat transfer. All the properties of the system vary with the temperature and composition during the propagation. Phase transitions are also contemplated. These last features allowed the obtainment of realistic solutions, readily comparable with the experimental values presented in Durães et al. (2006a). Adaptive numerical methods were applied in the resolution. The solution profiles are fast moving steep fronts, which were validated by experimental results in Durães et al. (2006b). The experimental combustion velocities were used to adjust the kinetic constant of the model, in order to give it a good predictive capability.

The most important novelty of the model is the assumption of variable temperature and composition thermophysical properties. This implied a wide bibliographic data review for the properties, namely the heat capacity, density, thermal conductivity and emissivity, of the system components (Fe₂O₃, Al, Fe, Al₂O₃ and air). However, the available data for the temperature dependence of some component properties was very scarce, making them unreliable.

Therefore, there were selected some of the least reliable properties: Fe_2O_3 and Al thermal conductivity, and Al, Fe_2O_3 and Fe_2O_3 densities. The sensitivity of the model towards those properties was tested. This was done in two ways: for the Fe_2O_3 thermal conductivity, due to a considerable lack of information, it was assumed non-temperature dependence and its value was tested; for the remaining properties it was assumed linear temperature dependence for temperatures beyond a known value, and its slope was tested. The kinetic constant adjusted in Durães et al. (2006b) and a stoichiometric ratio of reactants were used in all tests. The results monitored were the asymptotic thermal wave propagation velocity (v) and the average maximum front temperature (T_{max}). Some of the results are presented in the following Table.

	$k_{\text{Fe}_2\text{O}_3}$	$\rho_{\text{Fe}_2\text{O}_3}$	k_{Al}	v (m/s)	T_{max} (K)
Ref. run	const.	const.	const. for $T > 1300$ K	0.0273	4608
Test 1	const., 5×ref.	const.	const. for $T > 1300$ K	0.0284	4611
Test 2	const., 10×ref.	const.	const. for $T > 1300$ K	0.0284	4615
Test 3	const.	slope -0.2	const. for $T > 1300$ K	0.0273	4608
Test 4	const.	slope -0.3	const. for $T > 1300$ K	0.0273	4607
Test 5	const.	const.	$T > 1300$ K, slope 0.02	0.0299	4612
Test 6	const.	const.	$T > 1300$ K, slope 0.03	0.0299	4614

It is concluded that the model seems relatively insensible in relation to the temperature variation of most of the properties studied, including the less reliable one, the thermal conductivity of Fe_2O_3 . This property must be increased by a factor of 5, at least, to produce visible changes on the results. The highest sensitivity detected concerned the thermal conductivity of Al, which reasonably affects mainly the propagation velocity. The influence of non homogeneous mixing of the reactants was also tested, using randomly generated initial reactant concentration profiles centred on the average value. The velocity and temperature profiles were significantly affected, becoming oscillatory.

References

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