Fe_2O_3/Al thermite systems

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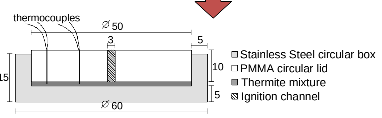
Motivation

Simulation of self-propagating high-temperature synthesis processes.

Fe_2O_3/Aluminum Thermite Combustion → $\alpha_A A + \alpha_B B \rightarrow \alpha_C C + \alpha_D D$

Features and Assumptions

- One or two-dimensional
- Disk shaped sample with radius R and thickness Z
- Sample confined in a steel cup with a PMMA top lid
- Negligible relative movement between species
- Limiting reactant A



Models

Radial Propagation

1D Model

$$\rho_M C_{PM}\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[k_M\left(r\frac{\partial T}{\partial r}\right)\right] + Q\cdot\Re - \left[\left(U_{steel/air} + U_{PMMA/air}\right)\left(T - T_0\right) + 2\sigma\varepsilon_M\left(T^4 - T_0^4\right)\right]/Z$$

$$\frac{dW_A}{dt} = -\alpha_A \Re$$

Ignition simulated as a spatial pulse

$$t = 0 \quad \begin{cases} 0 \le r \le R_0 & \Rightarrow \quad T = T_{igni} \\ r > R_0 & \Rightarrow \quad T = T_0 \end{cases}$$

Inner boundary – symmetry condition

$$t > 0; \quad r = 0 \quad \Rightarrow \quad \frac{\partial T}{\partial r} = 0$$

Outer boundary

$$t > 0; \quad r = R \quad \Rightarrow \quad k_M\frac{\partial T}{\partial r} = -\left[U'_{steel/air}\left(T - T_0\right) + \sigma\varepsilon_M\left(T^4 - T_0^4\right)\right]$$

Radial and Angular Propagation

2D Model Thermal Balance

$$\rho_M C_{PM}\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[k_M\left(r\frac{\partial T}{\partial r}\right)\right] + \frac{1}{r^2}\frac{\partial}{\partial \phi}\left(k_M\frac{\partial T}{\partial \phi}\right) + Q\cdot\Re - \left[\left(U_{steel/air} + U_{PMMA/air}\right)\left(T - T_0\right) + 2\sigma\varepsilon_M\left(T^4 - T_0^4\right)\right]/Z$$

Angular boundary conditions

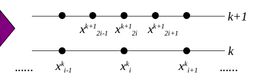
$$t > 0; \quad r > 0 \quad \Rightarrow \quad \begin{cases} T(\phi = 0) = T(\phi = 2\pi) \\ \frac{\partial T}{\partial \phi}(\phi = 0) = \frac{\partial T}{\partial \phi}(\phi = 2\pi) \end{cases}; \quad r = 0 \quad \Rightarrow \quad \frac{\partial T}{\partial \phi} = 0$$

Numerical Algorithm

General modelling conditions described in: Brito et al., 2005, Durães et al., 2006, Brito et al., 2007

- Static AMOL – classifiable as h-refinement.
- Spatial derivatives estimated by finite differences (FD) and/or high resolution schemes (HRS).
- Approximations FD – recursive algorithm of Fornberg.
- Approximations HRS – NVSF with flux limitation, e.g., MINMOD or SMART.
- Temporal integration: DASSL (BDF) or RKF45 (Runge-Kutta-Fehlberg 4th-5th order).

- $k = M$
- for $i = 1, \ldots, 2^k - 1$
- estimate U_i^n (order n derivative at node i) by FD
- if collocation criterion is met:
  - select intermediate nodes of level k+1: $x_{2i-1}^{k+1}; x_{2i}^{k+1}; x_{2i+1}^{k+1}$
- $k = k + 1$ repeat for $k = M, \ldots, N - 1$



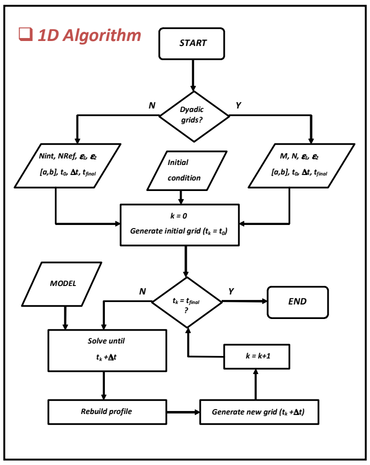
Criterion C1 σ – Oscillations capture

$$\delta_1 = U_i^n \times U_{i-1}^n$$
$$\delta_2 = U_{i+1}^n \times U_i^n$$
$$\left|U_i^n \times \Delta x\right| > \varepsilon_1 \quad \text{or} \quad \begin{cases} \delta_1 \le 0 \\ \delta_2 \le 0 \end{cases}$$
$$\text{and} \quad \sqrt{\frac{1}{2}\sum_{k=-1}^{1}\left(\left|U_{i+k}^n\right| - \frac{\left|U_{i-1}^n\right| + \left|U_i^n\right| + \left|U_{i+1}^n\right|}{3}\right)^2} > \varepsilon_2$$

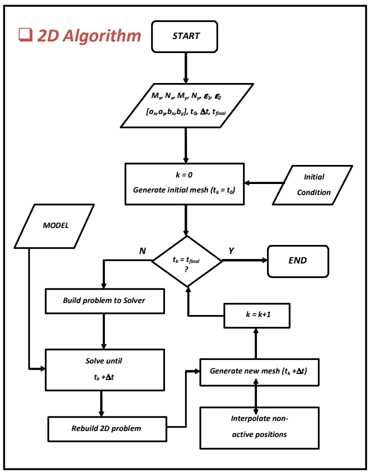
Criterion C2 – High values detection

$$\delta_1 = U_i^n - U_{i-1}^n$$
$$\delta_2 = U_{i+1}^n - U_i^n$$
$$\left|U_i^n \times \Delta x\right| > \varepsilon_1 \quad \text{or} \quad \delta_1 \times \delta_2 \le 0$$
$$\text{and} \quad \frac{\left|\delta_1\right| + \left|\delta_2\right|}{2} > \varepsilon_2$$

1D Algorithm



2D Algorithm



References

- P. Brito, L. Durães, J. Campos, A. Portugal, Chem. Eng. Sci., 62, 5078 (2007).
- L. Durães, P. Brito, J. Campos, A. Portugal, in Computer Aided Chemical Engineering, Vol. 21A, p. 365, Marquardt, W., Pantelides, C., Eds. (Elsevier, 2006).
- P. Brito, L. Durães, J. Campos, A. Portugal, 2005, in: Proc. of CHEMPOR 2005, Chem. Eng. Dept., Coimbra, p. 157 & CD-ROM.

Results

A	Fe_2O_3
B	Al
C	Fe
D	Al_2O_3
E	air

$Q\|_{T_0}$ (J/kg)	T_0 (K)	P (Pa)	T_{igni} (K)	T_{react} (K)	R (m)	R_0 (m)
5322746	298.15	101325	2300	1200	0.025	0.0015
Z (m)	τ (s)	T' (K)	Δr (m)		$\upsilon_{air\,0}$	
0.0015	0.1	1000	1×10^{-5}		0.392	
α_A	α_B	α_C	α_D	ω_A		ω_B
-1	-0.33792	0.69943	0.63848	0.747		0.253

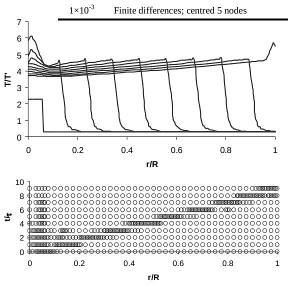
$$\Re = H\left(T - T_{react}\right)K$$ → Kinetic model

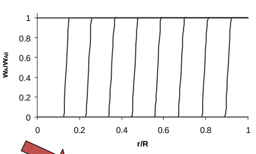
Zero order; non-temperature dependent kinetic constant

1D Model

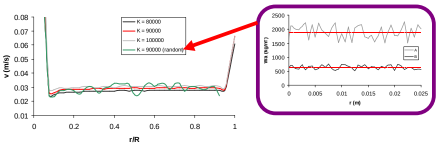
RKF45 tols.	Algorithm tol. ε_1	Algorithm tol. ε_2	Finite diff. approximations	1st level grid
1×10^{-6}	1×10^{-1}		centred; 5 nodes	uniform; 40 intervals
Criterion	*Derivative*		*Routine*	*Interpolation*
C2	1st		gridgen1	cubic splines; 7 nodes
Time step	*Spatial derivative scheme*			*Maximum refinement level*
1×10^{-3}	Finite differences; centred 5 nodes			2

Δt = 0.1 s





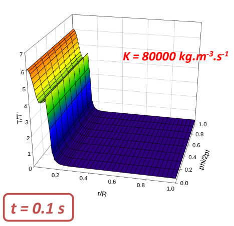
K = 80000 kg.m^{-3}.s^{-1}



- Radial propagation tends to constant velocity;
- Propagation velocity proportional to K value;
- Introduction of random initial profiles replicates experimental variations in the thermal front velocity.

2D Model

RKF45 ATol	Algorithm tol. ε_1	Algorithm tol. ε_2	Finite diff. approximations	1st level dyadic grid
1×10^{-5}	1×10^{-1}		centred; 5 nodes	uniform; 2^5 intervals in *r* and 2^3 in ϕ
Criterion	*Derivative*		*Routine*	*Interpolation*
C52/C2	1st		gridgen6	cubic splines; 7 nodes
Time step	*Spatial derivative scheme*			*Maximum refinement level*
1×10^{-3}	Finite differences; centred 5 nodes			2 in *r*; 0 in ϕ



t = 0.1 s

- *In a first approach, uniform mixing provides a residual influence of angular propagation;*
- *Results compare with 1D model.*

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