

NUMERICAL MODELING OF MULTIPHASE REACTING FLOWS

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A model for simulating multiphase reacting flows with shock waves is proposed. The model considers flows of reacting solid particles in a multicomponent gaseous flow. Several fractions of solid particles of both various size and material are included in the model. Solid particles can either burn in the presence of an oxidizer or decompose at high temperatures of the gas. The flow dynamics is described by the following set of equations

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \bar{u}) = \sum_k^{N_r} \sum_i^{N_g} J_{ik}^{(g)}, \quad (1)$$

$$\frac{\partial \rho \bar{u}}{\partial t} + \nabla(\rho \bar{u} \bar{u} + p) = - \sum_j^{N_s} \bar{F}_j + \sum_k^{N_r} \sum_i^{N_g} (\bar{u} \delta^-(J_{ik}^{(g)}) + \bar{u}_k \delta^+(J_{ik}^{(g)})), \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \nabla((\rho E + p) \bar{u}) = - \sum_j^{N_s} (\bar{F}_j \bar{u}_{sj} + q_j) + \sum_k^{N_r} \sum_i^{N_g} (E \delta^-(J_{ik}^{(g)}) + E_k \delta^+(J_{ik}^{(g)})), \quad (3)$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla(\rho Y_i \bar{u}) = \sum_k^{N_r} J_{ik}^{(g)}, \quad \frac{\partial \sigma_j}{\partial t} + \nabla(\sigma_j \bar{u}_{sj}) = \sum_k^{N_r} J_{jk}^{(s)}, \quad (4-5)$$

$$\frac{\partial \sigma_j \bar{u}_{sj}}{\partial t} + \nabla(\sigma_j \bar{u}_{sj} \bar{u}_{sj}) = \bar{F}_j + \sum_k^{N_r} (\bar{u}_{sj} \delta^-(J_{jk}^{(s)}) + \bar{u}_k \delta^+(J_{jk}^{(s)})), \quad (6)$$

$$\frac{\partial \sigma_j E_{sj}}{\partial t} + \nabla(\sigma_j E_{sj} \bar{u}_{sj}) = \bar{F}_j \bar{u}_{sj} + q_j + \sum_k^{N_r} (E_{sj} \delta^-(J_{jk}^{(s)}) + E_k \delta^+(J_{jk}^{(s)})), \quad (7)$$

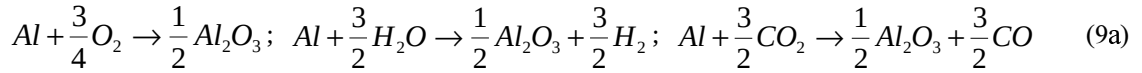
$$\frac{\partial n_j}{\partial t} + \nabla(n_j \bar{u}_{sj}) = \sum_k^{N_r} N_{jk}^{(s)}. \quad (8)$$

Here $\rho = \varepsilon \rho_g$, ρ_g is the gas phase density, $\sigma_j = \varepsilon_j \rho_{sj}$, ρ_{sj} are the mean and maximum thermodynamic density of particles of fraction j , $\bar{u}, \bar{u}_{sj}$ are the velocities of the gas and fraction j , $\varepsilon = 1 - \sum_j \varepsilon_j$ is the volume fraction of the gas phase in the mixture, r_j , n_j , $\varepsilon_j = \frac{4}{3} \pi r_j^3 n_j$ is the radius, concentration, and volumetric fraction of the j th fraction of particles, $E = e + \bar{u}^2/2$ is the total energy of the gas phase, $e = e(p, \rho_g)$ is the internal energy of the gas phase, $E_{sj} = c_{sj} T_{sj} + \bar{u}_{sj}^2/2$ is the total energy of the j th particle fraction, $\bar{u}_{sj}$ is the particle velocity of fraction j , p is the pressure of the gas and condensed phase, $\bar{F}_j = 0.5 \pi r_{sj}^2 n_j \rho C_{Dj} |\bar{u} - \bar{u}_{sj}| \cdot (\bar{u} - \bar{u}_{sj})$ is the interaction force between the gas and solid phases, $C_{Dj} = 24(\text{Re}_j)^{-1} + 4.4(\text{Re}_j)^{-1/2} + 0.42$, $J_{ik}^{(g)}$ is the mass flow of the i th gas component in the k th reaction, $J_{ik}^{(s)}$ is the mass of the i th condensed component in the k th reaction, $q_j = 2 \pi r_{sj} n_j \lambda c_p^{-1} \text{Nu}_j \left\{ \zeta_p (T - T_{sj}) + \frac{1}{2} \text{Pr}^{-1/3} (\bar{u} - \bar{u}_{sj})^2 \right\}$ is the heat flux to the j th particle fraction from the gas, Y_i is the mass fraction of the i th component in the gas mixture, $\delta^-(a) = (-1) \cdot \min(0, \text{sign}(a)) \cdot a$, $\delta^+(a) = (+1) \cdot \max(0, \text{sign}(a)) \cdot a$ is an auxiliary function, E_k is the specific energy of the products formed in the k th chemical reaction (the value of E_k is determined from equality of the energy of initial and end reaction

products), $\bar{u}_k$ is the velocity of gas and condensed particles formed in the k th products (the value of $\bar{u}_k$ is determined from equality of momentums of the initial and end reaction products), N_g is the number of components in the gas phase, N_s is the number of condensed phases, N_r is the number of reactions, $N_{jk}^{(s)} = n_j(\sigma_j)^{-1} J_{jk}^{(s)}$ is the number of particles of the j th phase formed (consumed) in unit volume per unit time in the k th reaction, $Re_j = 2r_{sj}\rho_g|\bar{u} - \bar{u}_{sj}|\mu^{-1}$ is the Reynolds number for the j th fraction of particles, $Pr = \mu c_p \lambda^{-1}$ is the Prandtl number, $Nu_j = 2 + 0.6 Re_j^{1/2} Pr^{1/3}$ is the Nusselt number, μ, c_p, λ are viscosity, specific heat, and thermal conductivity of the gas, which are function of temperature.

The gas is described by the equation of state of an ideal gas with a constant specific heat. Solid particles are incompressible.

For burning of solid particles (Al) we assumed the following model: Al oxide is solid and the reactions considered are



The ammonium nitrate decomposition reaction is represented by a global formula



The burning law is $dr_{sj}/dt = -r_{sj}(1 + 0.276\sqrt{Re_j})/t_{bj}$ (10a)

where the burning time $t_{bj} = K_j(2r_{sj})^n/\phi$ with $\phi = (Y_{CO_2} + Y_{H_2O} + Y_{O_2})/\sum_i Y_i$;

$K_{Al} = 4 \cdot 10^6 [sm^{-n}]$, $n = 2$ are constants deduced from experiment.

The model of solid oxidizer decomposition is based on the following law of variation in the particle size:

$$d_{0sj}^2 - d_{sj}^2 = k_{sj}t. \quad (11)$$

Here d_{0sj} is the initial particle diameter corresponding to time instant $t = 0$ (time is measured from the instant of particle ignition), d_{sj} is the particle diameter at time t , k_{sj} is a constant (set for ammonium nitrate equal to $4.8 \times 10^{-7} m^2/s$, this corresponds to the initial rate of ammonium nitrate decomposition of 3 mm/s).

For the burning law written in the form of Eq.(11), the reduction rate of the radius of oxidizer particles reads

$$dr_{sj}/dt = -k_{sj}/(8r_{sj}). \quad (10b)$$

The mass fluxes $J_{j,k}^{(g)}, J_{j,k}^{(s)}$ are written with regard for (10 a,b).

The results of calculations by this model are presented below.

We solved two problems

1. Initiation of detonation in an aluminum-air mixture.
2. A tube 2 m long is open at one end, 150 g AN and 30 g Al together with hot combustion products of an initiating propellant charge are injected at the opposite tube end for 1 ms, Al particle size is 10^{-5} m. The injected particles are aggregated to a 1 mm size and then break up over a 2-m distance

Problem 1. Simulated was 1-D initiation of detonation in an aluminum suspension in air. The Al density was 330 g/m³, particles were assumed spherical 3.5 micron in radius.

The initiation energy was deposited in two computational cells in amounts of 0.25 and 2 MJ/m². The pressure profiles for the two versions are shown in Fig.1 at time instants ranging between 0.15 and 0.90 ms). Detonation is initiated only at 2 MJ/m², in this case the shock velocity passes through a minimum and in the latter case it reaches the CJ level monotonically from above.

The results are compared with the available experimental data. According to [1], the initiation energy depends significantly on the particle size and shape. For ultrafine particles not exceeding 1 micrometer the measured initiation energy was 0.25 MJ/m² and, for Al flakes the measured initiation energy is 3.4 MJ/m². The calculated initiation energy for flakes which are assumed spherical of a mass-equivalent radius is several-fold less than the measured ones. This means that mass transfer coefficients and ignition temperatures for the particles should be slightly changed to fit the experimental data. There is a physical reason for that because of the difference in the

particle shapes and of the presence of hydrocarbon coating on real particles. Inclusion of the particle shape factor in calculations in [1] definitely increased the initiation energy.

It is noteworthy that the CJ parameters calculated by the gasdynamic code (the CJ plane was set at the point where the Mach number equals unity) agree quite satisfactorily with thermodynamic calculations: the CJ pressure and temperature are equal 22.3 bar and 4300 K, while their thermodynamic counterparts are 23.9 bar and 4222 K, respectively.

Similar results were also obtained for an ammonium nitrate-air (the amount of ammonium nitrate is 330 g/m³): in gasdynamic calculations the pressure and temperature at the CJ plane are 16.6 bar and 1961 K, their thermodynamic counterparts are 115.7 bar and 1977 K, respectively.

Problem 2. The calculated pressure fields are displayed in Fig.2. It is seen that in the mixture ejected from the tube aluminum reacts violently with the products of ammonium nitrate decomposition.

Thus a model of reacting flows in which several reactions between different species and phases take place concurrently is developed. The model is capable of adequately describing nonsteady phenomena with shock and detonation waves.

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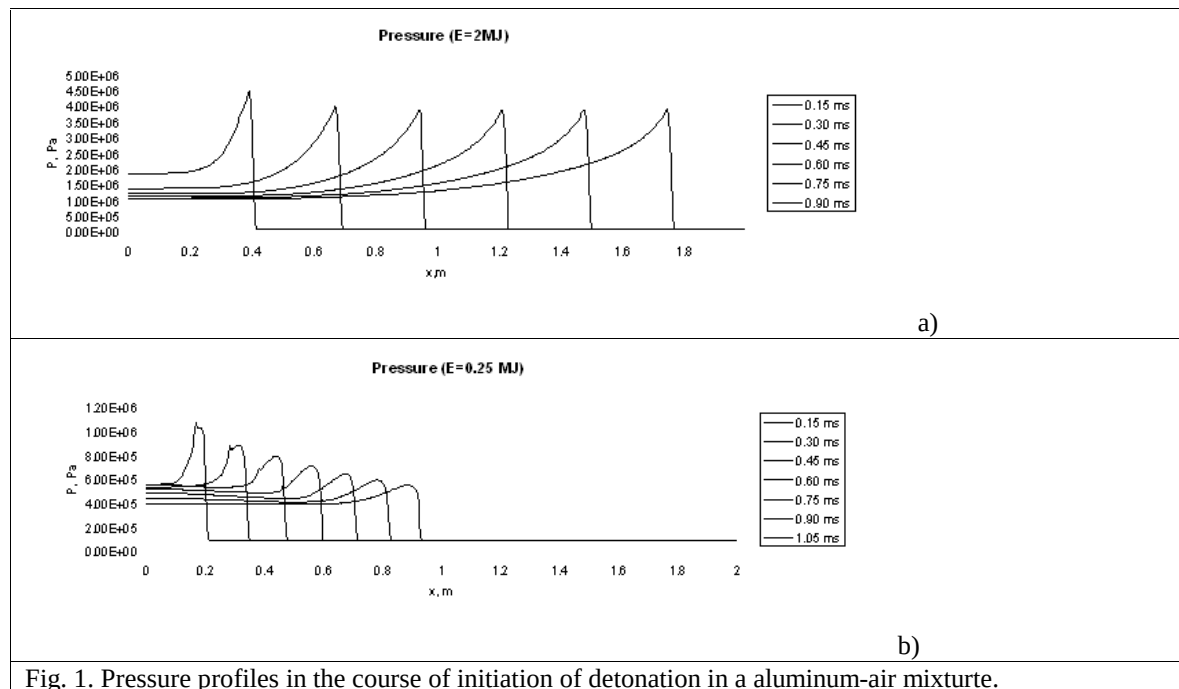


Fig. 1. Pressure profiles in the course of initiation of detonation in an aluminum-air mixture.

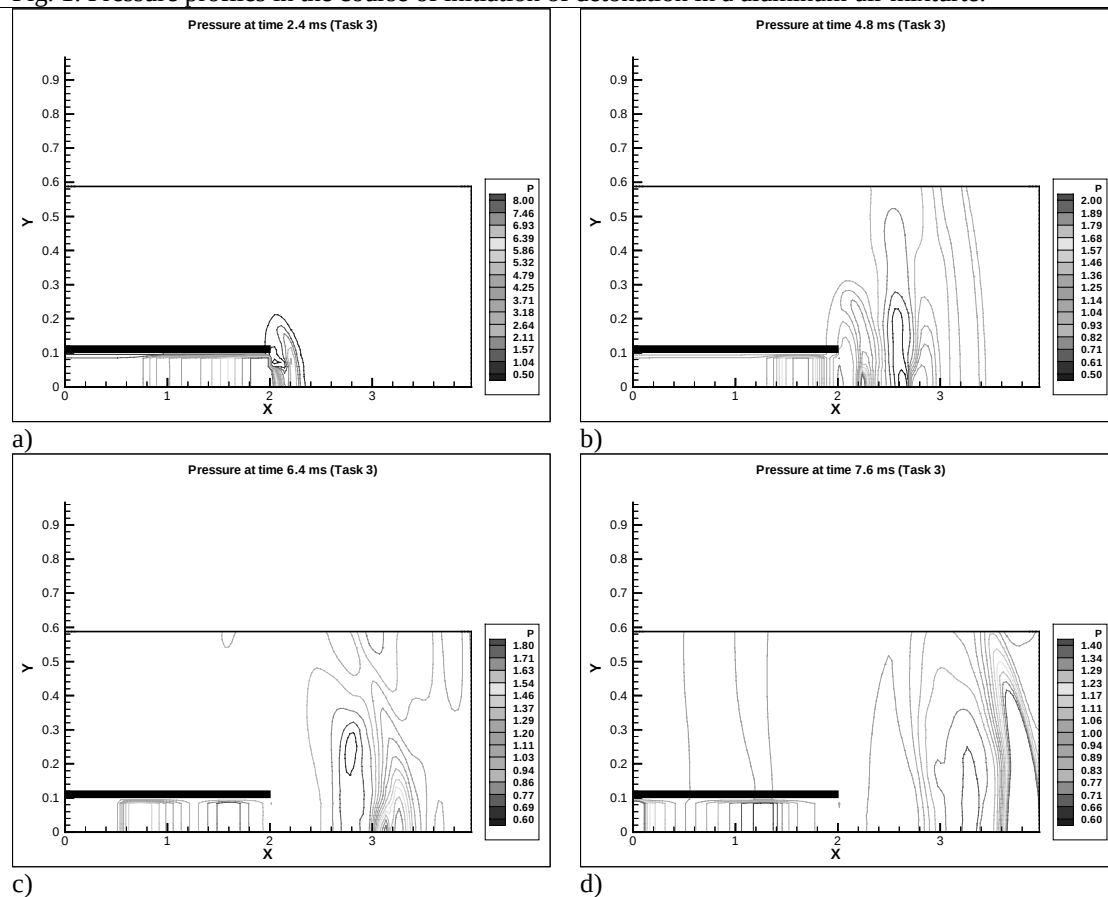


Fig. 2. Flow pattern in a tube and outside it after injection of burning AL-AN mixture (pressure, task 2)