Simulation of high-speed nonequilibrium heterogeneous turbulent flows with phase transition

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Abstract. In this paper the method of modelling of high-speed nonequilibrium two-phase turbulent flows with phase transition in disperse phase is presented. The method proposed in this paper has the following features: 1) the mathematical model includes conservation equations for gas and solid particles, as well as the equations for gas vibration molecular energy, conservation of species and phase transition equation for particles; 2) the equations for the particles are solved mixed Euler-Lagrange formulation; 3) the solver algorithm is two-way coupled; 4) a special turbulence model taking into account the effect of flow compressibility is implemented. The main case considered in this paper is crystallization process of aluminium oxide Al2O3 particles in underexpanded jet flow with cross-flow at different angles of attack. Simulation results for jets of different configuration are presented.

1. Introduction

Determination of parameters of high speed jets with admixture of solid phase is a very important problem in applied technical physics. Such type of flows can be seen in different systems and objects in civil area as well as special ones. And the parameters of these flows can be crucial to design.

Computational fluid dynamics today is one of the most important and powerful tools for investigation of multiphase flow. Nevertheless, it should be noted that the methods for investigating multiphase flows with phase transition by now are not quite well developed. Particle phase transition models have been usually treated using Lagrange technique. However, the handicaps of this technique are well-known and include two-way coupling difficulties, problems dealing with particle continuity equation in case of intersection of particle trajectories, treating dense particulate flows, etc. On the other hand, Euler approach lacks these disadvantages, but needs much more computational resources in case of polydispersed flow.

The main purpose of this work is to develop a robust method which would lack some of the disadvantages of the classical techniques and would allow to perform efficient simulations of high-speed nonequilibrium heterogeneous flows.

The method proposed in this paper has the following features:

1) The mathematical model includes conservation equations for gas and solid particles, that is conservation of mass, momentum and energy. In addition, the equations for gas vibration molecular energy, conservation of species and dimensionless particle crystallization radius are solved.

2) The equations for gas are solved in the Euler’s form, and for the particles – in mixed Euler-Lagrange formulation.
3) A two-way coupled solver algorithm is used.
4) A special turbulence model developed by the authors is implemented. The model takes into account turbulence anisotropy as well as effects of compressibility on turbulent mixing.

2. Mathematical model

2.1. Governing equations for the gas flow

The main system of equations for gas phase includes continuity equation, momentum equation, total energy equation, vibrational energy equations for each vibrational mode and mass conservation laws for each of the components of the reacting mixture.

The formulation of these equations is quite common (e.g. see [1]) and thus is omitted here.

In turbulent flows extra mass, energy and stress fluxes are added. For their calculation K-ε-Vn turbulence model was used [2]. For calculation of the formation rates of the chemical components system of reactions from [3] and [4] were implemented.

Solution methods for the gas flow system are given in many works (e.g. see [4]-[6]) and thus are not stated here.

2.2. Governing equations for a discrete phase

Polydisperse mixture of particles is represented as a set of L groups, each characterized by the values of the radius \( r_\alpha \), density \( \rho_\alpha = n_\alpha \cdot m_\alpha \), velocity components \( u_{\alpha,j} \) and temperature \( T_\alpha \).

It is supposed that the particles are spherical, chemically inert with respect to gaseous phase and do not interact with each other.

For each group of particles (\( \alpha=1,2,...,L \)) governing equations include [7]:

1). Continuity equation

\[
\frac{\partial \rho_\alpha}{\partial t} + \frac{\partial \left( \rho_\alpha u_{\alpha,j} \right)}{\partial x_j} = 0
\]

(1)

2). Momentum equation

\[
\rho_\alpha \frac{d \dot{u}_{\alpha,j}}{dt} = f_{\alpha,j}
\]

(2)

3). Thermal energy equation

\[
\rho_\alpha C_S \frac{dT_\alpha}{dt} = q_{\text{phase,}\alpha} - q_{\text{conv,}\alpha} - q_{\text{rad,}\alpha}
\]

(3)

Here \( \frac{d}{dt} \) is a total time derivative along the particle trajectory; \( f_{\alpha,j} \) - is force acting on particles; \( q_{\text{phase,}\alpha} \) - heat flux due to phase transition; \( q_{\text{conv,}\alpha} \) - convective heat flux; \( q_{\text{rad,}\alpha} \) - radiative heat flux; \( C_S \) - heat capacity of particles.

In case of Al2O3 particles, the following formulae are implemented:

\[
f_{\alpha,j} = \rho_\alpha C_f \left( u_j - u_{\alpha,j} \right) = \frac{3}{8} C_{D,\alpha} \rho \left( u_j - u_{\alpha,j} \right) \left| \vec{v} - \vec{V}_\alpha \right| \rho_\alpha
\]

\[
q_{\text{conv,}\alpha} = \rho_\alpha C_q \left( T_a - T_\alpha \right), \quad C_q = \frac{3}{2} \frac{Nu \cdot \lambda}{r_\alpha^2 \rho \delta \varphi}
\]

\[
q_{\text{rad,}\alpha} = \rho_\alpha \exp(C_{\text{rad}}),
\]

\[
C_{\text{rad}} = \begin{cases} 
1.25 \cdot 10^{-2} T_a - 0.5, \quad T_a < 1000, \\
10 + 2 \cdot 10^{-3} T_a, \quad 1000 < T_a < 2000, \\
7.143 \cdot 10^{-3} T_a - 0.286, \quad T_a > 2000
\end{cases}
\]

(6)
\[
\frac{q_{\text{phase},a}}{\rho_a} = 3q_{a} \frac{\psi^2}{r_a} \alpha (T_M - T_a)^{1.8}
\]

where \( q_{a} \) - is latent heat of phase transition; \( T_M \) is onset temperature of equilibrium crystallization; \( \psi \) is dimensionless radius of crystallization (0 ≤ \( \psi \) ≤ 1, where 0 corresponds to liquid particle and 1 - to the solid one); \( a \) is constant determining the crystallization interphase velocity [8]; \( a = 0.64 \cdot 10^6 \) is an empirical constant.

The crystallization model is written in the following form:

\[
\frac{d\psi}{dt} = -a \frac{T_M - T_a^{1.8}}{r_a} F_{cr}(T_a)
\]

where \( F_{cr}(T_a) \) is a function determining the crystallization onset and termination (for aluminum oxide crystallization begins at temperature being equal 0.83 \( T_a \) and terminates at temperature above \( T_M \)).

In case of high combustion intensity, temperature of gas can exceed melting temperature of particles in some regions. The melted zone is then determined from the consistency condition \( q_{\text{conv},a} = q_{\text{phase},a} \cdot \).

The liquid phase is assumed to transfer initially to the metastable solid \( \gamma \) phase. The transition process from the \( \gamma \) phase to the stable \( \alpha \) phase begins as soon as any portion of the \( \gamma \) phase has appeared. This is described by the equation of the form:

\[
\frac{dC_a}{dt} = A \exp \left( -B / T_a \right), \quad 0 < C_a < 1
\]

where \( C_a \) is \( \alpha \)-phase fraction; \( A,B \) are constants [9].

Drag coefficient is determined via Henderson’s formula [10] and Nusselt number – via Drake-Kawano’s formula [11].

Thermal and dynamical impact of particles on gas phase is determined as follows:

\[
F_{a,i} = \sum_{\alpha=1}^{L} f_{\alpha,i}, \quad F_{a} = \sum_{\alpha=1}^{L} \left( q_{\text{conv},a} - q_{\text{a},a,i} \right)
\]

2.3. Notes on discrete phase treatment
As it has been already mentioned, one of the goals that the authors are trying to pursue in scope of the present work is to develop a robust method for simulation of non-equilibrium flows with discrete phase.

Eulerian approach is rather resource-consuming in case of polydispersed flow, as it involves solving at least five partial differential equations for each size group of particles. Another issue is that Euler approach does not allow to trace history of individual particles along their tracks. This is a rather tricky problem in a case of Al2O3 phase transition, due to hysteresis of phase transition (solidification and melting begin at different temperature levels). One of the ways to solve it in the framework of fully Eulerian approach was shown in [1].

Classical Lagrangian approach is rather simple from the numerical point of view. Nevertheless, there are problems with solving continuity equations for particles in Lagrangian approach. The main issue here is that particle trajectories have rather complex geometry and can repeatedly overlap within the computational domain. This also complicates the two-way coupling between gas and particles. This problem is very difficult to resolve even in 2d case (e.g. see [12]), not to mention the 3d one.

In view of the above said, in this paper a mixed approach is introduced. As it can be seen from the previous section, the equations of motion, energy and phase transition are written in Lagrangian frame (see eqs. (2),(3) and (8),(9)) and the continuity equation (1) – in Eulerian frame. Coupling issues (impact of particles on gas – see eq. (10)) are also resolved with the help of Eulerian approach.
To explain the algorithm let us consider the flow with a pronounced x-directional flow. Let the finite volume grid be structured in that direction.

1. At the inlet, the seeding points of the particles are supposed to match the gas-flow grid.
2. Equations (2), (3), (8) and (9) are solved for the first $\Delta x$ “layer” in x direction.
3. The positions of the particles after passing through the layer do not coincide with the gas-flow grid. However, as $\Delta x$ is rather small, then no intersections of the particulate trajectories should occur. Thus, the particulate parameters could be easily interpolated to the grid points of the gas-flow.
4. The process is repeated on every other $\Delta x$ layer.

Continuity equations for the particles are solved on gas-flow grid by the method similar to the gas-flow equations (see [4]-[6]).

3. Case studies
The developed method was verified in different case-studies of multiphase jet flow.

3.1. Case 1
The first case was described in [12]. The jet has 0.4 atm (5.9 psia) static pressure and 2500 K static temperature at the nozzle exit (Mach number is 2.35). Three particulate groups are considered: 1.5 μm, 3 μm and 6 μm.

(a) Results from [12]. Classical Lagrange model  
(b) Present work. Mixed Euler-Lagrange model

Figure 1. Axial profiles of the gas and particle temperatures on the jet centerline

Figure 2 shows axial profiles of alpha-phase fraction. These results are in good agreement with the results of [12], where crystallization of 1.5 μm particles begins approximately at a distance of 16 nozzle radii and fraction of alpha-phase reaches ~1.6·10$^{-3}$ (see figures 6 and 7 of [12]).

The results for gas and particulate temperature in comparison with the results of [12] are shown in figure 1.
3.2. Case 2
The case was described in the work of F. Zavelevich et al [7]. It represents a typical solid rocket engine plume with engine thrust 12 tons at 31 km altitude.

(a) Results of [6]. Classical Lagrange model  
(b) Present work

Figure 3. Axial temperature distribution in plume of typical solid rocket engine at 31 km altitude.

1- calculation results without gas-particles coupling, 2- two-way coupled calculation.

The computation results in comparison with the results of [7] are shown in figure 3. As it can be seen, they are in good agreement.

Here one can see a very important practical result: particles “ignite” the gas mixture intensifying afterburning. In non-coupled calculations the afterburning cannot be seen.

3.3. Case 3
The previous calculations were performed for 2d jets. A cross flow of a model rocket engine is considered as a 3d case.

Flow parameters are given in Table 1 Flow composition is given in mass fractions (particles are not taken into account).

Table 1. Flow parameters at nozzle outlet

| T<sub>a</sub>, K | U<sub>a</sub>, m/s | P<sub>a</sub>, atm | H<sub>2</sub> | H<sub>2</sub>O | CO | CO<sub>2</sub> | N<sub>2</sub> | HCl | Al<sub>2</sub>O<sub>3</sub> |
|-----------------|-----------------|-----------------|----------|----------|----|----------|--------|-----|-----------------|
| 1780            | 3000            | 0.5             | 0.3      | 0.042    | 0.12e-4 | 0.57    | 0.8e-5 | 0.378 | 0.01            | 0.4 |
This leads to the substantial intensification of chemical reaction of H2 and CO with oxygen from the air, and to the increase of combustion products - H2O and CO2 (see Figure 4).

![Graph showing spatial distribution of H2O and CO2](image)

**Figure 4.** Altitude 80 km. Spatial distribution of H2O (a,b) and CO2 (c,d) mass fractions at different angles of attack (a,b) – 0°, (c,d) - 68°

As it is shown on figure 5, lighter particles are drifted more than the heavier ones. The cross-section of the flow resembles a horseshoe.

Table 2 shows that aftercombustion of H2 and CO leads to significant increase of H2O and CO2 in the jet, especially at greater angles of attack (for comparison: at nozzle outlet mass fraction of H2O equals to 0.12e-4 and CO2 - to 0.8e-5).

| Angle of attack, ° | 0    | 20   | 40   | 60   | 68   |
|-------------------|------|------|------|------|------|
| $C_{CO_2,\text{max}}$ | 0.0009 | 0.0015 | 0.002 | 0.012 | 0.0165 |
| $C_{H_2O,\text{max}}$ | 0.0054 | 0.0089 | 0.012 | 0.040 | 0.0488 |
Figure 5. Altitude 80 km. Spatial distribution of density of $\text{Al}_2\text{O}_3$ at angle of attack $68^\circ$ for minimal size group $0.5 \mu$ (a,b) and for the maximal size particles $7 \mu$ (c,d). The distribution is given in different planes: (a, c) – in XY plane ($Z=0$), (b,d) – in YZ plane with X=2000 m.

4. Conclusions

In this paper a method of simulation of heterogeneous non-equilibrium flows has been introduced. The method is based on mixed Euler-Lagrange approach. The calculation results presented here show good agreement with the works of other authors. The developed method allowed to obtain some insights into the structure of plumes at different heights, taking into account the influence of the particulate phase. The approach developed in this paper can easily be used for different types of particulate media undergoing phase changes provided that the crystallization laws are known.

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