Numerical modeling of two-phase high speed jet with non-equilibrium solid phase crystallization

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Abstract. The main purpose of the paper is to demonstrate that the Euler approach is fully applicable to the multiphase flows with discrete phase undergoing phase transitions. It is carried out using the example of a jet flow with aluminium oxide particles non-equilibrium crystallization. The jet is strongly underexpanded. The non-equilibrium molecular effects are being taken into account. The obtained results of the simulations are in good agreement with the works of the other authors. The developed Euler approach proved itself to be the most robust in flows with complex flow geometry.

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 flows with significant particle volume fraction (>10%), necessity to analyze a great number of particle trajectories in order to maintain statistical stability of the solution, etc. On the other hand, Euler approach lacks these disadvantages, but the Euler modeling techniques for particulate flows with phase transitions for now are developed rather poorly. This provides a high motivation for the present work.

This paper proposes a method for simulation of two-phase jets with solid phase non-equilibrium crystallization. The method 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 vibration gas molecular energy, conservation of species and dimensionless particle crystallization radius are solved.
2. The equations for gas and particles are solved in the Euler’s form.
3. A two-way coupled solver algorithm is used.

2. Governing equations for gas in state of thermal and chemical non-equilibrium
First of all, let us write down the system of equations for gas phase.
The main system of equations includes:

1. Continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0$$

2. Momentum equation

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} \left( \rho u_i u_j + \delta_{ij} p - \tau_{ij} \right) = 0$$

3. Total energy equation

$$\frac{\partial}{\partial t} \left( \rho E \right) + \frac{\partial}{\partial x_j} \left( \rho u_i \left( E + \frac{p}{\rho} \right) + q_{i,j} + q_{v,i,j} + \sum_s V_{s,j} \rho_s h_s - u_i \tau_{ij} \right) = -Q_R$$

4. Vibrational energy equation for m-th vibrational mode

$$\frac{\partial}{\partial t} \left( E_{v,m} \right) + \frac{\partial}{\partial x_j} \left( E_{v,m} u_j + q_{v,m,j} + E_{v,m} V_{s,j} \right) = S_{v,m}, \quad m = 1, 2, ..., N_M$$

5. Mass conservation law for the s-th reacting mixture component

$$\frac{\partial}{\partial t} \left( \rho C_s \right) + \frac{\partial}{\partial x_j} \left( \rho C_s u_j + \rho C_s V_{s,j} \right) = \dot{w}_s, \quad s = 1, 2, ..., N_C - 1$$

In these equations: \( \rho \) - mixture density; \( u_j \) - j-th component of the velocity vector; \( p \) - pressure; \( \tau_{ij} \) - shear stress tensor; \( E \) - specific total energy; \( h_s \) - specific enthalpy for the s-th component; \( \rho_s \) - density of the s-th component; \( V_{s,j} \) - diffusion speed for the s-th; \( q_{v,i,j} \) - vibrational energy heat flux; \( q_{i,j} \) - translational-rotational energy heat flux; \( Q_R \) - heat losses due to radiation; \( E_{v,m} \) - volume specific vibrational energy for m-th vibrational mode; \( q_{v,m,j} \) - m-th mode vibrational energy heat flux; \( S_{v,m} \) - vibrational energy source; \( N_M \) - number of vibrational energy modes; \( C_s = \rho_s / \rho \) - mass fraction of the s-th component; \( \dot{w}_s \) - s-th component production rate; \( N_C \) - number of gas mixture components.

In turbulent flows extra mass, energy and stress fluxes are added. For their calculation \( K-\varepsilon - V_n \) turbulence model was used [1]. For calculation of the formation rates of the chemical components system of reactions from [2] and [3] were used.

Solution methods for the gas flow system are given in many works (e.g. see [3]-[5]) and thus are not stated here.

3. Governing equations for particles

The main case considered in this paper is crystallization process of aluminum oxide \( \text{Al}_2\text{O}_3 \) particles in underexpanded jet flow.

Polydisperse mixture of particles is represented as a set of \( N \) groups of particles, each of which is characterized by the values of the radius \( r_{\alpha} \), density \( \rho_s = n_s \cdot m_s \), velocity components \( u_{a,j} \) and temperature \( T_{a} \).

For each of N groups (\( \alpha = 1, 2, ..., \)), under the assumptions that the particles are spherical, chemically inert to the gaseous phase, and do not interact with each other, equations describing the motion of \( \text{Al}_2\text{O}_3 \) particles can be written as [6]

1) Particle continuity:

$$\frac{\partial \rho_a}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho_a u_{a,j} \right) = 0$$

2) Particle momentum:
\[
\frac{\partial u_{a,i}}{\partial t} + u_{a,i} \frac{\partial u_{a,i}}{\partial x_j} = C_f \left( u - u_{a,i} \right) \tag{7}
\]

where \( C_f = \frac{3 C_{D, \alpha} P \left[ \bar{V} - \bar{V}_a \right]}{8 r_a P_{Al_2O_3}} \); \( P_{Al_2O_3} \) - Al2O3 density; \( C_{D, \alpha} \) is computed using Henderson’s formula [7].

3) Particle energy:

\[
\frac{\partial T_a}{\partial t} + u_{a,i} \frac{\partial T_a}{\partial x_j} = \frac{C_q}{C_s} \left( T - T_a \right) + \frac{q_{phase,\alpha}}{C_s \rho_a} - \frac{q_{rad,\alpha}}{C_s \rho_a} \tag{8}
\]

where \( C_q = \frac{3 Nu \cdot \lambda}{2 \rho_{Al_2O_3} r_a^2} \); \( Nu \) is Nusselt number [8], \( \lambda \) is gas mixture heat conductivity; \( q_{rad,\alpha} \) is radiative heat flux.

Phase transition heat is determined the following way:

\[
\frac{q_{phase,\alpha}}{\rho_a} = 3 q_c \psi^2 \frac{r_a^2}{T_m - T_a} \tag{9}
\]

where \( q_c \) - is latent heat of phase transition; \( T_m \) is onset temperature of equilibrium crystallization; \( \psi \) is dimensionless radius of crystallization (\( 0 \leq \psi \leq 1 \), where 0 corresponds to liquid particle and 1 - to the solid one); \( a \) is constant determining the crystallization interphase velocity [9].

As it is rather hard to solve Stephan problem for each of the particles, in this paper the approximate crystallization introduced in model is used.

\[
\frac{d\psi}{dt} = -a \left( T_m - T_a \right)^{1.8} F_{cr} \left( T_a \right) \tag{10}
\]

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

As the problem is considered from the Euler’s point of view then the derivative in left-hand side of the equation is considered as substantial.

\[
\frac{\partial \psi}{\partial t} + u_{a,i} \frac{\partial \psi}{\partial x_j} = -a \left( T_m - T_a \right)^{1.8} F_{cr} \left( T_a \right) \tag{11}
\]

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 \( \frac{dC_\alpha}{dt} = A \exp \left( -B/T_a \right) \), which yields:

\[
\frac{\partial C_\alpha}{\partial t} + u_{a,i} \frac{\partial C_\alpha}{\partial x_j} = A \exp \left( -B/T_a \right) \tag{12}
\]

where \( C_\alpha \) is \( \alpha \)-phase fraction; \( A, B \) are constants [10].

As the crystallization process begins and terminates at two different values of temperature, the onset function \( F_{cr} \) should depend on the history of particles along their streamlines. In Lagrange domain this is not a problem, while in the Euler domain it is rather tricky to represent \( F_{cr} \) correctly, as streamlines are not actually considered in this case.

Two ways could be considered to resolve the problem of \( F_{cr} \) non-locality. The first way to go is to actually reconstruct streamlines from the solution data and to use them to determine the value of \( F_{cr} \) at
a given point. This seems to solve the problem, however, this method has all the disadvantages of the Lagrange approach.

Another way to deal with the problem is to consider $F_{cr}$ as a transported scalar and to solve the appropriate convection equation for it.

$$\frac{\partial F_{cr}}{\partial t} + u_{a,j} \frac{\partial F_{cr}}{\partial x_j} = S_{cr}$$

(13)

The initial value of $F_{cr}$ is zero. The source term is zero everywhere except regions with $T<0.83T_m$. The maximum value of $F_{cr}$ is limited by one.

In case of strong aftercombustion, the gas temperature can exceed the melting temperature of the particles and the crystallized particles can begin to melt. In this case the melted zone is determined from the following consistency relation:

$$\alpha = \alpha (x,y,z)$$

(14)

4. Numerical scheme for the particle equations

Equations (6)-(8), (11)-(13) have a similar structure in 3d Cartesian frame $(x,y,z)$:

$$\frac{\partial f_a}{\partial t} + \tilde{u}_a \frac{\partial f_a}{\partial x} + \tilde{v}_a \frac{\partial f_a}{\partial y} + \tilde{w}_a \frac{\partial f_a}{\partial z} = S_a$$

(15)

where $u_a, v_a, w_a$ are the corresponding particle velocity components.

Let us consider a dimensionless coordinate frame, taking in account the shape of the computation domain:

$$\xi = \xi(x) = x/L, \quad \eta = \eta(x,y,z), \quad \zeta = \zeta(x,y,z)$$

(16)

where $L$ is characteristic dimension.

In the new frame steady state form of the equation (15) will be as follows:

$$\frac{\partial f_a}{\partial \xi} + \tilde{v} \frac{\partial f_a}{\partial \eta} + \tilde{w} \frac{\partial f_a}{\partial \zeta} = S_a$$

(17)

where $\tilde{v} = L\eta, \quad \tilde{v} = \frac{L\eta v_a}{u_a}, \quad \tilde{w} = L\zeta, \quad \tilde{w} = \frac{L\zeta w_a}{u_a}, \quad \tilde{S}_a = \frac{LS_a}{u_a}$

The numerical solution of equation (17) is performed with the explicit-implicit predictor-corrector method (explicit for convection and implicit of the source).

Predictor step:

$$(f_a)_{j,k}^{n+1} = (f_a)_{j,k}^{n} + \Delta \xi \tilde{S}_a^{n} - \Delta \xi \tilde{v} \frac{\partial (f_a)_{j+1,k}^{n} - (f_a)_{j,k}^{n}}{\Delta \eta} - \Delta \xi \tilde{w} \frac{\partial (f_a)_{j,k+1}^{n} - (f_a)_{j,k}^{n}}{\Delta \zeta}$$

(18)

Corrector step:

$$(f_a)_{j,k}^{n+1} = (f_a)_{j,k}^{n} + \Delta \xi \tilde{S}_a^{n+1} - \Delta \xi \tilde{v} \frac{\partial (f_a)_{j+1,k}^{n+1} - (f_a)_{j,k}^{n+1}}{\Delta \eta} - \Delta \xi \tilde{w} \frac{\partial (f_a)_{j,k+1}^{n+1} - (f_a)_{j,k}^{n+1}}{\Delta \zeta}$$

(19)

By linearizing the source $\tilde{S}_a^{n+1} = \tilde{S}_a^{n+1} + \left(\frac{\partial \tilde{S}_a}{\partial f_a}\right)^{n+1} \left[(f_a)_{j+1,k}^{n+1} - (f_a)_{j,k}^{n+1}\right]$, we get the solution value at (n+1) step for $\xi$ coordinate:
where \( \Delta (f_{a,j,k}^{\text{corr}}) \) is the explicit function increment at the corrector step:

\[
\Delta (f_{a,j,k}^{\text{corr}}) = \frac{\Delta \tilde{\xi}}{\Delta \eta} \left[ (f_{a,j,k}^{\text{corr}}) - (f_{a,j,k}^{\text{corr}}) \right] - \frac{\Delta \tilde{\eta}}{\Delta \zeta} \left[ (f_{a,j,k}^{\text{corr}}) - (f_{a,j,k}^{\text{corr}}) \right]
\]

(21)

The continuity equation has the following form in the frame \((\xi, \eta, \zeta)\):

\[
\frac{\partial}{\partial t} (\rho_a J) + \frac{\partial E}{\partial \xi} + \frac{\partial F}{\partial \eta} + \frac{\partial G}{\partial \zeta} = 0
\]

(22)

where \( E = \frac{\tilde{\xi}}{J} \rho_a u_a, \quad F = \frac{\tilde{\eta}}{J} (\eta_a u_a + \eta_a v_a + \eta_a w_a), \quad G = \frac{\tilde{\zeta}}{J} (\zeta_a u_a + \zeta_a v_a + \zeta_a w_a) \) \((J)\) is the Jacobian).

In steady state:

\[
\frac{\partial E}{\partial \xi} + \frac{\partial F}{\partial \eta} + \frac{\partial G}{\partial \zeta} = 0
\]

(23)

which can be solved by explicit Korte method [5].

5. Results

The developed method was verified in three case-studies of multiphase jet flow.

5.1. Case 1

The first case was described in [8]. 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.

The results for gas and particulate temperature in comparison with the results of [8] are shown in figure 1. Figure 2 shows axial profiles of alpha-phase fraction. These results are in good agreement with the results of [8], where crystallization of 1.5 μm particles begins approximately at a distance of 16 nozzle radii and fraction of alpha-phase reaches \(~1.6 \times 10^{-3}\) (see figures 6 and 7 of [8]).

(a) Lagrange model [8]  
(b) Euler model, present work  

Figure 1. Axial profiles of the gas and particle temperatures on the jet centerline.
5.2. Case 2
The case was described in the work of F. Zavelevich et al [6]. It represents a typical solid rocket engine plume with engine thrust 12 tons at 31 km altitude.

The computation results in comparison with the results of [6] 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.

5.3. Case 3
The previous calculations were performed for 2d jets. In 3d case with cross-flow (even when cross-flow angles are insignificant) Lagrange simulations are connected with certain difficulties because
particulate trajectories can become rather complex, which causes troubles with computation of particulate density. The Euler model, on the other hand, does not have this problems and thus is considered preferable for cross-flow cases.

Figure 4 shows particulate density distribution for typical solid rocket engine with 55 tons of thrust at 50 km altitude.

![Figure 4](image)

(a) 0.5 μm particles  
(b) 6 μm particles

**Figure 4.** Particulate density distribution in XY plane for jet in cross-flow (cross-flow angle is 30°).

As it can be seen, smaller particles are more carried away by the cross-flow than the larger ones.

6. Conclusions

This work has demonstrated that the Euler technique can be successfully implemented in investigation of multiphase flows with phase changes in the particulate phase.

The calculation results presented here show good agreement with the works of other authors.

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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