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Effect of the condensed particles on a flow of combustion products in a Laval nozzle

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Abstract. The specialized multifunctional software package is developed for the numerical simulation of the flow of products of combustion in a Laval nozzle. The complex has a friendly graphical user interface of input-output and wide possibilities for visualization of simulation results directly in the process of calculating. Particles moving in the gas stream are exposed to the action of hydro-mechanical forces due to its interaction with the carrier gas environment, as well as mass forces caused by the gravitational field. Performed parametric calculations have shown that the interaction of particles with the combustion products, even with a relatively small volume fraction may lead to a qualitative change in the internal flow in the Laval nozzle, and thereby influence the characteristics of the nozzle.

1. Introduction

Multiphase flow is significantly non-equilibrium process. The various phases are not necessarily in the equilibrium with each other [1] even if each phase is in local thermodynamic equilibrium. Therefore, that the system of equations describing such a flow were closing, it is necessary to determine the transfer velocities of mass, energy and momentum between the phases. The forces of various natures act on a particle moving in a gas flow. These forces are hydromechanics and mass forces [2, 3]. Hydromechanics forces are caused by the interaction of the particles with the carrier gas phase. The forces of resistance due to friction and pressure are forces of this type. Also forces arising from parameter gradients existing in the carrier-phase flow are such forces. This type includes rising forces caused by acceleration and deceleration of the particles in the gas flow. Mass forces are determined external physical fields such as gravitational, electrostatic and other fields. Forces acting on the particle as it move along a curved path and also forces generated during rotary motion of the carrier or discrete phases, for example, Coriolis forces are the same type of forces. In general, all of the listed forces are no stationary. The degree of influence on the particle depends on its relative size, structure of the gas flow in the channel with variable cross section and its mode parameters [3-6]. In most cases, it is possible to take into account the aerodynamic drag force only. Two-speed model are typically used to account for the interaction of particles with a flow of combustion products. In this model the particle field is represented continuous medium with the appropriate density [7, 8]. This approach works well; however it has several disadvantages. At first it is not possible to describe the situation where the particles move in different directions in single point of space, which can occur when the particles rebound from the obstacle. At second the description of the particle size distribution leads to the necessity of considering multiple continuums.
2. The physical model of the motion of particles in the gas flow

In the construction of mathematical and computational models that describe the interaction of condensed particles with combustion products in channels withvariable cross section, we shall proceed from the following basic assumptions:

- the movement of the carrier medium is described by the system of gas dynamics equations;
- the particles of condensed phase have a spherical shape;
- the particles undergo aerodynamic drag force and the force of gravity only;
- the processes of collision, fragmentation and coagulation can be neglected;
- an exchange of energy, impulse and mass in general case is a result of the interaction of individual particles with the gas flow;
- mutual particles affect at each other is through the interaction of the gas flow.

As a basic model, which describes the interaction of the particles with the gas flow of the combustion products the Sand Bag model [9] was taken. This model has been successfully used in the description of the dynamics of entry into the dense layers of the Earth's atmosphere the originally destroyed body [10] which do not experience further fragmentation, as well as cratering model for the description of the dynamics of soil release from crater [11]. Individual pieces of the object or release interact with the atmosphere, resulting in accelerated or decelerated, thus exchanging with impulse, energy, and, in general, mass. In addition to the force interaction and heat and mass transfer the change of the density of the gas component is taken into account in the model by reducing its volume by the amount of volume of the condensed phase of matter. The same situation may occur when the condensed particles are moving in a flow of combustion products in a Laval nozzle.

All the variety of particles can be divided into separate conglomerates according to their size, speed and location. In this case, any interaction of conglomerate with the gas stream can be described by a single representative which bearing of all the average parameters of conglomerate particle, and also the number of particles in the form of the total mass of the conglomerate. Since the processes of collision, crushing and particle coagulation are neglected in this model, the only possibility of their interaction with each other is mutual influence through the changed by them gas-dynamic parameters of the carrier medium.

3. Mathematical model of the interaction of particles with the flow

Let’s take into account only the mechanical interaction of particles with the gas flow. A mathematical model describing the gas flow perturbation due to the interaction of particles in a Laval nozzle in the two-dimensional axially symmetric approximation is a gas-dynamic system of equations with the additional terms describing the exchange of energy and impulse. This system in a conservative form is:

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial (r \rho v)}{\partial r} + \frac{\partial (\rho u)}{\partial z} = 0
\]

\[
\frac{\partial (\rho u)}{\partial t} + \frac{1}{r} \frac{\partial (r \rho vu)}{\partial r} + \frac{\partial (\rho u^2)}{\partial z} = -\frac{\partial p}{\partial z} + \delta I_z \tag{1}
\]

\[
\frac{\partial (\rho v)}{\partial t} + \frac{1}{r} \frac{\partial (r \rho v^2)}{\partial r} + \frac{\partial (\rho uv)}{\partial z} = -\frac{\partial p}{\partial r} + \delta I_r
\]

\[
\frac{\partial (\rho E)}{\partial t} + \frac{1}{r} \frac{\partial (r v (\rho E + p))}{\partial r} + \frac{\partial (u (\rho E + p))}{\partial z} = \delta E
\]

where \( u \) and \( v \) – axial and radial components of velocity \( \vec{w} \) respectively; \( \delta I_z, \delta I_r, \delta E \) - changing the impulse component and the gas flow energy due to the interaction with a condensed phase material; \( \rho \) - the total density of the carrier gas flow, which generally in the case when the flow is a mixture of \( N \) component, is given by
\[ \rho = \sum_{i=1}^{N} \rho_i \]  

To close the system (1) the equation for the pressure in a medium are used

\[ p = \sum_{i} p_i, \quad p_i = p_i(\rho_i, \varepsilon_i) \]  

where pressure of each components of the medium \( p_i \) is determined by the equation of state given in analytical form or in tabular form. In addition, if in the task the parameters of air at a given height \( h \) are required, then they are determined by the standard tables of the Earth’s atmosphere

\[ \varepsilon_a = \varepsilon_a(h), \quad \rho_a = \rho_a(h) \]  

To solve the system of equations (1) - (4) the large particles method was used [12]. The main idea of the method of large particles is splitting into the physical processes of the original non-stationary system of equations. At the first stage the system is solved under the assumption instantaneous retardation substances i.e. without convective terms and at the second stage the mass transfer and corresponding impulse and energy transfer are calculated.

Consider now a collection of particles that occupy at the moment a certain volume. The total number of particles that need to be considered in the problem, can be very large, therefore, it is advantageous to combine the individual particles which are placed in a small spatial region and which have close on the value parameters such as size, speed, etc. into a single conglomerate. Interaction of any conglomerate with the gas flow can be described by its single representative. It’s necessary to calculate the interaction of the representative with the gas flow, and then get the change in the total energy, mass and momentum of the conglomerate by multiplying the corresponding changes in the values obtained for a single representative on the actual number of particles in the conglomerate.

Dynamics of a particle-representative having a spherical shape according to our assumption is described by a system of ordinary differential equations, including the equation of motion, momentum change equation due to hydrodynamic and exchange forces and energy change equation:

\[ \frac{dr_i}{dt} = \vec{\mathbf{\dot{w}}}_i \]

\[ \frac{d(m_i\vec{\mathbf{\dot{w}}}_i)}{dt} = m_i(\vec{\mathbf{\dot{F}}}_i + \vec{\mathbf{\dot{g}}}) \]

\[ \frac{d(m_i\varepsilon_i)}{dt} = m_i\vec{\mathbf{\dot{F}}}_i\vec{\mathbf{\dot{w}}}_i \]  

where \( m_i \) – mass, \( \vec{\mathbf{\dot{w}}}_i \) – velocity, \( \varepsilon_i \) – full energy, \( \vec{r}_i \) – the radius vector of the particle-representative, respectively.

The strength of the aerodynamic braking per unit mass of the \( i \)-th particle-representative is given by

\[ \vec{\mathbf{\dot{F}}}_i = 3\rho_i \frac{C_{D_i} \vec{\mathbf{\dot{a}}}}{4\rho_i \vec{\mathbf{\dot{r}}}_i^2} \]  

where \( \vec{\mathbf{\dot{a}}} = \vec{\mathbf{\dot{w}}} - \vec{\mathbf{\dot{w}}}_i \), \( \rho_i \) – density of condensed substance of particle.

To determine the resistance coefficient of the particle moving in a gas stream, it is necessary to know the Reynolds number, which defined by its size

\[ \text{Re} = \rho_i |\vec{\mathbf{\dot{a}}}|d/\eta \]  

For a spherical solid particle in the region of small Reynolds numbers (\( \text{Re} = 10^4 - 1.0 \)) the Stokes formula could be used

\[ C_{D_i} = 24 \text{Re}^{-1} \]  

In a wide range of Reynolds numbers (\( \text{Re}_a = 10 - 10^3 \)) the empirical formula could be used [3]

\[ C_{D_i} = 12 / \sqrt{\text{Re}} \]
This system of equations is solved locally at the point in space (computational cell) inside of which the considered particle-representative is placed. If at the same time at this cell there are several particle-representatives, there shall be a joint decision of several systems. Obtained change of mass, momentum and energy of representative particles which are calculated in the same cell are added, whereby they become sources of the corresponding values for the carrier gas environment. It is necessary to satisfy a number of conditions that limit of the integration time step for stability of calculations in accordingly with described algorithm.

At the diffuser part of the nozzle the particles intensely collide with the walls. Therefore, the Sand Bag model was modified to take into account of the adhesion processes and reflection particles to/from the nozzle walls. The sticking coefficient can vary from zero (no adhesion) to one (complete adhesion). When the reflection factor equal one the specular reflection occurs, while a decrease reflection occurs at a smaller angle and partial adhesion.

4. Testing of model
When the particles are so small that their size is comparable to the mean free path of the particles, it is necessary to take into account an Cunningham amendment or the Millikan resistance factor. The simplest expression of this amendment [13] is:

\[
C_c = 1 + 1.275 \frac{2\lambda}{d}
\]  

where \(\lambda\) - free path, \(d\) - particle diameter.

As a test of the model the calculations were conducted to determine the steady-state rate of subsidence in the air for a particle under the influence of gravity. Two variants of calculations were performed. At the first case the initially resting particles with diameter 0.1- 10 μm are accelerated in a gravitational field till stationary velocity, while at the second case the initially moving particles slowed down to it. In both cases the times of getting settling rate were the same and coincide with the data of [13].

5. Results of simulations
Parametric calculations were performed for the same size of the particles, which ranged from 1 μm to 100 μm. The initial volume fraction of the particles coming to the nozzle input changed from \(10^{-7}\) to \(10^{-4}\). Only the force interaction was studied. In some calculations the number of particles-representatives reached about \(10^5\). With the some volume fraction smaller particles have a significant influence on the flow of products of combustion in connection with considerably intensive exchange. Characteristic changes in the flow of combustion products are following: appearance of subsonic zone inside the diffuser of nozzle in close proximity its axis of symmetry; appearance of the field of reverse flow inside the convergent part of the nozzle in close proximity the place where the nozzle wall begins to narrow; total or partial removal of the sound line in the critical section of the nozzle at high volume fractions of small particles; increased volume fraction of particles in the axial region of the expanding part of the nozzle; oscillation of output nozzle parameters, including traction. The presence of particles leads to loss of traction to 5% in some calculations. Another feature of the flow in the nozzle is a sharp expansion of the gas flow in the expanding supersonic part of the nozzle. Particles-representatives disperse in this region to the extent that not every calculation cell there is at least one representative. This leads to spatial fluctuations of environmental parameters, caused by nonuniformity of particle-representatives distribution in the nozzle channel. Analysis of the simulation results revealed the need of algorithm for separation peripheral conglomerates into several parts when they move towards the axis of the nozzle.
Figure 1. The velocity field in the cylindrical part of the nozzle: а – in the absence of the particles, b - particle diameter is 1 μm, the initial volume fraction is $10^{-5}$.

The figure 1 illustrates the results of the effect of particle influence at the velocity field into the vicinity of the cylindrical part of the nozzle immediately prior to constriction. The dots indicate the position of the particle-representatives. The presence of particles increases the effective viscosity of the gas + particles substances whereby there is a swirling motion with the strong upflow near the nozzle wall. Inside of this vortex some of the particles move on loop-like path.

The distribution of representative particles is shown in Figure 2 at the moment of their release on the steady-state solution. Here clearly visible the region of formed vortex motion, in which the volume fraction of the particles is significantly lower than the input value. Also note that on the nozzle axis in its output the volume part of particles fractions is strongly increased, forming spatial accumulations of the condensed phase.

Figure 2. Particle's distributions inside of the nozzle.
6. Conclusion
The developed software complex allows performing calculations internal flows in channels of variable section in the 1D-3D approximations. There is the possibility of simulating multiphase flows and multimediu. Physics-chemical properties of the medium may be given in tabular form directly or calculated during the simulation. The complex is equipped with a convenient GUI for easy input of the parameters of simulated tasks, and dynamic graphical visualization of the calculated gas-dynamic parameters.

Conducted parametric calculations have shown that the interaction of particles with the combustion products, even with a relatively small volume fraction may lead to a qualitative change in the internal flow in the Laval nozzle, and thereby could influence at it characteristics.

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