NUMERICAL STUDY OF MULTIPHASE DROPLET FLOW IN NOZZLE PLUME AT VACUUM CONDITIONS

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Introduction

Processes occurring in multiphase nozzle and plume flows are of key importance for problem of spacecraft contamination produced by control thrusters. This paper presents some results of continuation of the study of droplet nozzle and plume flows in transitional regime [1].

Euler-Lagrange description of the droplet nozzle-plume flows is implemented in this study utilizing separate consideration of the phases on the basis of appropriate models for the carrier phase and the probe droplet model for the dispersed phase. Phase coupling is realized with a procedure of temporal-spatial averaging of trajectory parameters of the probe droplets in each computational cell providing source interphase transport terms.

At the Euler stage of the algorithm a hybrid Navier-Stokes (NS)/Direct Simulation Monte Carlo (DSMC) approach is used to simulate the flow in different regimes, from a dense flow inside the nozzle, through very fast expansion near the nozzle lip, to rarefied, free-molecular flow in the back flow region.

The Lagrange stage of the algorithm provides descriptions of motion, heating, evaporation/condensation of the droplets.

Detailed description of algorithm of the Lagrange stage as well as discussion of closing relations for the interphase drag, heat and mass transfer are presented in [2]. Special attention is paid to regimes of transitional and rarefied flows characterized by moderate and high Knudsen numbers.

Mathematical Model

The two-dimensional and axisymmetric Navier-Stokes equations are solved with a shock-capturing MUSCL TVD scheme. The standard van Leer's formula with the \textit{minmod} slope limiter is used for reconstruction of cell-faced variables from cell-centered ones. The viscous terms are approximated by the central finite differences and the HLLEM approximate Riemann solver is employed to calculate the inviscid fluxes. The HLLEM solver is constructed to be robust near low densities and, therefore, it is particularly appropriate for simulation of rapidly expanding flows. For low-Reynolds-number regimes, the initial rarefaction effects are taken into account by means of imposing velocity slip and temperature jump boundary conditions on solid walls. For this purpose, the slip conditions are used. Time stepping is performed with the explicit Runge-Kutta scheme.

The DSMC code SMILE developed in the Computational Aerodynamics Laboratory, Institute of Theoretical and Applied Mechanics is utilized for kinetic modeling. Intermolecular collisions are computed by the Variable Hard Sphere (VHS) model. The number of collisions is calculated by the majorant frequency method. In the case of a polyatomic gas, the energy redistribution between rotational and translational degrees of freedom is obtained in accordance with the Larsen-

Borgnakke model. Up to 9.6×10^6 molecules are used to simulate the flows under consideration.

In the course of hybrid simulations, a coupling of Navier-Stokes solver and the DSMC method is based on the use of the NS solver in the nozzle and in the plume core and the DSMC method in the in the neighborhood of the nozzle lip and in the backflow region. Flow parameters on the boundaries of the DSMC computational domain, which are located inside the nozzle and in the central part of nozzle plume, are taken from a previous Navier-Stokes simulation. The velocity distribution function, which is needed to provide necessary boundary conditions for the DSMC method, is specified as the local Maxwellian distribution. It is worth noting that, from the general viewpoint, the Chapman-Enskog distribution function is a natural choice for model particles coming into the DSMC computational domain at the boundary between the NS and DSMC domains. However, the Chapman-Enskog distribution function has a drawback: it becomes negative with deviation from the Maxwellian distribution. Moreover, it was demonstrated in a number of investigations that the Chapman-Enskog distribution function may not provide much improvements against the Maxwellian distribution. As this simulations also demonstrate, the simplest approach to NS/DSMC coupling based on the local Maxwellian distribution works quite well for the present conditions. An example of the hybrid simulation for a low-Reynolds-number conical nozzle is shown in Fig. 1. The thick and thinner red lines are the boundaries of computational domains for the continuum and kinetic simulation, respectively. The density contours are shown as solid (for Navier-Stokes) and dashed (for DSMC) curves. From this figure, close agreement between two solutions in the common part of two computational domains is evident.

The Lagrange stage of the algorithm provides descriptions of motion, heating, evaporation/condensation of the droplets. Ordinary differential equations of test droplet motion and evolution can be written as follows:

\[
\frac{d\bar{X}_p}{dt} = \bar{R}_p, \quad \bar{X}_p = \begin{pmatrix} \bar{r}_p \\ m_p \\ m_p \bar{V}_p \\ m_p c_p^0 T_p \end{pmatrix}, \quad \bar{R}_p = \begin{pmatrix} \bar{V}_p \\ J_{gp} \\ \bar{F}_{gp} \\ Q_{gp} \end{pmatrix},
\]

where \( \bar{r}_p, \bar{V}_p, m_p, c_p^0, T_p \) are the radius vector, velocity, mass, heat capacity, and temperature of disperse inclusions and \( J_{gp}, \bar{F}_{gp}, Q_{gp} \) are terms that describe interphase transfer of mass, momentum, and energy.

Phenomenological approach is used to close the model; the closing relations are based on experimental data on mass, momentum, energy interphase transfer. For gas/droplet nozzle plume
flows with a significant difference in phase densities, \( \rho_p/\rho_g \sim 10^3 \), the main contribution to interphase transfer of momentum is made by the interphase drag:

\[
\vec{F}_{gp} = \vec{F}_{int} \equiv \frac{c_D \pi d_p^2 \rho_p}{8} |\vec{V}_g - \vec{V}_p| (\vec{V}_g - \vec{V}_p), \quad c_D = c_D \left( \text{Re}_{gp}, \ M_{gp}, \ Kn, \ We_{gp}, \ldots \right),
\]

where

\[
\text{Re}_{gp} = \frac{d_p \rho_g |\vec{V}_g - \vec{V}_p|}{\mu_g}, \quad M_{gp} = \frac{|\vec{V}_g - \vec{V}_p|}{\sqrt{\gamma p_g / \rho_g}}, \quad \text{Kn} = \Lambda/ d_p, \quad \text{We}_{gp} = \rho_g d_p |\vec{V}_g - \vec{V}_p| / \sigma_p.
\]

here \( \mu_g \) is the gas viscosity, \( \Lambda \) is the mean free path in the carrier phase, and \( \sigma_p \) is the surface tension coefficient.

Possible modes of droplet deformation and break-up due to interphase velocity lag are presented in diagram proposed by Gelfand (see Fig. 2). Domains shown by the Roman figures are: I corresponds to droplet deformation and break-up in the vibrational, “parachute”, and parachute + stamen” modes; II corresponds to droplet deformation and break-up in the “stripping” mode, III corresponds to droplet deformation and “explosive” break-up.

![Fig. 2. A diagram of droplet deformation and break-up modes in flows with phase velocity lag.](image)

Conditions under study correspond to domain depicted by red in Fig. 2. It ensures possibility to ignore droplet deformation and break-up, as well as droplet inner flow. Thus, it is possible to use approximations of \( c_D \) for solid particles valid in a wide range of flow parameters (see, e.g., [3]):

\[
c_D = 2 + (c_{D0} - 2) \exp \left( -3.07 \sqrt{k} \left( \frac{\text{Re}_{gp}}{\text{Re}_{gp}} \right) \frac{M_{gp}}{\text{Re}_{gp}} \right) + g \left( \frac{M_{gp}}{\text{Re}_{gp}} \right) \exp \left( \frac{\text{Re}_{gp}}{2M_{gp}} \right)
\]

\[
g \left( \text{Re}_{gp} \right) = \frac{1 + \text{Re}_{gp} \left( 12.278 + 0.548 \text{Re}_{gp} \right)}{1 + 11.278 \text{Re}_{gp}}, \quad h \left( M_{gp} \right) = \frac{5.6}{1 + M_{gp}} + 1.7 \sqrt{\frac{T_p}{T_g}}
\]

here \( k \) is the ratio of the specific heats of the carrier phase, and \( c_{D0} \) is the drag coefficient at \( M_{gp} = 0 \). This approximation is valid in a wide range of Mach and Reynolds numbers and, as we see, ensures \( c_D \) approaches to 2.0 at high values of the Knudsen number.
In the framework of a phenomenological description of interphase transport the contact heat transfer may be written as follows:

\[
Q_{gp} = \pi \lambda_g d_p Nu \left( T_g - T_p \right).
\]

Mass transfer due to diffusion and at conditions close to boiling can be respectively written as:

\[
J_{gp} = \pi D d_p Sh \left( \rho_v - \rho_s \left( T_p \right) \right), \quad J_{gp} = -\frac{Q_{gp}}{h_v}.
\]

Summarizing the above one can write:

\[
J_{gp} = \pi D d_p Sh \left( \rho_v - \rho_s \left( T_p \right) \right) \left( 1 - \delta \right) \frac{Q_{gp}}{h_v} \delta
\]

here \( \lambda_g \) is the carrier phase heat conductivity, \( D \) is the dispersed phase vapor diffusion coefficient, \( \rho_s \) is the saturated vapor density at the dispersed phase temperature, \( \delta = p_{ps}/p_g \), \( h_v \) is the latent heat of evaporation,

\[
Nu \left( Re_{gp}, \ M_{gp}, \ Kn, \ We_{gp}, \ ... \right) = \frac{d_p \beta_{gp}}{\lambda_g}
\]

is the Nusselt number and

\[
Sh \left( Re_{gp}, \ M_{gp}, \ Kn, \ We_{gp}, \ ... \right) = \frac{d_p K_{gp}}{D}
\]

is the Sherwood number.

To close the model Nusselt and Sherwood number approximations based on [4] were used

\[
Nu = \frac{2 + 0.552 Re_{gp}^{0.5} Pr^{0.33}}{1 + 3.42 \frac{M_{gp}}{Re_{gp} Pr}}, \quad Sh = \frac{2 + 0.552 Re_{gp}^{0.5} Sc^{0.33}}{1 + 3.42 \frac{M_{gp}}{Re_{gp} Sc}}
\]

here \( Pr \) is the Prandtl number, \( Sc \) is the Schmidt number.

Vaporization and condensation can significantly influence on the interphase mass, momentum, and energy transport. According to data [5] corrections accounting for vaporization/condensation can be introduced using the Spalding number,

\[
Br = c_D \left( T_g - T_p \right)/h_v
\]

\[
c_D \left( 1 + Br \right)^{0.2} = c_{D0}, \quad Nu \left( 1 + Br \right) = Nu_0, \quad Sh \left( 1 + Br \right) = Sh_0.
\]

The equations of the Lagrangian stage are solved by the Adams method.

To calculate the spatial distribution of gas-dynamic functions of the disperse phase and terms that describe interphase interaction we used the procedure of space-time averaging of trajectory
parameters of the probe particles that simulate the disperse phase. The procedure of averaging for a certain function $\varphi$ can be written as:

$$
\langle \varphi \rangle_i = \frac{\sum_{l \in \{ij\}} \hat{\eta}_l \int_0^{\tau_{ij}} \varphi \, dt}{\sum_{l \in \{ij\}} \hat{\eta}_l \tau_{ij}},
$$

$$
n_{pij} = \frac{\sum_{l \in \{ij\}} \hat{\eta}_l \tau_{ij}}{V_{ij}},
$$

where $\tau_{ij}$ is the residence time of the probe particle $l$ in the cell $\{ij\}$, $\hat{\eta}_l = n_{p0} V_{p0} S / N_p$ is the numerical flux of the disperse inclusions associated with the $l$-th probe particle, $n_{pij}$ is the numerical concentration of disperse inclusions in the cell $\{ij\}$, $V_{ij}$ is the volume of the computational cell $\{ij\}$, $S$ is the cross-sectional area through which disperse particles enter the computational domain, and $N_p$ is the number of probe particles; the subscript 0 indicates the parameters at the entrance to the computational domain. Summation is performed over all probe particles within the cell $\{ij\}$.

Effect of the dispersed particles on the carrier gas flow accounts in course of the following iteration procedure:
- at the first (eulerian) step, equations of the carrier gas are solved;
- at the second (lagrangian) step, trajectories of the probe particles are calculated using the obtained carrier phase flowfield;
- at the third (phase coupling) step, a time-spatial averaging procedure is performed for each computational cell in order to determine distributions of the dispersed phase parameters;
- at the fourth step the data obtained at the previous step are used to calculate the source terms of the governing equation of the carrier phase. These terms are incorporated in computation at the next eulerian step.

Results and Discussion

To validate the proposed algorithm a number of test computations have been carried out. In.

(a): variation in time of the droplet diameter (air temperature, $T_g = 1000$ K, ambient pressure, $p_g = 10^5$ Pa, initial temperature and diameter of the kerosene droplet, $T_d = 300$ K and $D_d = 1$ mkm, respectively, droplet velocity, $V_d = 10 - 100$ m/s); (b): the angular distribution of the droplet mass flux in the plume flow (droplet diameter, $D_d = 2.5$ mkm,)

![Graph](image-url)
particular, heating and evaporation of droplet in an air flow as well as angular distribution of droplet mass flux in a nozzle plume were simulated at conditions corresponding to known experimental data [6] and independent computations [7], respectively.

Comparison of the obtained results (see Fig. 3) demonstrates good agreement with independent data. Stratification of the droplet flow is demonstrated with limiting droplet trajectory corresponding to the angle 40°.

Fig. 4. Temporal evolution of the droplet diameter squared, (a), and the droplet temperature, (b), for hexane. The conditions are: \( T_g = 437 \) K, \( T_{p,0} = 281 \) K, \( D_0 = 1.76 \) mm, ambient air pressure is equal to one standard atmosphere, and \( R_{e_p,0} = 110 \)

To validate the proposed model for droplet evaporation in a convective air flow temporal evolution of the diameter squared and the temperature for hexane droplet are compared to experiments at a moderate evaporation rate. The simulation correspond to hexane droplet with an initial diameter and temperature of \( D_0 = 1.76 \) mm and \( T_{p,0} = 281 \) K, correspondingly, suspended in quiescent air (see Fig. 4 (a)) and in a convective flow with relatively large initial Reynolds number of \( R_{e_p,0} = 110 \) (see Fig. 4 (b)), the gas temperature, \( T_g = 437 \) K, in this case is nearly one hundred degrees above the liquid boiling point.

Predicted linear time dependence of surface area agrees with the experimental data. It is seen that the proposed model should be modified to be able to consider high rates of interphase mass transfer.

Nevertheless, the proposed model can provide adequate description of droplet flows in a wide range of flow parameters including highly rarefied flows.

On the basis of this model computations of the nozzle flow of a gas-droplet mixture have been conducted for conditions of experimental setup of the Institute of Thermophysics, Novosibirsk, Russia. The stagnation pressure is \( p_0 = 3390 \) Pa, the total temperature 293.15 K, the carrier gas is \( \text{N}_2 \), the nozzle-throat radius is \( r_c = 5 \) mm, the radius of the generatrix in the throat cross section is 5 mm, the radius of the exit cross section is 9.55 mm, the design Mach number is 2.84.

The computations show that at conditions under study high Mach numbers of the relative motion of droplets are reached only behind the nozzle exit for comparatively large drops (about 10µm and greater), see Fig. 5 (g). The droplet flows are highly stratified. Relatively low Weber numbers (see Fig. 5 (c, f)) confirm validity of the assumption to neglect of droplet deformation and inner flows.
Fig. 5 (a, b, c). Distributions of the Mach, Reynolds, and Weber numbers for the relative motion of droplets in the “experimental” nozzle of the Institute of Thermophysics of the Siberian Branch of the Russian Academy of Sciences. Droplet diameter 0.1\,\mu m.
Conclusions

Simulations of heating and evaporation of a quiescent droplet and a droplet in a convective flow of ambient gas were carried out. Comparison of the obtained results with experimental data and independent computations demonstrated good agreement for low and moderate evaporation rates.

Validation of the proposed algorithm confirms that it is able to describe adequately mass, momentum, and energy interphase transport in droplet nozzle and plume flows at low pressure conditions.

It was demonstrated that the droplets suspended in the flow are not responsible for the dispersed phase involved in the backflow and therefore are not responsible for spacecraft contamination.

REFERENCES