## CALCULATION OF NONEQUILIBRIUM TWO-PHASE, TWO-DIMENSIONAL FLOWS IN AN INITIAL CONDENSATION ZONE

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Finite-difference methods are improved to calculate two-dimensional transonic and supersonic flows in nozzles taking into account the kinetics of nonequilibrium phase transitions. A comparison with experimental data testifies to the improved accuracy of the methods under consideration.

Calculations of high-speed, two-phase flows, taking into account the kinetics of homogeneous or heterogeneous condensation, find ever-increasing application for designing power-generating plants, aircraft, and other present-day production equipment [1, 2]. Mathematical models of such calculations are usually [3] based on the following prerequisites: the two-phase medium is considered as interpenetrating continua; flow is adiabatic and moves in an initial condensation zone with a single velocity; pressure is induced only by a vapor (a gas), whose properties are approximated by the equation of state of a perfect gas; viscosity and heat conduction manifest themselves only at the interaction of the phases; homogeneous condensation is described in terms of the Frenkel–Zel'dovich nucleation theory; the condensation-induced growth of drops, having a constant temperature throughout the entire volume, is determined by one of the known Knudsen, Bouler, et al. formulas [4].

The total set of equations for such flows includes the equations of conservation, state of phases, and the kinetic equations for formation and growth of a condensing phase. The experience gained in one-dimensional the calculations and comparison with experimental results of different authors [4] have shown that sufficiently accurate results are attained if the Frenkel formula for a nucleation rate is used in the kinetic equations

$$I = \lambda \sqrt{\frac{2\mu\sigma}{\pi N_{\rm A}}} \frac{P}{k\rho' T''} \exp\left(-\beta \frac{4\pi\sigma}{3kT''} \xi_{\rm cr}^2\right),$$

where  $\lambda$  or  $\beta$  are the correction coefficients (usually one of them is introduced) dependent on the pressure, and the growth rate is determined by the Knudsen formula

$$\theta = \frac{\alpha_{\kappa}P}{\rho' \sqrt{2\pi RT}} \left( 1 - \sqrt{\frac{T''}{T'}} \right)$$

or by a more exact formula derived at the Central Boiler-Turbine Institute (CBTI):

$$\theta = \frac{\alpha_{\rm s} c_p \rho''}{r \rho'} \sqrt{\frac{RT''}{2\pi}} \frac{T' - T''}{1 + \frac{c_p T''}{r} - \frac{2\sigma}{r \rho' \xi}}$$

This is illustrated in Fig. 1, which shows the error of maximum overcooling calculation in experimentally investigated nozzles, which characterizes the onset of spontaneous condensation.

It is noteworthy that  $\lambda$  (or  $\beta$ ) practically has an effect only at the beginning of a spontaneous condensation zone (minimum pressure in the curves; see the figures), while the drop growth rate influences drop sizes behind the zone; of importance, the choice of a particular formula for  $\theta$  has a very small effect on a pressure rise in the spontaneous condensation zone ("a condensation jump") [4].

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Fig. 1. Accuracy of the calculation of initial condensation parameters (data of [4]): a)  $\Delta \bar{T} = 1 - \Delta T_{exp}^{max}/\Delta T_{calc}^{max}$ ; b)  $K = d_{exp}^{mod}/d_{calc}^{mod}$ ;  $\delta$ ) confidence interval (90% reliability).

The set of equations for a two-dimensional flow of a nonequilibrium condensing vapor has the form [1]:

$$\begin{aligned} \frac{\partial a}{\partial t} &+ \frac{\partial b}{\partial x} + \frac{\partial c}{\partial y} = 0, \\ a &= \begin{vmatrix} \rho \\ \rho u \\ \rho v \\ \rho v \\ \rho v \end{vmatrix}, \ b = \begin{vmatrix} \rho u \\ P + \rho u^2 \\ \rho uv \\ \rho uv \\ \rho uv \\ (i + w^2/2) \end{vmatrix}, \ c = \begin{vmatrix} \rho v \\ \rho uv \\ P + \rho v^2 \\ \rho v (i + w^2/2) \\ \frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} + v \frac{\partial f}{\partial y} + \frac{\partial (f\theta)}{\partial \xi} = I^*, \\ I^* &= I \frac{2}{\sqrt{2\pi} \omega \xi_{cr}} \exp \left[ -\frac{(\xi/\xi_{cr} - 1)^2}{2\omega^2} \right], \\ s &= \frac{\int_{\xi_{cr}}^{\infty} f\xi^3 d\xi}{\xi_{cr}}, \ T' = \frac{\int_{\xi_{cr}}^{\infty} T'_{\xi} f\xi^3 d\xi}{\xi_{cr}}, \\ \xi_{cr} &= \frac{2\sigma}{\rho' R T'' \ln (P/P_s)}, \\ \rho &= \rho' s + \rho'' (1 - s), \ i = i' s + i'' (1 - s), \\ i' &= c'T', \ i'' = \frac{\varkappa}{\varkappa - 1} \frac{\rho}{\rho''}. \end{aligned}$$

The inlet pressure and temperature, the pressure behind the nozzle, and the dispersion composition of moisture, if available, in the inlet cross section are assumed as the initial conditions. As regards the wall, the no-leakage condition is given.

Numerical solution of this system is usually made by one of the finite-difference methods of through-counting developed in the one-phase gas dynamics. Most often, Godunov's method is employed [5-9], which allows the first order of accuracy and uses the piecewise-constant approximation of parameters of both phases of the flow. In essence, this indicates the validity of the liquid phase "freezing" hypothesis within the limits of a calculation cell. The modified difference scheme proposed by V. P. Kolgan [10] increases the order of accuracy along the coordinates since the piecewise-linear approximation of parameters is used. In these methods, discontinuity decay is calculated by the one-phase gas dynamics relations that is not always justified [11]. The



Fig. 2. Pressure distribution along the CBTI nozzle axis (experiment [13]);  $P_0 = 0.1 \text{ MPa}$  [I)  $T_0 = 384 \text{ K}$ ; II) 399 K]: a) calculations by Godunov's method; b) Kolgan's method; c) one-dimensional calculations  $\omega = |(M/s)(ds/dx)/(dM/dx)|$ .

process of moisture release is described by differential equations of "the Hill chain" [1, 12], which simplifies the algorithm of solution but imparts, however, essential limitations to the relations for the drop growth rate because it is possible only under the assumption of independence of the growth rate from drop sizes (the Knudsen formula is used).

The reliability and accuracy of the methods is illustrated in Figs. 2 and 3, showing a comparison with experimental data on pressure distribution along the axis for condensing vapor flows in flat Laval nozzles. Figure 2 gives comparison with the experiments conducted at the CBTI [13], and Fig. 3 with experiments of G. Dyarmathy and H. Meyer [14]. The examples considered cover, in fact, the entire investigated range of a vapor expansion rate, which is the main governing parameter of nonequilibrium condensation flows.

As is seen, the above methods allow sufficiently exact determination of the location of a spontaneous condensation zone. However, gas dynamic parameters of the flow in the spontaneous condensation zone appear to be essentially different. Godunov's method practically does not show a pressure rise typical of this region and gives a rather distorted, in this sense, flow pattern. Moreover, it gives rise to a large error in the determination of the nozzle outlet pressure (in the given examples, the pressure behind the nozzle is prescribed lower than the predicted value). As regards Kolgan's method, the results are closer to the experimental data; in some cases a pressure rise is seen in the condensation zone but on the whole the difference between the calculated and the experimental values is still great. It is noteworthy that Kolgan's method possesses a worse, compared to Godunov's method, convergence and even for steady-state flows the large number of iterations does not eliminate "a numerical saw" [18]. To illustrate it, the vertical segments in Fig. 3b are made to show the numerical solution range after 4000 iterations (the counting time on a network is 90 min). Godunov's method at a given relative error of 0.3% per 100 iterations requires 2100 iterations (20 min).

As analysis has shown, the main reason for insufficient accuracy of calculations in the spontaneous condensation zone is the large difference in relaxation times of the vapor and liquid phases. Inspection of curves  $\omega(x)$  in Figs. 2 and 3 reveals that the gradients of the liquid-phase parameters in the spontaneous moisture-release zone are by 2-3 orders of magnitude higher than those of gas dynamic quantities. Therefore, though the method of averaging the vapor phase parameters accepted in discontinuity decay calculations is sufficient, for liquid phase parameters it is not. The situation does not essentially change with network reduction in size. The question of the possibility of calculation on such a small-meshed network, at which neglect of changing the liquid phase parameters is sufficiently justified, is left open, since it requires an increase of both the computational accuracy and the service life of the computer. Note that such a situation may take place in other problems of nonequilibrium gas dynamics concerned with different-scale relaxation processes.



Fig. 3. Pressure distribution along the axis of Dyarmathy's nozzle No. 1 [14],  $P_0 = 0.0635$  MPa,  $T_0 = 389$  K (a) and Dyarmathy's nozzle No. 3 [14],  $P_0 = 0.0632$  MPa,  $T_0 = 392$  K (b). Designations are the same as in Fig. 2.

It is obvious that the accuracy of calculations in the above region may be improved by considering a real (i.e., much larger than in the accepted methods) change in the parameters of the condensing phase. As a more simple tool, introduction of some effective degree of moisture  $s_{eff} = ks$  may be proposed, to be used only at the stage of calculating the increment of gas dynamic parameters. As is seen from the figures, the improves the convergence with experiments in some cases, in particular, in calculations by Kolgan's method (the figures at the curves in Figs. 2 and 3 are the values of k; k = 1 is not indicated). The calculations conducted show that introduction of  $s_{eff}$  has an effect only in the spontaneous condensation zone, changing neither any point at the beginning of it nor any other characteristics of the flow, including also flow pulsation frequencies under condensation instability conditions. The most suitable k values are 2-3; at larger values, the iteration process may fail to converge. Introduction of k in Kolgan's method does not improve the convergence and in some cases promotes "driving" of a solution.

A more complete account of the moisture release effect is attained by introducing, as proposed in [15], additional terms into the difference equations of continuity and energy, which determine directly a change in the mass and enthalpy of the condensing phase in a computation cell while preserving the piecewise-constant approximation of gas dynamic quantities. For the steady-state flow, these equations may be written [15], using the stationary analog of Godunov's scheme [16], as

$$A_{(k)}^{n-1/2} = A_{n-1/2} + E_n - E_{n-1} + G_{(k)}^{n-1/2},$$
  
$$D_{(k)}^{n-1/2} = D_{n-1/2} + (EF)_n - (EF)_{n-1} + H_{(k)}^{n-1/2}, \quad k = 0, \ 1, \ 2, \ \dots,$$

where the additional terms

$$G_{(k)}^{n-1/2} = \alpha \rho' u_{(k)} h_y [s_{(k)}^{n-1/2} - s_{n-1/2}],$$
  

$$H_{(k)}^{n-1/2} = \rho' u_{(k)} h_y \{ \alpha (i_{(k)} - i_{(k)}^{''}) [s_{(k)}^{n-1/2} - s_{n-1/2}] + \beta s_{(k)} [i_{(k)}^{(n-1/2)} - i_{n-1/2}^{'}] \}$$

are calculated through iterations that specify the semiexplicit character of the calculation scheme.

The results of our calculations (see solid curves in Figs. 2 and 3) prove to agree essentially better with experiment. In this method, moisture release is calculated by direct solution of a kinetic equation without using "the Hill chain," thus allowing consideration a wider class of drop growth equations, while interaction of the flows in neighboring cells (discontinuity decay) is determined from the relations for two-phase flows [11]. But the latter circumstance, as calculations have shown [17], has a small effect on results and yields only 15-20% of an actual pressure "jump."

All the calculations were made on an EC-1061 computer, using the problem-oriented package of applied programs "Moist Vapor."

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