SIMULATION OF PHASE ADSORPTION PROCESSES IN THERMAL PROCESSES

Academician Boris DRAGANOV

INSTITUTE OF ENGINEERING, KIEV, UKRAINE

The essence of analysis is that is entered a function \( \phi \) \((z_1, z_2, z_3, \tau)\), which indicates the probability that in the vicinity of a given point in space at time \( \tau \) is the \( i \)-th phase or that a given point of space belongs to the set of points the \( i \)-th phase.

This probability can be represented as the volume concentration of the \( i \)-th phase in a given point in space.

In the equation of motion we introduce the function \( k \)-interaction between the components of the flow. \( i \) is considered that the rate tensor is deformed, \( \delta^{ij} \) determined by the field of barycentric velocity, for mixtures \( v \).

\[
\begin{align*}
\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho_i v)}{\partial x} &= I_{1i}, \\
\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho_i v)}{\partial x} &= -I_{x}; \\
\rho \left( \frac{\partial u_i}{\partial t} + \frac{\partial (\rho_i v)}{\partial x} \right) &= \sigma \frac{\partial v}{\partial x} + \sigma \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x}.
\end{align*}
\]

The hypothesis of local equilibrium in phase permits:
- phases are two-parameter medium;
- thermodynamic functions of each phase depend only on the thermodynamic parameters of state (and the true density \( \rho^w \); temperature \( T \))

\[
\begin{align*}
u_i &= u_i (\rho_i^w, T_i), \\
p_i &= p_i (\rho_i^w, T_i), \\
s_i &= s_i (\rho_i^w, T_i), \\
T_i \frac{d_i}{dt} &= -p_i \left( \frac{1}{\rho_i^w} \right).
\end{align*}
\]

In the representation of the equation use the notation: the internal energy of the mixture can be taken as an additive for internal energies of phase. Then \( p\mu = \rho_1\mu_1 + \rho_2\mu_2 \).

It is considered that the effect of the mixture (\( \rho, i = 1, 2, \ldots, N \), where \( \rho \) – density) is directly expressed through the physical and chemical parameters. The system of equations of one-dimensional two-phase media in Eulerian variables \( x, t \) in terms of cylindrical symmetry, where \( \rho_1, \rho_2 \) – given the density of the phases; \( t \) – time, \( x \) – coordinate; \( v \) – velocity; \( I_{ij} \) – the intensity of the phase transition \( (I_{12} = I_{21}) \); \( u_1, u_2 \) – the internal energy; \( \rho \) – density of the mixture; \( q \) – heat flux; \( \sigma, \sigma^0 \) – the stress tensor, respectively, in the radial and circumferential directions; \( T \) – the temperature; \( p_i \) – the pressure; \( s_i \) – entropy.

A theoretical analysis of flows with condensation, which is based on the concept of nuclei formation (nucleation).

For a deeper approach is analyzed within a mixture of \( n \) components, which one can condensed. It includes the kinetic relation for the distribution function of droplet size, the values of the coefficients \( a, \) condensation and thermal accommodation \( \beta \).

An integral part of the condensation process is nucleation. For conditions of steady-state nucleation M. Vollmer, determines the rate of nucleation \( I \):

\[
I = bN \frac{3kT}{\sigma} B \exp(-B),
\]

where \( N \) – number of vapor molecules per unit volume; \( b \) – number of molecules which are
condensed in a collision with a unit surface per unit time; $k$ – Boltzmann’s constant; $\sigma$ – surface tension coefficient of liquid (which is independent of the radius $r$ of the drop).

Based on the kinetic theory of the value of $b$ determined by the formula:

$$b = \frac{a_k p}{\sqrt{2 \pi m_1 k T}},$$

where $a_k$ – condensation coefficient equal to the ratio the number of condensable vapor molecules to the number of molecules incident on the surface of the medium; $m_1$ – mass of the molecule.

Dimensionless factor

$$B = \frac{\sigma}{kT} \left( \frac{4 \pi V^2}{3} \right)^{1/2} n_{xp},$$

where $V$ – the volume occupied by one molecule of the liquid; $n_{xp}$ – the number of molecules in a drop of critical size.

For given external conditions, drops to a critical size are among the unsaturated vapor and evaporates, droplets size of supercritical ($r > r_{xp}$) – in an environment supersaturated vapor, and hence grow.

R. Becker and W. Doering received more accurate expression for the rate of formation of nuclei and condensation. Their calculation formula differs from the M. Folmer formula by pre-exponential factor:

$$f_r = \frac{S_1 a}{3 k T n_{xp} \sqrt{3 \pi B}} f_r,$$

where $S_1$ – surface area of the couple.

$$f_r = \frac{\chi}{n_{xp}^{1/2}} f_r.$$