Modeling the dynamics of a gas-droplet substance in nozzles, taking into account the phase transition

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Abstract. The paper studies the process of cluster formation, condensation and evaporation in a viscous flow of a two-phase gas-droplet mixture in nozzles and free jets. The simulation results obtained using the gas-kinetic scheme and the method of moments are presented. The system of equations is solved with the second order accuracy finite volume method and using the approximate AUSM+up or HLL methods for solution of the Riemann problem.

1. Introduction

Phase transition processes, which are the transonic flow around aerodynamic surfaces, in turbine units of aircraft engines and steam-gas units of thermal power plants, are essential to modern technologies, to aerodynamics and other fields. There are technologies of vacuum deposition of gas to form coatings [2], smoothing coatings by bombarding the surface with the help of an ionized cluster beam of inert gases [3], etc. In addition, condensation can provoke indignation in the throat region of the Laval nozzle, similar to shock waves, which are caused by the heat liberation of vaporization.

The work studies the process of cluster formation, condensation and evaporation during the flow of a two-phase gas-droplet substance in nozzles and jets in the outer region. Condensation and evaporation of xenon and water vapor have been investigated. The two-phase substance is a multicomponent gas (carrier gas and vapors of the condensing substance) and clusters (drops) of the condensing substance. It is believed that the gas phase and the droplets are in mechanical equilibrium.

There are methods that introduce kinetic intermolecular interactions, for example, gas-kinetic schemes [4,10]. In the kinetic methods, the particle association probabilities are used, depending on the internal energy, the number of inner degrees of freedom, and relative particle velocities. However, they are very expensive to compute. To simulate the condensation process, we use two approaches. One of them is the kinetic approach (quasi-chemical model of condensation [10]) and other is the continuum approach (the method of moments [1], it is supplemented by the evolution equation for the mass concentration of the condensing phase).

2. Mathematical model. Method of moment

As a mathematical model of gas, the Navier-Stokes equations are used, written in a weakly divergent form:

\[
\]
\[ \frac{\partial U}{\partial t} + \frac{\partial (F - F_c)}{\partial x} + \frac{\partial (G - G_c)}{\partial y} = S, \]

Other paragraphs are indented (BodytextIndented style).

\[
U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho Q_0 \\ \rho Q_1 \\ \rho Q_2 \\ \rho \alpha \\ \rho \alpha_{max} \end{bmatrix}; \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \\ \rho uQ_0 \\ \rho uQ_1 \\ \rho uQ_2 \\ \rho \alpha \\ \rho \alpha_{max} \end{bmatrix}; \quad G = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho E + p)v \end{bmatrix};
\]

\[
F_\alpha = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{yy} \\ u\tau_{xx} + v\tau_{xy} - q_x \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \quad G_\alpha = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{yy} \\ u\tau_{yy} + v\tau_{yy} - q_y \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \quad S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \delta(r - r_c)J \end{bmatrix}.
\]

Drops (clusters) formed during the condensation process are described using the droplet size distribution function \( f(x,t,r) \), \( r \) - is the radius of the spherical drop.

Assuming the mechanical equilibrium of the gas and liquid phase (droplets), the negligible volume fraction of the liquid phase, the spherical shape of the droplets and the absence of collisions between the droplets (the droplet phase does not generate pressure), the distribution function satisfies the General Dynamic Equation (GDE) [5]. The general dynamic equation describes the dynamics of droplets (clusters), the process of nucleation, condensation growth and evaporation.

The general equation of droplet dynamics for homogeneous condensation is written as:

\[ \frac{\partial f}{\partial t} + \frac{\partial (uf)}{\partial x} + \frac{\partial (ff)}{\partial r} = \delta(r - r_c)J, \]

\( J \) - homogeneous nucleation rate, \( \delta(r - r_c) \) - delta-function, \( r_c \) - droplet critical radius, \( \dot{r} \) - droplet growth rate.

Multiplying equation (2) by \( r^k \) (\( k \) is the natural number) and integrating along the radius from \( r_c \) to \( \infty \), we get an infinite chain of moment equations – chain of the Hill [1]:
\[
\frac{\partial}{\partial t} (\rho Q_k) + \frac{\partial}{\partial x_j} (\rho U_j Q_k) = (r^*_k)^k \rho J + k \rho Q_{k-1} \frac{\dot{r}}{J}, \quad k=1, \infty \tag{3}
\]

\[
\rho Q_n = \int_{x} r^n f(x, t, r) dr - \text{moments of the n-th order.}
\]

We consider the first four moments that have physical meaning. In this case: \(Q_0\) - equals the number density of droplets per unit mass, \(Q_1\) - sum of radii of all clusters, \(Q_2\) - sum of the squares of the radii of all clusters (estimate of the surface area of all clusters), \(Q_3\) - sum of cubes of radii of all clusters (estimation of the volume of all clusters). Instead of the moment \(Q_3\) it is convenient to use the mass fraction of the liquid phase \(\alpha = 4\pi \rho Q_3 / 3\), \(\rho_1\) - liquid phase density.

In this work, we consider the version of the method of moments (MM), in which the evolution of the liquid phase is described by a finite number of moment equations derived from the general equation of the dynamics of the cluster-droplet size distribution function [1], \(Q_0, Q_1, Q_2, \alpha\) and the equation for \(\alpha_{\text{max}}\) - mass fraction of the condensing phase at the beginning of the calculation. To simulate evaporation, the adaptation homogeneous nucleation rate, which is described in the article [8], was used:

\[
C_{v_{\text{mix}}} = (1 - \alpha_{\text{max}}) C_{v_a} + \alpha_{\text{max}} C_{v_V} + \alpha (C_l - C_{v_V}),
\]

\[
C_{p_{\text{mix}}} = (1 - \alpha_{\text{max}}) C_{p_a} + \alpha_{\text{max}} C_{p_V} + \alpha (C_l - C_{p_V}),
\]

\[
R_{\text{mix}} = (1 - \alpha_{\text{max}}) R_a + \alpha_{\text{max}} R_V - \alpha R_l,
\]

\[
\gamma_f = \frac{C_{p_{\text{mix}}}}{C_{v_{\text{mix}}}},
\]

\[
T = \frac{(E - u^2 / 2) + \alpha L_0}{(1 - \alpha_{\text{max}}) C_{v_a} + \alpha_{\text{max}} C_{v_V} + \alpha (C_l - C_{v_V})},
\]

\[
p = \rho T R_{\text{mix}},
\]

\[
\alpha_f^2 = \gamma_f \frac{p}{\rho},
\]

\[
L = L_T + L_0, \quad L_T = C_{p_V} - C_l,
\]

\(T\) – temperature of the mixture, \(\alpha_f\) - frozen velocity of sound of the mixture; \(L\) – latent heat of vaporization.

The right sides of the equations for the moments are written using the parameters calculated in the classical theory of nucleation. \(J\) is the homogeneous nucleation rate (the number of nucleation centers formed per unit volume per second); \(\dot{r} = dr/dt\) is the droplet grows rate; \(r_\ast\) is the critical radius (in this case, the lower limit of the radius).
\[ J = \frac{\rho_c^2}{\rho_s} \sqrt{\frac{2\sigma}{\pi m^3}} \exp \left( -\frac{4\pi R_c m T}{3} \right), \] (7)

\[ S = \frac{p_c}{p_s} \quad \text{- saturation ratio}, \] (8)

\[ r_c = \begin{cases} \frac{2\sigma}{\rho_c R_c T \ln S}, & \text{if } S > 1 \\ 0, & \text{if } S \leq 1 \end{cases} \] (9)

The growth of a drop is described by the Hertz-Knuth model [18] for the free-molecular regime of a multicomponent gas flow around a cluster-drop.

\[ \frac{dr}{dt} = \beta \frac{p_c - p_{S,r}}{\rho_i \sqrt{2\pi R_y T}} \] (10)

\[ p_{S,r} = p_s \exp \frac{2\sigma}{\rho_i R_y T r_{hull}} \quad \text{- saturated pressure for the surface of a drop of average radius,} \]

\[ r_{hull} = \begin{cases} \sqrt{\frac{Q_0}{Q_i}}, & \text{if } \alpha > 10^{-6} \\ 0, & \text{if } \alpha \leq 10^{-6} \end{cases} \] (11)

\[ \beta \] is the evaporation coefficient [1]. The value obtained by Tishkin(1946) \( \beta = 0.1 \) for ice has been used in this study.

In the algorithm the case \( r_{hull} \approx 0 \) (for example, \( r_{hull} \leq r_\ast \)) is considered in special way.

The system of equations (1), (4) is solved with the second order accuracy finite volume method [6] and using the approximate AUSM+up [7] (adaptation is in the appendix) and HLL [11] method for solving the Riemann problem. The approximation in time is performed by the second-order Runge-Kutta method. Viscous terms were approximated using central differential approximation.

3. Mathematical model. Kinetic method

In the quasi-chemical condensation model, it is believed that the condensing phase consists of a mixture of clusters consisting of an arbitrary number of molecules. Each component of the mixture is modelled using the perfect gas model. Assumption is that the number of monomers significantly exceeds the number of large-sized clusters. It means that the reaction of addition (detachment) of monomers have a dominant role in the process of growth and destruction of clusters.

\[ M_i + M_{i-1} \xrightarrow{\gamma_i} M_{i+1} \quad i = 1, 2, \ldots \] (12)

In the present case cluster size distribution functions (it means the number of clusters of size \( i \) in a kilogram of the mixture) along the streamline (in case when diffusion is off) can be determined by solving an infinite ordinary differential system [20-21]:

\[ \rho \frac{d\gamma_i}{dt} = W_i = I_{i-1} - I_i \quad i = 2, 3, \ldots \] (13)

which is supplemented by the condition preserving of the number of atoms of condensable and inert gases:
The molecular weight of the mixture is given by
\[ m_\Sigma = (\gamma_A + \sum_{i=1}^{\infty} \gamma_i)^{-1}. \]

The expression for the Gibbs potential of the mixture is
\[ G(p,T,\gamma) = \gamma_A G_A(p,T) + \sum_{i=1}^{\infty} \gamma_i G_i(p,T) + T S_\Sigma(\gamma), \]
where \( S_\Sigma(\gamma) = R \sum_{i=1}^{\infty} \gamma_i \ln x_i + \gamma_A \ln x_A \), \( x_i = \gamma_i m_\Sigma \), \( x_A = \gamma_A m_\Sigma \).

\[ G_j(p,T) = RT \ln(p / p_0) + G_j(T), \quad j = A, 1, 2, ... \]

\[ G'_i(T) = i G'_i(T) + B(T)i^{2/3}, \quad i = 2, 3, ..., B(T) = \sigma(T)(36\pi)^{1/3} N_A(m_i / \rho_L(T))^{2/3} \]
\( G'_i(T), G'_j(T), G'_k(T) \) - taken from the directory [19].

Corresponding thermal and caloric equations of state are
\[ \rho = \left( \frac{\partial G}{\partial p} \right)_T = \frac{p m_\Sigma}{RT}. \]
\[ h = \gamma_A H_A^0(T) + \gamma_i H_i^0(T) + \sum_{i=2}^{\infty} i \gamma_i H_i^0(T) + B(T) \left( 1 - T \left( \frac{\sigma(T)}{\sigma(T)} - \frac{2 \rho_L(T)}{3 \rho_L(T)} \right) \right) \sum_{i=2}^{\infty} i^{2/3} \gamma_i \]

According to kinetic equations (12), expressions for the right parts (13) can be written as:
\[ I_i = v_i e_i \left( \frac{\gamma_i}{e_i} - \frac{\gamma_i}{e_i} \right), \quad e_i = \exp \left[ i \ln x_i - \left( \frac{G_i(p,T) - i G_i(p,T)}{RT} \right) \right]. \]

The expression for the rate of addition of monomer to \( i \)-mer is
\[ v_i = \alpha_i 4 \pi \rho^2 N_A^\frac{1}{3} \left( \frac{3 m_i}{4 \pi \rho} \right)^{1/2} \left( 1 + i^{-1} \right)^{1/2} \left( 1 + \delta_i \right)^{1/2} \frac{RT}{(2\pi m_i)^{1/2}}, \quad i=1, 2, 3,... \]
\( m_i \) - molecular weight of condensable gas; \( \alpha_i \) - condensation coefficient.

When studying the condensation process in the nozzles, it is usually assumed that in the receiver the condensing gas is in a stable state and the cluster size distribution function is close to the delta function and can be calculated from the conditions of thermodynamic equilibrium. If pressure and temperature are known, then the amount of supersaturation \( s = p / p_H \) can be found from a nonlinear algebraic equation:
\[ F(s) = \sum_{i=1}^{\infty} \left( 1 + \frac{\gamma_A}{\gamma_i} \right)^{1/2} \exp \left[ \ln s + \frac{i G_L(p,s,T) - G_i(p,T)}{RT} \right] - 1 = 0, \]
Other the distribution function can be found from the equilibrium conditions:

\[ G_i(p, T) + RT \ln x_i = i(G_i(p, T) + RT \ln x_i) = i\left(G_i(p/s, T) + RT \ln s\right). \]

Using equation (19), system of equations (13) - (14) can be rewritten as:

\[ \rho \frac{d\gamma_i}{dt} = v_{i-1}\gamma_{i-1} - \left(\frac{v_e_i e_{i+1}}{e_{i+1}} + \frac{v_e_i e_i}{e_{i+1}}\right)\gamma_i + \frac{v_e_i e_{i+1}}{e_{i+1}}\gamma_{i+1}, \quad i = 2, 3, \ldots \quad (22) \]

\[ \gamma_i = \gamma_0 - \sum_{i=2}^{n} i\gamma_i. \quad (23) \]

Using equations of the form (22) of infinite dimension is impossible in practice. And thus, systems of finite dimension \(N\) are used which are obtained from system (22). Additionally, it is assumed that \(I_N = 0\). In the system (22) the equations for \(\gamma_i\) with \(i > N\) and in (23) corresponding terms are removed. However, if \(N\) is not large enough, the solution is not accurate. Therefore, in practice [22], stretch function \(n_i, \quad i=2,3,\ldots,N\) \((n_1=1, \quad n_N>>N, \quad n_i=dn/di \geq 1)\) is used, which indicates the number of molecules in the cluster with the number \(i\). The abridged system is approximated by a completely implicit difference scheme. The resulting nonlinear difference system is solved by the iteration scheme. At each iteration, a system of linear algebraic equations with a tridiagonal matrix is solved using the sweep method.

4. Numerical results

4.1. Homogeneous condensation in the shock tube

The phenomenon of condensation in a fan of rarefaction waves arising in the process of disintegration of a discontinuity in a shock tube is investigated. The initial stage of the flow arising after rupture of the membrane in a flat shock tube is considered (figure 1). The pipe has a length of 1 meter, filled with wet nitrogen, the membrane is located exactly in the middle, the pressure in the high-pressure chamber is \(p_4 = 1.0\) bar, the humidity is \(S_4 = 0.82\). In the low-pressure chamber \(p_1 = 0.3\) bar, humidity \(S_1 = 0.246\). Temperature everywhere \(T_1 = T_4 = 295K\). Mass fraction of water vapour in both chambers of the pipe at the beginning of the process is 0.013744.

The calculation was performed using an algorithm that implements the method of moments on a uniform computational grid of \(N = 1000\) cells \((\Delta x = 1/N\) m), with a time step \(\Delta t = 0.0005\Delta x\) until time point \(t = 0.001\) s.

Figure 1. X-t diagram of the flow in the shock tube.
Figure 1 shows the $X_t$ diagram of the flow in the shock tube resulting from decay of discontinuity. The rarefaction wave (RW) propagates to the high-pressure chamber area, the shock wave (SW) propagates in the low-pressure chamber area and contact discontinuity (CS). The temperature drop in the region of propagation of rarefaction waves (RW) and, especially, in region 3 in figure 1 leads to the emergence of supersaturation, due to which the formation of clusters and their growth with release of heat of condensation occur. The most active condensation process takes place near the closing characteristic of the second RW fan family in region 3. At the same time, gas trajectories emanating from the region of the initial rupture point just to the left of the instantaneous point almost immediately fall into the zone of strong rarefaction and low temperatures 1, which leads to a change in the parameters to the left of the contact discontinuity and the formation in the initial period of time in the zone between RW and CS of the fan of compression waves with time of the shock entering the shock wave (condensation shock) figure 2a, b.

Figure 2. Contour lines of the temperature field (a) and density (b).

Figure 3 shows the pressure distribution along the pipe for an adiabatic flow (blue line) and condensed flow (red line) at a point in time. One can see a sharp increase in pressure in the condensation shock at the end of the RW fan, as well as a slight increase in pressure in zones 3 and 2 of figure 1. In general, the algorithm based on the method of moments qualitatively correctly describes the physical effects that occur in shock tubes with a wet gaseous medium, and the calculated results quantitatively correspond to the calculations of [9].

Figure 3. Pressure distribution at time $t = 10^3$ s. The blue line is the adiabatic flow. The red line is the flow with condensation.
4.2. Xenon condensation in a shock tube quasi-two-dimensional system

The physical properties of xenon are taken from [13]. Considered a conical nozzle with throat radius \( r_{cr} = 0.00007 \) m, exit area radius \( R = 7r_{cr} \), length of the supersonic part \( L = 120r_{cr} \), temperature in the receiver \( T_k = 293 \) K, nozzle inlet pressure \( p_k = 3, 4, 4.5, 5 \) atm. The simulation results are shown in the figure 4.

![Figure 4](image)

**Figure 4.** Distribution of physical parameters after the nozzle throat. a - temperature, b – pressure relative to inlet pressure, c - concentration of the liquid fraction.

For the inlet pressure \( p_k = 3 \) atm, the processes of nucleation and condensation proceed unnoticed, therefore the flow parameters (temperature and dimensionless pressure) are equal to the parameters of the adiabatic flow (figure 4 a, b). In the case when the pressure \( p_k > 3 \) atm in the supersonic part at a distance of 1 mm from the nozzle throat, condensation and active heat generation of condensation begin in the flow, leading to a difference in pressure and temperature in the flow from the values in the adiabatic flow. The strongest effect of inlet pressure on flow parameters is observed at \( p_k > 4.5 \) atm. In this case, the mass fraction of the liquid phase can reach 0.23 (\( p_k = 5 \) atm, figure 4 c).

4.3. Condensation and evaporation of water vapor in a Laval nozzle 1D and 2D

Simulated experiment is described in [12]. The pressure in the receiver was considered to be 60 kPa, the temperature was 287.6 K, and the partial pressure of water vapor in the receiver was 1 kPa (mass fraction of water vapor). The origin of the coordinate system is located at the center of the nozzle throat. The scheme of the computational domain is shown in figure 5, and the results of calculations in comparison with experiment [12] in figure 6.

![Figure 5](image)

**Figure 5.** Scheme of the calculated flat nozzle.
Other the distribution function can be found from the equilibrium conditions: It can be said that the condensation process began to affect the macro parameters of the mixture in one cm away from the throat (figure 8). At a distance of 1.8 centimeters from the throat the monomers contain more than 70% of the mass, 30% are contained in clusters ranging in size from 100 to 1000 molecules. At a distance of 3.2 cm the monomers contain about 20% of the mass of water, 80% are contained in clusters larger than 800 molecules. Despite the fact that the difference between the distribution function at distances of 3.2 cm and 9 cm from the throat is small (Figure 9), nevertheless, the mass fraction of water monomers is about 2%. The remaining water molecules are contained in clusters larger than 900 molecules. Large clusters grow due to a decrease in the concentration of clusters ranging in size from 1 to 10 molecules, while the concentration of clusters ranging in size from 1 to 10 molecules practically does not change.
When solving the problem in a two-dimensional formulation (figure 10), it can be seen that the concentration distribution of the liquid fraction is uniform along the vertical section of the nozzle, if you do not take into account the boundary layer.

![Figure 10. Mass fraction of liquid along the nozzle axis in 2D.](image)

To study the evaporation, a numerical experiment was conducted in which a pressure shock forms in the nozzle. For this purpose, as the boundary condition, the outlet pressure was assumed to be constant with the value 2kPa. In figure 11 and figure 12 are the results of evaporation of a liquid that occurs behind a pressure shock.

![Figure 11. Pressure distribution along the nozzle axis with pressure shock.](image)  ![Figure 12. Mass fraction of liquid fraction along the nozzle axis with evaporation.](image)

In the two-dimensional formulation of the problem, we see (Figure 13) the growth of the boundary layer behind the shock wave. The temperature grows near the boundary layer. Evaporation is less intense, in contrast to the one-dimensional formulation of the problem.

**Conclusion**

The method of moments cannot give a complete picture of the nucleation process. And the method of moments does not describe the cluster size distribution function, which can be obtained using the methods [4,10,15]. It is also impossible to study in detail the behavior of particles during sticking using the velocity distribution function of particles [14], considering the interaction potentials of molecules at the moment when the partial pressure of the condensing phase exceeds the gas saturation pressure. However, with the help of moments, you can get a general idea of the behavior of the gas-droplet mixture, you can predict the appearance of pressure surges, temperature. Using the method of moments, you can determine how much of the substance will condense (or evaporate) and you can determine at what point in time this will happen. With the help of the moments, it is even possible to restore approximately the particle size distribution function [16]. The calculations using the methods of moments are performed at almost the same speed as the Navier-Stokes equations are solved.

**Acknowledgments**

This work was partially supported by Government program of basic research of Russian academy of science (contract #AAAA-A17-117021310372-6).
Figure 13. Contour a) – mass fraction of liquid, b) – mach number, c) – temperature.

Appendix. Adaptation AUSM+up method for MOM

The inviscid flow in the AUSM + -up scheme is divided into the mass flow and the pressure flow:

\[ F_{i+\frac{1}{2}} = \frac{\bar{m} + |\bar{m}|}{2} \Psi^+ + \frac{\bar{m} - |\bar{m}|}{2} \Psi^- + \tilde{p}N, \]

\[ \Psi = (1, u, v, E, Q_0, Q_1, Q_2, \alpha, \alpha_{\text{max}})^T, \]

\[ N = (0, n_x, n_y, 0, 0, 0, 0, 0)^T. \]

The indices L and R denote the left and right cells.

Mass flow:

\[ \bar{m} = M_{\frac{1}{2}} a_{\frac{1}{2}} \begin{cases} \rho_L, & M_{\frac{1}{2}} > 0, \\ \rho_R, & M_{\frac{1}{2}} \leq 0. \end{cases} \]

\[ M_{\frac{1}{2}} = M^* + M^- + M^\rho, \]

\[ M^\pm = \begin{cases} \frac{1}{2}(M \pm |M|), & |M| \geq 1, \\ \pm \frac{1}{4}(M \pm 1)^2 \pm \frac{1}{8}(M^2 - 1)^2, & |M| < 1. \end{cases} \]
\[
M_p = -K_p \max(1 - \sigma \frac{M_L^2 + M_R^2}{2}, 0) - \frac{P_R - P_L}{\rho_R + \rho_L}^2 \cdot \frac{C_L}{2} \cdot \frac{C_R}{2} \cdot a_{\|/2},
\]

\[
a_{\|/2} = \min(C_L, C_R),
\]

\[
\tilde{C}_{L,R} = \frac{C_{L,R}^2}{\max(C_{L,R}, |U_{L,R}|)}.
\]

\[
C_{L,R} = 2 \gamma_{L,R} \left( \frac{1 - \gamma_{L,R}}{2} \gamma_{L,R} + 1 \left( \frac{P_{L,R}}{\gamma_{L,R}} \right) \right).
\]

Pressure flow:

\[
\tilde{p} = P^+ |_{u_L} \cdot P^+ |_{u_R} \cdot P^+ |_{u_u} \cdot P^+ |_{u_u}.
\]

\[
P^+ = \begin{cases} 
1/2 (1 \pm \text{sign}(M)), & |M| \geq 1, \\
1/4 (M \pm 1)^2 (2 \mp M) \pm \alpha M (M^2 - 1), & |M| < 1.
\end{cases}
\]

\[
P_u = -K_u \cdot P^+ \cdot \rho_R - \frac{\rho_R - \rho_L}{2} \cdot a_{\|/2} \cdot (U_R - U_L).
\]

The coefficients for solving the Riemann problem are \( K_p = 0.25, K_u = 0.025, \alpha = 3/16, \sigma = 1. \)

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