Applying the relaxation model of interfacial heat transfer to calculate the liquid outflow with supercritical initial parameters

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Abstract. A comparative numerical simulation of the supercritical fluid outflow on the thermodynamic equilibrium and non-equilibrium relaxation models of phase transition for different times of relaxation has been performed. The model for the fixed relaxation time based on the experimentally determined radius of liquid droplets was compared with the model of dynamically changing relaxation time, calculated by the formula (7) and depending on local parameters. It is shown that the relaxation time varies significantly depending on the thermodynamic conditions of the two-phase medium in the course of outflowing. The application of the proposed model with dynamic relaxation time leads to qualitatively correct results. The model can be used for both vaporization and condensation processes. It is shown that the model can be improved on the basis of processing experimental data on the distribution of the droplet sizes formed during the breaking up of the liquid jet.

1. Introduction

De-pressurization of vessels and pipelines in power plants, filled with water under high pressure, leads to a release of superheated water with a drastic pressure decrease in the area of rupture, formation of compression waves in the surrounding medium and further formation of the jet of the boiling-up coolant [1]. If thermodynamic parameters of the coolant (pressure, temperature) are in the supercritical region, there is a case when parameters of the fluid at outflowing pass not only through the curve of saturation and «boiling», but through the curve of «condensation» as well [2]. The process of adiabatic expansion, as a rule, is non-equilibrium and its description frequently requires a thermodynamic non-equilibrium two-temperature model of steam-water mixture motion [3]. In the simulation of vaporization in real conditions it is necessary either to set the parameters of the heterogeneous mechanism of bubbles formation (e.g. [4]), or to use a different (phenomenological) approach (e.g., relaxation [5]). In particular, in [4] it is proposed to set the number of vaporization centres added with asymptotic models of bubbles growth as an empirical parameter. Due to the use of a bubble structure to describe the two-phase medium, this approach loses its adequacy at large ($\alpha > 0.3 - 0.5$) volumetric steam qualities.

Earlier, authors of [6] based on the performed analysis proposed a simple relaxation model for the description of thermal and dynamic processes, involving water boiling at de-pressurization of high pressure vessel. The model assumes droplet structure of the liquid-vapor flow, which is
typical at high differential pressure «vessel – atmosphere». This paper is an attempt to generalize
this model to the case of non-equilibrium condensation.

There are many experimental studies of the features of the stationary jet outflow of
superheated steam and boiling coolant on the obstacle under high pressure. For example, authors
of [7] measured the impact of the steam jet on the obstacle and the pressure distribution over the
obstacle radius. They showed similarity of the stationary outflow of the superheated steam and
that of the gas jet. Experimental study of the stationary outflow of boiling coolant from the pipe
end on the barrier in an industrial scale was carried out in [8]. An adequate calculation of the
characteristics of the wave action on the barrier at small times is of great interest in modelling
the flow of the coolant both with subcritical and supercritical parameters.

2. Governing equations

The present study considers an axisymmetric problem of water coolant outflow from high pressure
vessel with the aim to obtain the characteristics of wave impact on the outer barrier and other
parameters of the outflow. Numerical simulation is carried out in the absence of the phase slip,
and given that the vapor and liquid phases can be in a metastable state. The system of model
equations includes the Euler equations in the axisymmetric approximation:

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

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

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

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

added with the equation for interphase mass transfer:

\[
\frac{\partial}{\partial t} (\rho r X) + \frac{\partial}{\partial z} (\rho r X) + \frac{\partial}{\partial r} (\rho r X) = \Gamma
\]

\[
\Gamma = \rho (X S - X) \theta
\]

Here, \(z, r\) are the axial and radial coordinates, \(u, v\) are the axial and radial components of
velocity, \(\rho\) is the density, \(p\) is the pressure, \(E\) is the specific internal energy, \(X\) is the steam quality
and \(X_s\) is the equilibrium steam quality (at given \(p\) and \(E\)), \(\Gamma\) is the rate of steam generation,
and \(\theta\) is the relaxation time. The system of equations (1)-(6) is closed by the equation of state
(relationship between \(p, E, \rho, X\)).

Calculation of properties of steam and water in sub- and supercritical condition was performed
using the software package TTSE [9]. The program code was developed to solve a wide class
of problems on de-pressurization of the vessels or pipelines with superheated water coolant with
the use of computer complex LCPFCT [10].

Due to low density of steam the droplet structure of the two-phase medium is typical even
at small steam qualities (but moderate and large volumetric ones) [11], and can be used in the
modelling of intensive evaporation of liquid. To determine the relaxation time in (6), an analytic
relaxation model [6] is used (as mentioned above), constructed on the basis of the asymptotic
solution of the thermal problem in superheated water droplets of the same size:

\[
\theta = \frac{R^2}{\pi^2 a}
\]
In a real situation, the droplet size distribution takes place [12]. Therefore, according to the existing spectrum, it is necessary to calculate an effective droplet size. The droplet size is easy determined from the simplified analysis of instability of «water-steam» interface: the droplet size corresponds to the length of waves, the fastest destroying the interfacial surface, and is determined by critical Weber number \(\text{We}_{cr}\) approximately equals to 2\(\pi\) (water, liquid metals) [11, 13]. According to the model, at the micro-level of drops the heat required for vaporization is supplied from the superheated liquid. The temperature of the droplet surface is equal to the steam temperature [14]. To calculate the relaxation time we proposed the formula [6].

\[
\theta = \begin{cases} \frac{\sigma^2 \rho_i^2}{4 \alpha L \rho V^2 (P - P_S)^2}, & P - P_S > \frac{\rho L^2}{2 (\frac{\rho L}{\rho V} - 1)^2 C_{P,L}} \\ \frac{\sigma^2 (\frac{\rho L}{\rho V} - 1)^4 C_{P,L} T^2}{\alpha L \rho V^2 L^2}, & P - P_S \leq \frac{\rho L^2}{2 (\frac{\rho L}{\rho V} - 1)^2 C_{P,L}} \end{cases}
\]

(8)

Here, \(\sigma\) is the surface tension coefficient, \(\alpha\) is the thermal diffusivity, \(C_{P,L}\) is specific heat of liquid and \(L\) is the enthalpy of phase transition. To use the relaxation model not only for evaporation, but condensation as well, we substantially modified the equation of state of two-phase medium, which closes the system of equations (1)-(6) to the case of existence of not only saturated, but supercooled steam. Although the size of drops formed in the condensation may change from the case of jet disintegration [11, 13], the formula (7) was used for test calculations. Simulation was carried out in two versions: a) with fixation of the relaxation time; b) taking into account its dependence on locally varying parameters (dynamic relaxation model, as well as in the paper [5]).

The relaxation time \(\theta\) (7) is proportional to the square of the drop size, that is very sensitive to the value of this parameter. In addition, the characteristic size of the drop, according to the model, is determined by the magnitude of the critical Weber number \(\text{We}_{cr}\) and formally must reach this value asymptotically for long times. Therefore, the correct choice of the characteristic (effective) size remains an important problem. The most reasonable approach is to analyze the real distribution of droplets in sizes obtained from experiments on fragmentation of boiling-up jet upon its outflow from a pressure vessel (see, for example, the review [15]). Figure 1 presents a concrete example of such a droplet size distribution [12]. The right maximum of the distribution curve is associated with the classical jet fragmentation, which is determined by the \(\text{We}_{cr}\) and exists both for the hot and cold (no boiling up) liquid outflow. The left maximum is explained by the fragmentation of large droplets, caused by their explosive effervescence [12, 16] and for a cold liquid is not observed.

Applying the procedure for deriving the relaxation equation for a monodisperse medium [6] to a polydisperse discrete distribution, we obtain the following model evolution equations for the mass content of the liquid drops \(X_{drop} = \sum_i X_i\):

\[
\delta X_{drop} \approx \frac{C_{P,L}}{L} \sum_i X_i \delta T_i
\]

(9)

\[
\frac{dX_{drop}}{dt} = -\frac{C_{P,L}}{L} \sum_i X_i \frac{\delta T_i}{\theta_i}
\]

(10)

where \(\theta = R_i^2 / \pi^2 a\), \(\delta T_i = (T_0 - T_s(P)) \exp(-t/\theta_i)\)

The procedure for choosing the effective (characteristic) droplet size is proposed as follows: the solution of equation (9) is compared with the exponent \(\exp(-t/\tau_{eff})\), where the parameter \(\tau_{eff}\) is chosen so that this exponent, simultaneously with the exact solution (9), reaches a dimensionless sensation, for example, 0.01. This is equivalent to the generally accepted definition of boundary layer thickness in fluids.
The analysis shows that in a wide range of design parameters for water the equilibrium model is adequate with sufficient accuracy at \( \theta < 10^{-6} \) s. Therefore, it was logical to "cut off" droplets of small size, for which, for example, \( \theta < 10^{-6} \) s (for the experiment (Figure 1), this corresponds to drops with \( R < 1.3 \mu m \)). Then we can assume that the liquid in small droplets instantly cools, forming a thermodynamically equilibrium vapor-liquid medium together with the vapor. In this case, relaxation takes place only on larger drops.

\[
X, \quad R_{\text{drop}}
\]

Figure 1. Dependence of the volume content of the liquid on the droplet radius at a distance of 60 mm from the cut of the nozzle at a water temperature of 473K and a pressure of 8MPa [12]

The characteristic radius of the droplets for the distribution in Fig. 1 calculated according to the proposed procedure with «cut-off» of small drops, is equal to 9.8 \( \mu m \), which corresponds to a relaxation time value of \( 5.8 \times 10^{-5} \) s. The use of an exact solution with a full spectrum of drops substantially reduces the characteristic relaxation time, and it is not practical to use it.

For this reason, it is clearly inappropriate to use the so-called sauter mean size as a characteristic size, which is acceptable when the character of the heat exchange on droplets of different sizes is the same. Unfortunately, in many experiments to investigate the fragmentation of drops, namely this parameter is given (for example [16]).

In our opinion, for the logical completion of the relaxation model construction, it is necessary to carefully analyse all available experimental data on the distribution of droplets in the jet of boiling liquid, depending on the initial pressure and temperature. Then, based on the algorithm proposed above, we get a reasonable empirical formula for the effective droplet radius and relaxation time. Further comparison with a verified more complete program or an appropriate precision experiments will make the final model choice.

3. The calculation results

Earlier in [2] it was shown that a small change of initial parameters leads to a significant change in the nature of a supercritical fluid outflow, in particular, to a change in direction of phase transition. The present work provides calculations of the outflow of water in the supercritical state in a wide range of parameters at different initial parameters and different geometry of the computational domain.

Both equilibrium and non-equilibrium relaxation models of the phase transition were used. The thermodynamic equilibrium model of two-phase medium was, in fact, obtained from the general system (1)-(4) with its closing by the equation of state of the equilibrium two-phase mixture. A fixed relaxation time \( \theta = 10^{-4} \) was chosen in accordance with the relaxation model (7) for the experimentally determined droplet sizes of \( 10^{-5} \) m [12].

In the numerical calculation, a dynamic relaxation model was also used. The relaxation time was determined from expression (8), which includes the local parameters of the mixture. It
turned out that both at evaporation and condensation, the relaxation time varies in the range from $10^{-6}$s to $10^{-3}$s, and the main change occurs in the range from $10^{-5}$s to $10^{-4}$s. These values are in good agreement with the experimental data on relaxation time during steam condensation in Laval nozzles. In particular, in [16] it was shown that the characteristic relaxation time is of the order of $10^{-5}$s.

Figure 2 shows the calculation results of spatial distribution of normalized pressure gradient and steam quality for the case of the boiling up water jet outflow and its impact on the barrier. Profiles are calculated at time of 0.3 s after de-pressurization for the dynamic relaxation model. Two pressure wave fronts are observed, as in the case of the outflow of a coolant located at subcritical parameters [17]. The first pressure front corresponds to the compression wave, the second front to the rarefaction wave. It can be noted that the difference in the fields of the pressure gradient for boiling and condensation processes is inessential. The amplitudes of the pressure waves for these cases are also close. A significant difference can be observed for fields of mass vapor content (Fig. 2, bottom). Inside the channel, both the boiling front (Fig. 2a) and the condensation one (Fig. 2b) propagate. The velocity of the condensation front is higher than the velocity of the boiling one. In both cases, the regions of sharp changes in the mass vapor content correspond to the regions of the fronts of the sudden change in pressure.

![Figure 2](image_url)

**Figure 2.** Spatial distribution of normalized pressure gradient (top) and steam quality (bottom) at time $t = 300$ µs for initial conditions $P_0 = 23$ MPa, $T_0 = 370^\circ$C (a) and $T_0 = 380^\circ$C (b)

Fig. 3, 4 shows axial distributions of steam quality calculated by three models at different points in time. It is seen that inside the channel the calculation results obtained by the equilibrium model and for the dynamic relaxation time coincide with graphical accuracy. The small value of the relaxation time (8) is most likely due to the close to zero value of the surface tension $\sigma$ in the near-critical region. At a greater distance from the nozzle the relaxation time increases to values of $\theta \approx 10^{-4}$s. This leads to an increasing deviation of the results of the calculation on the dynamic model from the equilibrium model and the approximation of the results with a fixed relaxation time.

4. Conclusion

We have performed a comparative numerical simulation of the supercritical fluid outflow on the thermodynamic equilibrium and non-equilibrium relaxation models of phase transition for different times of relaxation: fixed, based on the experimentally determined radii of the drops, and dynamically changing, depending on local parameters. The application of the proposed model with dynamic relaxation time leads to qualitatively correct results. The model can be
Figure 3. Axial distribution of steam quality for the initial conditions $P_0 = 23$ MPa, $T_0 = 365^0$C (a) and $T_0 = 385^0$C (b), $t = 90 \mu s$ (1 - equilibrium model; 2 - fixed relaxation time $\theta = 10^{-4}$s; 3 - dynamic relaxation model).

Figure 4. Axial distribution of steam quality for the initial conditions $P_0 = 23$ MPa, $T_0 = 365^0$C (a) and $T_0 = 385^0$C (b), $t = 150 \mu s$ (1 - equilibrium model; 2 - fixed relaxation time $\theta = 10^{-4}$s; 3 - dynamic relaxation model).

used for both vaporization and condensation processes. It is shown that the model can be improved on the basis of processing experimental data on the distribution of the droplet sizes formed during the breaking up of the liquid jet.

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