Numerical modeling of the waves evolution generated by the depressurization of the vessels containing a supercritical parameters coolant

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Abstract. The development of power plants focuses on increasing the parameters of water coolants up to a supercritical level. Depressurization of the unit circuits with such a coolant leads to emergency situations. Their scenarios can change significantly with the variation of initial pressure and temperature before the start of depressurization. When the pressure drops from the supercritical single-phase region of the initial thermodynamic parameters of the coolant, either the liquid boils up, or the vapor is condensed. Because of the rapid pressure decrease, the phase transition can be non-equilibrium that must be taken into account in the simulation. In the present study, an axisymmetric problem of the outflow of a water coolant from the pipe butt-end is considered. The equations of continuity, momentum and energy for a two-phase homogeneous mixture are solved numerically. The vapor and liquid properties are calculated using the TTSE software package (The Tabular Taylor Series Expansion Method). On the basis of the computer complex LCFFCT (The Flux-Corrected Transport Algorithm) the program code was developed for solving numerous problems on the depressurization of vessels or pipelines, containing superheated water or gas under high pressure. Different variants of outflow in the external model atmosphere and generation of waves are analyzed. The calculated data on the interaction of pressure waves with a barrier are calculated. To describe phase transitions, an asymptotic relaxation model of nonequilibrium evaporation and condensation has been created and tested.

1. Introduction
In power plants, emergency depressurization of pipelines and tanks with water coolant under high pressure occurs with a sudden pressure decrease in the area of the rupture, with generation of compression waves in the surrounding space, and with further formation of the jet of boiling-up coolant [1]. At initial supercritical thermodynamic parameters of water coolant at coolant outflow, there may be not only evaporation of a superheated liquid, but condensation of superheated steam as well [2]. The process of adiabatic outflow may be non-equilibrium, therefore, its description needs a thermodynamically non-equilibrium two-temperature model of steam-water mixture motion [3]. Several approaches can be used to simulate non-equilibrium vaporization. The first approach is based on the calculation of parameters of the heterogeneous mechanism of bubble formation (see e.g. [4]). The second approach applies the phenomenological method (a relaxation approach) [5]. In the first approach, in [4] the number of ready vaporization
centers is set with the addition by asymptotic models of bubble growth. This approach is no more adequate at large volumetric steam qualities ($\alpha > 0.3 - 0.5$) due to the presence of a bubble structure for describing the two-phase medium.

In the earlier work [1], calculating the non-stationary boiling, the authors used the relaxation - phenomenological approach, based on experimental data [5]. The asymptotic analysis of the model [5] was conducted in [6], where a number of shortcomings and contradictions were revealed. In the same work [6], on the basis of the analysis we have proposed a simple relaxation model to describe thermal and dynamic processes, involving water boiling at depressurization of a high-pressure vessel. The model assumes the droplet structure of the liquid-vapor flow, which is typical at high differential pressure of "vessel–atmosphere.”

The aim of this work is to numerically simulate the phase transition and the evolution of pressure waves, generated at depressurization of pipes with water coolants in the supercritical state, and the interaction of pressure waves with an obstacle, as well as to test the asymptotic relaxation model of non-equilibrium boiling and condensation.

2. Governing equations

The present study considers the axisymmetric problem of the water coolant outflow from the high-pressure vessel. Characteristics of wave impact on the outer barrier and other outflow parameters are calculated. Numerical simulation is realized at a no-slip condition for phases, and given that the vapor and liquid phases can be in a metastable state. The system of model equations includes the equations of conservation of mass, momentum and energy in axisymmetric approximation added with the equation for interphase mass transfer:

$$\frac{\partial}{\partial t} (\rho r) + \frac{\partial}{\partial z} (\rho ru) + \frac{\partial}{\partial r} (\rho rv) = 0,$$  

(1)

$$\frac{\partial}{\partial t} (\rho ru) + \frac{\partial}{\partial z} (\rho ru^2) + \frac{\partial}{\partial r} (\rho r uv) = -r \frac{\partial p}{\partial z},$$  

(2)

$$\frac{\partial}{\partial t} (\rho rv) + \frac{\partial}{\partial z} (\rho r uv) + \frac{\partial}{\partial r} (\rho rv^2) = -r \frac{\partial p}{\partial r},$$  

(3)

$$\frac{\partial}{\partial t} (Er) + \frac{\partial}{\partial z} (ur (E + p)) + \frac{\partial}{\partial r} (vr (E + p)) = 0,$$  

(4)

$$\frac{\partial (\rho r X)}{\partial t} + \frac{\partial (\rho ru X)}{\partial z} + \frac{\partial (\rho r v X)}{\partial r} = \Gamma,$$  

(5)

$$\Gamma = \frac{\rho (X_s - X)}{\theta}. $$  

(6)

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 mass and $X_s$ is the equilibrium mass vapor content (at the 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 steam and water properties in sub- and supercritical condition was performed using the software package TTSE [7]. The program code was developed for the solution of a wide class of problems on depressurization of vessels or pipelines with superheated water coolant, using the computer complex LCPFCT [8].

Earlier, to describe the phase transition, we used the model, based on the processing of experimental data on relaxation time (transport) of “non-equilibrium – equilibrium boiling” [5]. Given the shortcomings of this model, we have developed a new analytical relaxation model, which is described in [6]. This model describes the non-equilibrium process of boiling and is based
on the solution of the thermal problem of superheated water droplets. Due to low steam density, the drop structure of the two-phase medium is characteristic even at small steam qualities (but moderate and large volumetric ones) [9], and can be used in the modeling of intensive evaporation of liquid. According to the model, at the micro level of drops, the heat required for vaporization is supplied from the superheated liquid. At that, the temperature of the droplet surface is equal to the steam temperature [10]. To calculate the relaxation time in [6] we proposed the formula:

$$\theta_L = \frac{R_k^2}{\pi^2 a_L}$$  \hspace{1cm} (7)

where $R_k$ is the drop radius, and $a_L$ is the thermal diffusivity of the fluid.

If the average droplet size is determined from the simplified analysis of the instability of interfacial "water-vapor" surface, the size of the droplet corresponds to the length of the waves, the fastest in destroying the interfacial surface, and is determined by a critical Weber number $W_{ecr} \approx 2\pi$ (water, liquid metals) [9, 11]. The formation of droplets determines the process of liquid fragmentation during boiling and the break-up of the liquid jet due to the Kelvin-Helmholtz instability.

From formula (7) given the radius of the droplets, calculated from the critical Weber number, we obtain formula [6]:

$$\theta_L = \begin{cases} \frac{\sigma^2 \rho_L^2}{4a_L \rho_V^2 (P-P_S)^2}, & P - P_S > \frac{\rho_L L^2}{2(\frac{\rho_V}{\rho_L} - 1)} C_{p,L} T \\ \frac{\sigma^2 (\frac{\rho_L}{\rho_V} - 1)^4 C_{p,L}^2 T^2}{a_L \rho_V^2 L^4}, & P - P_S \leq \frac{\rho_L L^2}{2(\frac{\rho_V}{\rho_L} - 1)} C_{p,L} T \end{cases}$$ \hspace{1cm} (8)

Here $\sigma$ is the surface tension coefficient, $a_L$ is the thermal diffusivity of the fluid, and $L$ is the enthalpy of the phase transition.

The formula (similar to (7)) for a regular thermal regime in the steam surrounding the drop may be obtained, considering the spherical layer filled with steam as a flat plate [12]:

$$\theta_V = \frac{R_k^2}{\pi^2 a_V} \left( 1 - \alpha \right)^{1/3} = \frac{1}{2} \left( \frac{\rho_L L^2}{2(\frac{\rho_V}{\rho_L} - 1)} C_{p,L} T \right)$$ \hspace{1cm} (9)

where $\alpha$ is the volumetric steam quality.

At large volumetric steam qualities $\alpha$, $\theta_V$ may be close to $\theta_L$. Therefore, in the general case, it is necessary to propose some interpolation ratio for total relaxation time, for example:

$$\theta = (\theta_L^2 + \theta_V^2)^{1/2}$$ \hspace{1cm} (10)

To use the relaxation model not only in evaporation but at condensation as well, it was necessary to substantially modify the equation of state for the two-phase medium, which closes the system of equations (1)–(6) in case of not only saturated, but super-cooled steam. Although the size of the drops formed in the condensation may differ from the case of the jet break-up [9, 11], the test calculations were based on the formula (10).

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 the supercritical fluid outflow, in particular, to a change in the direction of phase transformation. This work presents calculations of supercritical water outflow in a wide range of parameters and at different initial parameters as well as at different geometry of the computational domain.
Figures 1, 2 present the results, calculated for a spatial distribution of normalized pressure gradient and bulk steam quality for the case of end depressurization of the pipe channel with water-coolant in the model liquid-vapor atmosphere [13]. Figure 1 corresponds to the initial conditions of \( P_0 = 23 \) MPa, \( T_0 = 365^\circ\text{C} \), and figure 2 corresponds to \( P_0 = 23 \) MPa, \( T_0 = 385^\circ\text{C} \). Spatial distributions are calculated at times of 90, 210, 330 \( \mu\text{s} \) after depressurization for the relaxation time \( \theta \), corresponding to the radii of the drops \( R_k=1 \) \( \mu\text{m} \). The calculated results with the relaxation time \( \theta(R_k) \), corresponding to the drop radius of 1 \( \mu\text{m} \), with a graphical accuracy coincide with the results of the calculation for the equilibrium model. The thermodynamically equilibrium model of the two-phase medium was actually obtained from the general system (1)-(4) at its closure with the equation of state of the equilibrium two-phase mixture.

![Image of Figure 1](image1)

**Figure 1.** Spatial distribution of normalized pressure gradient (top) and steam quality (bottom) at time \( t = 90\mu\text{s} \) (a), \( t = 210\mu\text{s} \) (b) and \( t = 330\mu\text{s} \) (c) for initial conditions of \( P_0 = 23 \) MPa, \( T_0 = 365^\circ\text{C} \)

![Image of Figure 2](image2)

**Figure 2.** Spatial distribution of normalized pressure gradient (top) and steam quality (bottom) at time \( t = 90\mu\text{s} \) (a), \( t = 210\mu\text{s} \) (b) and \( t = 330\mu\text{s} \) (c) for initial conditions of \( P_0 = 23 \) MPa, \( T_0 = 385^\circ\text{C} \)

Figures 3 present axial distributions of steam quality, calculated with different functions of the relaxation time \( \theta \), obtained from equation (10) for different radii of the droplets (1 \(- R_k=1 \) \( \mu\text{m} \), 2 \(- R_k=5 \) \( \mu\text{m} \), 3 \(- R_k=10 \) \( \mu\text{m} \), 4 \(- R_k=25 \) \( \mu\text{m} \), 5 \(- R_k=50 \) \( \mu\text{m} \)) for initial data (a \(- P_0 = 23 \) MPa, \( T_0 = 365^\circ\text{C} \), b \(- P_0 = 23 \) MPa, \( T_0 = 385^\circ\text{C} \)) at time \( t = 330\mu\text{s} \).

The numerical calculation also served to determine the dynamic relaxation time \( \theta \) on (10), using local parameters of the mixture. A similar algorithm for dynamic calculation of \( \theta \) has been
used previously for the model [5] in [1, 3]. In the present work, the calculation on the formula (10) has proved that both at evaporation and condensation, the relaxation time varies in the range from $10^{-6}$ s to $10^{-2}$ s. These values are in good agreement with experimental data on the relaxation time during steam condensation in Laval nozzles. In particular, in [14] it was shown that the characteristic relaxation time is about $10^{-5}$ s. In the superheated liquid jet outflow, authors of [15] have experimentally obtained droplet sizes, the bulk of which lies in the range $1 - 10 \mu m$, which corresponds to the relaxation time $10^{-6} - 10^{-4}$ s.

Figure 4 shows axial distributions of the relaxation time $\theta$, obtained from equation (10) for different radii of the droplets (1 – $R_k=1 \mu m$, 2 – $R_k=5 \mu m$, 3 – $R_k=10 \mu m$, 4 – $R_k=25 \mu m$, 5 – $R_k=50 \mu m$) for initial data (a – $P_0=23$ MPa, $T_0=365^0C$, b – $P_0=23$ MPa, $T_0=385^0C$) at time $t=330 \mu s$.

![Figure 3](image1.png)

**Figure 3.** Axial distribution of steam quality at time $t=330 \mu s$ for the initial conditions $P_0=23$ MPa, $T_0=365^0C$ (a) and $T_0=385^0C$ (b)

![Figure 4](image2.png)

**Figure 4.** Axial distribution of the relaxation time at time $t=330 \mu s$ for the initial conditions $P_0=23$ MPa, $T_0=365^0C$ (a) and $T_0=385^0C$ (b)

4. Conclusion
The relaxation model has been modified taking into account heat transfer between the liquid droplet and ambient steam. Numerical simulation of the supercritical fluid outflow was realized
on thermodynamically equilibrium and nonequilibrium relaxation models of phase transition for different times of relaxation. It is found that the calculation results with the relaxation time $\theta = 10^{-6} \text{ s}$, which corresponds to a droplet size of 1 $\mu\text{m}$, with graphic accuracy coincide with the calculation results for the equilibrium model. The development of the proposed model is shown to lead to qualitatively correct results.

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