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Application of hysteresis in FEM modeling of vapor-liquid phase transitions

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Abstract. In this paper a new, phenomenological, temperature dependent hysteresis model of the vapor-liquid first-order phase transitions is introduced. For the modeling of the vapor–liquid phase transition a versatile ODE-based hysteresis model is implemented under the assumption of a local non-equilibrium condition that enables a certain level of supersaturation without phase change. The proposed modeling approach improves the existing equation-of-state type diffuse interface methods involved in homogeneous two phase flow models.

Vapor-liquid phase-change processes play an important role in many technological applications. Boiling and condensation processes are associated with high heat transfer efficiency. Applications of these processes are highly advantageous in power and refrigeration processes, for cooling electronic components in computers, for thermal control of aircraft avionics and spacecraft environments and so on [1], [2], [3], [4], [5]. The heat transfer and fluid flow associated with liquid-vapor phase-change processes have all the complexity of single-phase convective transport, plus additional elements resulting from motion of the interface, metastable phase stability, and dynamic interactions between the phases. Mathematical models for vapor-liquid phase transformations can be divided into two classes: diffuse interface models and sharp interface models [6]. The first class takes into account the internal structure of a phase boundary and resolves it as a steep but continuous transition. In the second class, phase boundaries are discontinuous transitions of the thermodynamical variables. With the diffuse interface method all governing equations can be solved over the entire computational domain without any a priori knowledge of the location of the interfaces. Interface tracking is completely avoided and topology changes are handled naturally without the need for any special procedures. Therefore diffuse interface is a popular tool for simulations of two-phase flows in engineering applications. In the diffuse interface model an order parameter or phase indicator is introduced to represent the transition between the phases. Generally the diffuse interface model consists of three balance equations of mass, momentum and energy, and of an evolution equation of the order parameter, i.e. it is a so called four equations model. This paper focuses on the fourth equation, on the governing equation of the phase transition. Equilibrium phase change models could not describe the experimentally observed supersaturation of vapor and therefore overestimate the rate of condensate formation and the resulting heat transfer coefficient [7]. The goal of this study is to increase the so-called equation-of-state type equilibrium models by enabling the occurrence of metastable states. The model formulation is a function of an intensive state variable (temperature), but this function is hysteretic. The proposed saturation temperature dependent upper limit of the allowable supersaturation ensures that unstable conditions could be always avoided.
In order to verify the effectiveness of the proposed model, it is implemented into a 2D finite element model of a transient non-isothermal two-phase flow in a horizontal tube [5]. Two hysteresis test examples with different coercive values are compared to a case study of an equation-of-state type model without hysteresis. The results obtained confirm that the time evolution of the temperature, and therefore the formation of condensate, are strongly influenced by the allowable supersaturation.

1. Phase transitions in van der Waals gas, meta-stable states

A thermodynamic process in which the system passes through a continuous succession of equilibrium states is called an equilibrium or quasi-static process. The equilibrium can be defined as the specific Gibbs free energy $g$ has a minimal value. For low temperature the absolute minimum of $g$ corresponds to a liquid state. At high temperature, $g$ reaches the absolute minimum at a high specific volume, i.e. in vaporous states. Phase transition occurs when the ‘vapor minimum’ reaches the level of the ‘liquid minimum’. Although the Gibbs potential may be the fundamental entity at phase transition, a more common description of a thermodynamic system is in terms of the form of isotherms. An isothermal equilibrium vapor-liquid phase transformation in the $P-v$ plane is represented by a function similar to those shown in Fig. 1a. The lines separating the single-phase regions from the two-phase regions are saturation lines or coexistence curves or binodal. The saturated liquid line and the saturated vapor line meet at the critical point. Between the single-phase regions lie two-phase regions, where two phases coexist in equilibrium [8].

Vapor-liquid phase transformation belongs to the so called first-order type phase transitions that are always accompanied by the release or absorption of energy in the form of latent heat, and specific internal energy and density suffer discontinuous jumps [9]. In equilibrium phase transitions at the same temperature and pressure, various compositions of two-phase mixture can occur. Suppose that a small quantity of heat ($Q = T \Delta S$) is injected into the phase mixture. The heat supply, the phase transition (vaporization) and a small quantity of matter transform from liquid to vapor. The temperature and pressure remain constant. Thus the specific heat capacity defined as $c_p = T \left( \frac{\partial s}{\partial T} \right)_p$ diverges [8]. The specific heat capacity jumps from one finite value to another finite value by passing through an intermediate infinity, see Fig. 1b. (This description is correct until very close to the critical point, in which region non-classical behavior dominates.) For numerical reasons the phase transition models approximate this discontinuity with an appropriate smooth function that will be presented in the following.

![Fig. 1. a) Schematic drawing of an equilibrium isothermal phase transition in the $P-v$ plane, b) Discontinuity and divergence of specific heat capacity at saturation temperature $T_s$](image)

For many real fluids the isotherms are well represented by the van der Waals equation of state [8]
\[ p = \frac{RT}{(v - b)} - \frac{a}{v^2}, \]  

where \( p \) is the pressure, \( T \) is the temperature, \( v \) is the specific volume, \( R \) is the gas constant, and \( a \) and \( b \) are material constants. A van der Waals isotherm is shown schematically in a \( P - v \) diagram in Fig. 2 for \( T < T_c \). The solid line between points A and D means the equilibrium line of phase transition. The dashed line is the isotherm resulting by extrapolation of the van de Waals equation of state for the liquid and vapor phases. Phases are meta-stable in the intervals between points A-B and D-C on the dashed region of isotherm. A meta-stable state means that the phase is stable to small disturbances. A necessary and sufficient condition for phase stability is that \( < \frac{\partial p}{\partial v} > T < 0 \) \[3\]. The region between points C and B is the unstable region. The locus of points of isotherms where \( \frac{\partial p}{\partial v} = 0 \) are termed spinodal curves \[8\]. The spinodal curves separate the unstable area from the meta-stable regions. Regions of metastable vapor and liquid exist between the saturation curves and the spinodal curves.

This study focuses on the water vapor-liquid phase transitions. The International Association for the Properties of Water and Steam (IAPWS) issues equation-based recommendations for state equations and for various thermophysical properties of water \[10\]. The characteristic curves of water in the \( P-v \) plane can be seen in Fig. 2. The coexistent curves and an example isotherm at \( T_s \left(p = 1 \times 10^6 \text{ Pa}\right) = 453 \text{ K} \) are calculated by IAPWS IF95 formulations. In the meta-stable/unstable two phase region the isotherm is approximated by extrapolation of the van der Waals equation of state. The constants in (1) have been defined for water as \( a = 27(R T_s)^3/64 P_c \) and \( b = R T_s / 8 P_c \), where the critical temperature is \( T_c = 647 \text{ K} \), and the critical pressure is \( P_c = 22.04832 \text{ MPa} \) \[11\].

There are several liquid-vapor phase transition problems where the isothermal condition assumption is not valid, since the phase change is thermally induced, accompanying only slight pressure variations. In these cases isobaric conditions can be considered and the equilibrium-non-equilibrium phase transitions could be investigated in the \( T - v \) plane. Water characteristic curves and an isobar curve at \( p_s \left(T = 453 \text{ K}\right) = 1 \times 10^6 \text{ Pa} \) are shown in Fig. 3. Temperature driven equilibrium phase transformation occurs along the solid line of the IAPWS IF95 formulation.

Non-equilibrium isobaric phase transition can be described on a small (elementary) subsystem named a cluster, which is initially in the vapor state and assume that the size of the cluster is small enough that it could be characterized by the property to be entirely either in liquid or vapor phase.
(local bistability). At constant pressure the supersaturation means that the temperature in the cluster decreases below the saturation temperature without condensation. In this context the saturation temperature is the earliest temperature where the condensation of a cluster may occur. For further decrease of temperature the cluster is in a meta-stable state, and at the latest at the vapor spinodal condition the vapor phase becomes unstable and the cluster is converted into liquid. On reheating a reverse transformation takes place, at latest at the liquid spinodal condition [6]. Hysteresis phenomenon could be appearing in meta-stable states, see arrow lines in Fig. 3. Hysteresis in isobaric non-equilibrium phase transformation means that the cluster could change its states at different temperatures from vapor to liquid and from liquid to vapor.

![Fig. 3. Characteristic curves of water vapor-liquid phase transitions in the $T - \nu$ plane. The arrows show the possible hysteresis observable in non-equilibrium phase transformations](image)

2. Equation-of-state type phase transition models

2.1. Apparent heat capacity method for isobaric phase-transition

Numerical simulations of phase transformation are frequently performed by applying simple laws of phase changes. Here, the phase transition criterion is usually defined by assuming that phase transformation occurs, if the temperature reaches the pressure defined equilibrium (saturation) temperature or in isothermal conditions the pressure reaches the equilibrium. These types of phase transitions most commonly can be described by so-called equation-of-state type of models. In these models the order parameter can be directly determined from the physical quantities appearing in general conservation laws. However, these formulations could suffer from singularity problems. This difficulty can be circumvented by assuming that the region where phase transition takes place covers a certain interval.

The so-called apparent heat capacity method is one of the most preferred methods for modeling problems in heat conduction with phase change [12], [13]. Latent heat effects due to phase change are incorporated in the apparent heat capacity. The advantage of this approach is that the temperature is the primary dependent variable that derives directly from the solution of the heat equation. The heat conduction in the two-phase system can be described by

$$C_p \frac{dT}{dt} - L \rho \frac{d\xi}{dt} - \nabla \cdot (\lambda \nabla T) = 0,$$

where $C_p$ denotes the effective volumetric heat capacity $C_p = c_p \rho_1 \xi + c_p \rho_2 (1-\xi)$, $c_p$ is the specific heat capacity, $\xi$ is the volume fraction of phase 1, $L$ the specific latent heat for change from
phase 1 to phase 2, $\lambda$ is the effective thermal conductivity of the mixture and subscript refers to the phase index. The first term in (2) represents the change in energy storage with respect to time. The second term represents the rate of the latent heat released during the change of phases. The third term represents the net energy flow by conduction. The latent heat can be incorporated into the heat capacity and (2) can be rewritten as

$$
\left(C_p - L\rho \frac{\partial \xi}{\partial T}\right) \frac{\partial T}{\partial t} = C_a \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T),
$$

where $C_a$ is the apparent heat capacity. Applying this method to the water vapor-liquid phase transformation, by assuming constant heat capacity of the pure phases and constant latent heat with parameters $c_{pv} = 2.08 \times 10^3 \text{kJ}/(\text{kgK})$ for water vapor, $c_{pl} = 4.2 \times 10^3 \text{kJ}/(\text{kgK})$, for water liquid, $L = 2.26 \times 10^5 \text{kJ/kg}$, then the apparent heat capacity functions have the shape similar those shown in Fig. 4. The Dirac-delta function has been approximated by Gaussian distribution with various $\Delta T$ according to

$$
\frac{d\xi}{dT} = \left(\frac{1}{\sqrt{2\pi} \sigma}\right) e^{-\frac{(T-T_s)^2}{2\sigma^2}},
$$

where $\sigma$ is selected so that $\text{erf}(\sigma \Delta T) = 1 - \delta$, $\Delta T$ is one-half of the assumed phase change interval, $T_s$ is the saturation temperature and $\delta$ is a sufficiently small positive number.

The effective heat capacity can be obtained from the apparent heat capacity divided by the average density $\rho$. The effective heat capacities with respect to the temperature at various $\Delta T$ are shown in Fig. 5. The volumetric heat capacities of pure phases are calculated as $C_{pl} = c_{pl}\rho_l$ and $C_{pv} = c_{pv}\rho_v$.

It can be seen that too small $\Delta T$ causes numerical difficulties, but too large $\Delta T$ causes release/absorption of heat at temperatures where phase transformations are still unexpected. It appears from the numerical solutions presented in [12] that the results obtained by approximating the phase change at a fixed temperature with a gradual change over a small temperature interval should be acceptable if $2\Delta T/|T_{\text{initial}} - T_{\text{end}}| < 0.1$. 

![Fig. 4. Apparent heat capacity of water at $T_s = 373$ K](image)
From the figure it can be seen that the maximum locations of the specific heat capacity functions are shifted from the location of transition temperature in the direction of higher temperature regions, i.e. the latent heat is mainly released before the transition temperature is reached. This displacement is caused by the large difference existing between the densities of the pure phases. This problem can be solved by the selection of the vapor mass fraction as an order parameter.

2.2. Barotropic state law for isothermal phase transformations

Delannoy and Kueny [14] proposed a formulation that strongly links the mixture density to the static pressure: they use a barotropic law \( p_\rho \), which describes the mixture density both in the pure phases and in the transition zone. This model has been used mainly in cavitating flow models with consideration of an isothermal homogeneous equilibrium mixture model. The barotropic state law \( p_\rho \) can be formulated as

\[
\rho = \begin{cases} 
\rho_i, & \text{if } p > p_s + \Delta p, \\
\rho_v, & \text{if } p < p_s + \Delta p, \\
\rho(p), & \text{if } p_s - \Delta p < p < p_s + \Delta p, 
\end{cases}
\]

(6)

where \( \Delta p \) is half-width of the transition from vapor to liquid. Three functions are usually used to ensure the transition between the vapor and the liquid:

- integration of analytical formula of speed of sound;
- polynomial connection;
- sinusoidal connection.

The most frequently used method in which the connection from liquid to vapor can be defined with a sinusoidal function is

\[
\rho = \rho_i + \rho_v + \rho_v - \rho_i \times \sin \left( \frac{p - p_s}{\frac{2}{c_{\text{min}}} \rho_i - \rho_v} \right),
\]

(7)

where \( c_{\text{min}} \) corresponds to the minimal speed of sound in the mixture. The parameter \( c_{\text{min}} \) can be approximated by \( c_{\text{min}} = 2c_v \sqrt{\rho_i / \rho_v} \) if \( \rho_i >> \rho_v \). For water at standard conditions \( c_{\text{min}} = 25 \text{ m/s} \) [14].

In this method the order parameter is the density, the variation of density describes the interface between the two phases.
3. Kinetic type phase transition models

In kinetic relaxation models, the phase transition is considered to be a molecular exchange process that develops during a finite time interval. Hence, the liquid would not immediately evaporate completely when the equilibrium vapor pressure is reached, but a time-dependent evaporation process starts [8]. The derivation of a kinetic model for a particular phase transition in a thermodynamical system consists of identifying the order parameter, which characterizes the difference between the two phases. The equations of state are determined by constructing the Helmholtz free energy density \( f \) or the Gibbs free energy density \( g \) as a function of order parameter \( \phi \) and absolute temperature \( T \). Then all relevant thermodynamic quantities are derived from free energy density functions. The free energy based phase transition models differ from each other in the form of the approximation of the free energy function and in the simplification considerations [9], [15].

3.1. The Landau theory and the phase field model

In the Landau theory of phase transition [16], it is assumed that the free energy density \( g \) can be represented in power series expansion of the form

\[
g = \sum_{i=0}^\infty g_i(T,P,\phi,N_1,N_2,\ldots,N_j)\phi^i, \tag{8}\]

where the coefficient functions \( g_i \) are analytic functions. The kinetics of the phase transition implies that the order parameter has to be a function of space \( x \) and time \( t \), that is \( \phi = \phi(x,t) \). If the order parameter \( \phi \) is a function, then the total free energy \( g \) must be a functional acting on a function space to which \( \phi \) belongs. The variational derivative \( \partial g/\partial \phi \) can be interpreted as a generalized thermodynamic force that tends to decrease the value of the total free energy. A possible kinetic equation is obtained by assuming that the order parameter \( \phi \) responds to the impact of this thermodynamic force at a rate proportional to its negative value. Therefore, in isothermal conditions, the so-called Ginzburg–Landau equation is obtained as the relaxation law

\[
b \frac{\partial \phi}{\partial t} = -\frac{\partial g}{\partial \phi}, \tag{9}\]

where \( b \) is a function of \( \phi \) and \( \partial g/\partial \phi \) is the variational derivative of a free-energy functional \( g \), which has minimum value at equilibrium states [9]. The kinetic equation of the order parameter is called as Cahn-Allen equation for non-conserving dynamics and Cahn-Hillard equation for conserving dynamics [9]. Both equations have been derived from the Landau-Ginsburg functional under the premise that the temperature is constant. The thermodynamically consistent phase field model has been described by Penrose and Fife [17].

It can be concluded that in the kinetic models the dynamics of pure phase transition have been studied very extensively but separately from fluid flow problems [15]. These methods require identifications of coefficient functions of the polynomial in (8). In most cases it is a very difficult task, and several assumptions have to be made to obtain an appropriate solution. For engineering applications the kinetic models are usually highly simplified. For example a simplified non-equilibrium relaxation model for one-dimensional flashing liquid flow has been developed in [18]. This model as a homogenous relaxation model takes into account the non-equilibrium evaporation leading to meta-stable conditions and predicts the mass flow rates and the pressure distributions for one-dimensional flashing water. The vapor generation rate \( \Gamma \) has been approximated by the first term of Taylor series as

\[
\Gamma = \rho \frac{D\phi}{Dt} = \rho \frac{\phi - \phi^*}{\tau}, \tag{10}\]
where \( \rho \) is the mixture density, \( \phi_e \) is the equilibrium vapor quality, \( \tau \) is the relaxation time, which is fitted as a power function of void fraction and pressure decay amount [18].

3.2. Statistical approach
Statistical models are based on the consideration of a local bistability hypothesis. The local bistability hypothesis consists in considering the first-order phase transformation as an ensemble of several independent simple transitions. This hypothesis goes back to the magnetic hysteresis models, which consist in subdividing the system for small elements in such a way that each single element has just two configurations in its free energy [19]. The system is then considered as a collection of independent bistable objects. This idea has been used in the last few years to study hysteresis and relaxation effects [20], [21]. The martensitic–austenitic phase transformations of shape memory alloys are the typical case for the thermodynamics of systems with hysteresis, described with the statistical method constructed on the local bistability hypotheses [20].

Basso et al. [21] proposed a hysteresis operator for thermally induced first-order phase transformations. Basso et al. find that the switching rules of phase change turn out to be identical to the rules governing the Preisach model of hysteresis [22], therefore all the methods developed for Preisach model can be immediately applied to describe the thermally induced phase transformations in solids. The difficulty in this development is that the Gibbs free energy functions of the pure phases have to be known in advance. This fact may create some difficulties for the applications of this approach to real cases. Applying a Preisach-type hysteresis model to fluid systems, the hysteresis memories have to be coupled to small volumes of fluids, which are in motion. These models are very complicated to handle numerically.

The original concept for shape memory alloys [20] has been modified for constructing a statistical model for water to describe cavitating flow in [23]. The fluid is considered as a set of independent clusters. Each cluster consists of the same number of water molecules and, thus, has the same constant mass. If a cluster grows, it has to change the volume occupied. This happens in cavitation due to decreasing pressure. The rate equation for vapor quality \( x \) \((x = m_v/m, m_v \) is the mass of vapor, \( m \) is the total mass) is formulated as

\[
\frac{dx}{dt} = (1-x)K_{l-v} - xK_{v-l}. \tag{11}
\]

The first part at the right hand side in (11) is the gain term the last part is the loss term. The gain of vapor clusters depends on the number of liquid clusters expressed by the liquid quality \((1-x)\), and further on the probability \( K_{l-v} \) of liquid clusters changing their state of aggregation from liquid to vapor. Then the probabilities are

\[
K_{l-v} = \frac{e^{-g(\nu_{bar}, p)/(k_BT/m_v)}}{\tau \int_{v_{min}}^{v_{bar}} e^{-g(\nu, p)/(k_BT/m_v)} dv}, \tag{12a}
\]

and

\[
K_{v-l} = \frac{e^{-g(\nu_{bar}, p)/(k_BT/m_v)}}{\tau \int_{v_{min}}^{v_{bar}} e^{-g(\nu, p)/(k_BT/m_v)} dv}, \tag{12b}
\]

where \( m_c \) is the mass of a cluster, \( \nu_{bar} \) is the specific volume at the energy barrier of the specific Gibbs free energy function, \( \nu_p \) and \( \nu_{min} \) are the smallest and greatest possible specific volume occupied by the molecules respectively, \( k_B \) is the Boltzmann constant and \( \tau \) is the relaxation time. The probability \( K_{v-l} \) differs from \( K_{l-v} \) only in the integration boundaries that cover the region of the
respective phase area. For the solution of (11), it is necessary to declare the specific Gibbs free energy functions. Equilibrium or non-equilibrium states can be obtained respectively, depending on the choice of the relaxation parameter.

4. The proposed hysteresis model

Phase equilibrium models are not able to predict the experimentally observed meta-stable states. The smoothing in the $C_p(T)$ or $\rho(p)$ functions are symmetric around the equilibrium state variable $T_e$ or $p_e$, therefore these models allow phase transformations before the local pressure or temperature reaches the saturation conditions and smoothing results in some supersaturation or superheating. While the latter cases are acceptable from thermodynamic point of view, the former assumption is there only for numerical reason. The kinetic models are more precise but the free energy functions and the relaxation time must be known in advance.

In this study a new method is proposed to model the vapor-liquid first-order phase transition occurring in flowing system, which is similar to the equation-of-state type models in its easy identification and in the macro-scale viewpoint, and similar to the statistic models, where the phase transition is described with a hysteresis function. The difference between the proposed and the equation-of-state type models is that with this new model the non-equilibrium phase transitions can be modeled. The difference between the proposed and the kinetics models is that the proposed hysteresis model does not contain relaxation time; therefore it is assumed that the predefined degree of supersaturation and superheating always occur. Under the above assumptions the knowledge of the free energy density function is replaced by the knowledge of the degree of supersaturation.

4.1. The model fluid

Similar to the model in [23], it is assumed in this study that the model fluid is an ensemble of clusters of molecules. A cluster is considered as an elementary subsystem. The size of the clusters should be selected so that subsystems are small enough portions of the system that are characterized by the property to be entirely either in liquid or vapor phase (local bistability), and it is large enough to could be characterized with thermodynamic variables. Each cluster consists of the same number of water molecules and it has a constant mass. Change of temperature modifies the volume occupied by a cluster, and this leads to the change of specific volume. The fluid clusters are characterized by a sharp existence function $x \in [0,1]$. If a cluster is in the vapor phase, the existence function is equal to 1, $x = 1$, and if a cluster is in the liquid phase, the existence function is zero, $x = 0$. (This assignment does not agree with the Landau formalism where the high temperature phase is set to 0 and the low temperature phase is 1, but only with our assignment can we obtain the hysteresis function in its common form.)

This study focuses on the thermally induced water vapor-liquid phase transition, since this condition can be frequently assumed in technological processes, therefore non-equilibrium phase transition can be studied on the isobar curve in $T-v$ plane. Theoretically the supersaturation (or superheating) of a cluster can approach the appropriate spinodal conditions. Physically, the meta-stable state becomes short-lived before the spinodal condition is reached [24], therefore the assumption that the spinodal condition is the upper limit of the supersaturation is not acceptable.

Assume, that each individual cluster that is in the vapor state can transfer into the liquid state in the temperature interval defined by $[T_s, T_s - \Delta T]$ and the vaporization of a cluster that is in liquid form can occur in the temperature interval of $[T_s, T_s + \Delta T]$. Consequently, this phase transformation is a switching process that shows hysteretic character, which can be seen in Fig. 6. In this way the thermally induced non-equilibrium vapor-liquid phase transformation of a fluid cluster is similar to the local bistability hypothesis assumption, which has been developed for magnetic materials.
The existence function $x$ of the individual water cluster switching from 0 to 1 and 1 to 0 around the saturation temperature $T_s$.

The upper limit of the acceptable supersaturation i.e. the value of $\Delta T$ has to be determined. The spinodal of vapor supersaturation is proportional to the relative pressure, $p/p_c$ where $p_c$ is the critical pressure [24]. In this study a relative temperature $T/T_c$ ($T_c$ is the critical temperature) based heuristic supersaturation limit is introduced. This limit is close to the coexistent curve and vanishes at the critical state (see in Fig. 7 the dotted line under the vapor binodal). The limit has been obtained by calculating a weighted specific volume $v_w$ from the liquid $v_l(T_s)$ and vapor specific volume $v_v(T_s)$ at the saturation temperature $T_s$, by a weighing factor of $\gamma = T_s/T_c$ as $v_w = \gamma v_v + (1-\gamma)v_l$. The vapor binodal, the spinodal decomposition curve and the hysteresis limit projected to the $T$-$P$ plane are shown in Fig. 8. Determination of the hysteresis limit at constant pressure $P$, is plotted in this figure as well. The proposed limit agrees with experimental data that can be found in the literature [2], [25]. The characteristic curves in Fig. 8 can be approximated in the form of $\log(P) = a/T + b$, for the vapor binodal with $a = -4.74 \times 10^3$, $b = 24.3$, for the vapor spinodal with $a = -1.58 \times 10^3$, $b = 19.3$ and for the hysteresis limit with $a = -4.33 \times 10^3$, $b = 23.7$. The value of $\Delta T$ can be expressed by

$$\Delta T = T_s \left( T_s - 680.33 \right) / \left( T_s - 7903 \right), \quad 350 \leq T_s \leq 600 \text{ (K)}. \quad (13)$$

The value of $T_s$ can be expressed by

$$T_s = \left( T_s - 680.33 \right) / \left( T_s - 7903 \right), \quad 350 \leq T_s \leq 600 \text{ (K)}. \quad (13)$$

**Fig. 7.** Isobars of water calculated by the van der Waals equation of state in the meta-stable regions and with IAPWS IF 95 formulation in the stable phase domains.
4.2. The applied hysteresis model

In this analysis it is assumed that the fluid is in motion while the phase transition occurs. Therefore an appropriate hysteresis model has to be selected to describe the phase transition in a flowing system. The Preisach-type hysteresis models are not acceptable, because it would be very complicated to handle the hysteresis memories bound to the moving volumes of fluid. A hysteresis model, which has only so called local memory, can resolve the moving fluid induced computational difficulty [26], [27]. This type of hysteresis model has been presented in [28] and is applied in this study. The hysteresis model is based on the simple statistics of a collection of elementary hysteresis operators corresponding to clusters of the fluid. In this way the process of phase transition is represented by a properly defined probability distribution function \( Z(Y) \) of a continuous random variable \( Y \), with expected value in the case of liquid-vapor transition \( \Delta T^+ = T_c + \Delta T/2 \) and for vapor-liquid transition \( \Delta T^- = T_c - \Delta T/2 \).

The hysteresis model has the form of a partial differential equation (PDE), which can be written as

\[
\phi = H[T], \quad \text{and} \quad \frac{\partial \phi}{\partial t} = \gamma \zeta(\psi T) \frac{\partial T}{\partial t},
\]

where \( H[T] \) denotes the temperature dependent hysteresis operator, \( \phi \in [0,1] \) is the order parameter of the phase transition. The function \( \phi \) is a smoothed version of the sharp phase existence function \( x \), and corresponds to the vapor mass fraction. The function \( \zeta(.) \) is a probability density function (PDF) corresponding to the hysteresis operator. The function \( \psi \) denotes the direction of the change in \( T \), and \( \gamma \) is a weighting function, which is responsible for the shape of the minor loops [28].

The hysteresis model can be identified by determining the PDF \( \zeta(.) \). In this work a Gaussian-type distribution function is assumed, \( \zeta \sim N(T_c, \pm \Delta T/2, \Delta T/4) \), where the selection of + or – depends on the increasing and decreasing curves, respectively. The variance of the PDF influences the steepness of the main hysteresis curves, which in this case is equal to \( \Delta T/4 \). Graphical interpretations for \( \zeta(.) \) with Gaussian PDF-s are shown in Fig. 9 and the corresponding distribution function \( Z(.) \) as main hysteresis loops can be found in Fig. 10. No hysteresis corresponds to a simple equation-of-state type model.

The proposed hysteresis model has several advantages. For example, because it has a local memory character, the local mass-fraction and local temperature determine unambiguously the hysteretic state of the local volume of fluid, and the temperature gradient can regulate the direction and gradient of the vapor mass-fraction through the hysteresis function. Another advantage of the model is that the
Numerical solution of the differential equation (14) can be acquired easily and the model implementation into field problems can be handled by coupling the ‘hysteresis’ state equation to the equations of the problem [5].

5. Case study: a transient two-phase flow with phase transition
In this section a hypothetical non-isothermal two-phase flow problem is presented. The model has been formulated in a finite element model-simulator. The assumed model set-up consists of a two-dimensional axially symmetric horizontal tube with diameter \( D \) and length \( L \). Water vapor close to the saturation conditions with constant velocity \( u = u_0 \) is assumed to enter into the tube. At a point some distance downstream of the entrance, the flow field is developed, vapor begins to condense and a thin liquid film evolves on the interior wall of the tube. The model is a hypothetical case study; the parameters are biased for demonstrative reasons. The goal with this example is the validation of the applicability of the proposed hysteresis model. The problem constructed can be solved on a simple PC within a relative short running time (CPU time is about 700s for the simulated time intervals on an Intel® Pentium® M 1.6GHz processor). The axially symmetric computational domain with the
appropriate boundary condition is depicted in Fig. 11. In the simulations presented the geometry parameters are \( L = 1 \text{ m} \), \( D = 0.2 \text{ m} \) and a non-uniform mapped mesh is used with 1300 elements.

For the sake of simplicity, in the examples presented, constant physical properties of the individual phases and constant saturation temperature have been assumed. The mass, momentum and energy-balances can be described with a homogenous equilibrium model, i.e. the physical properties can be calculated with mixing rules [29].

![Fig. 11. The computational domain and the initial and boundary conditions of the finite element model](image)

Usually, the diffuse interface can be characterized by the volume fraction \( \xi \), i.e. the shape of the interface between the phases is volume dependent. The relation between the order parameter of the phase transition \( \phi \) and the phase function of the diffuse interface is determined by \( \xi = \phi \rho / \rho_v \). These two parameters, \( \xi \) and \( \phi \), vary with temperature in different forms, since the rate of change of densities of the two phases is three orders of magnitude. Consequently, relatively large variations in mass fractions cause only a little vapor fraction deformations by decreasing temperature. However, in the low mass fraction domain, small variations cause large volume differences. It means that the same phase transition phenomenon manifested in different forms in mass rates than in volume rates and can be seen in Fig. 12. Assuming that the volume fraction is the order parameter with an inflection point at the saturation temperature, than the mass conversion is shifted above the saturation temperature. This is the reason why the volume fraction is not the order parameter of the phase transition in this case.

![Fig. 12. Vapor mass fraction as the order parameter \( \phi \). Vapor volume fraction, defined as \( \xi = \phi \rho / \rho_v \), has different characteristics](image)
A detailed description of the applied diffuse interface model for isothermal flow can be found in [6], in this paper the energy equation is presented. The energy balance of the system should be supplemented with an extra term due to the mass transfer induced latent heat release/absorption. The energy balance can be formulated as

$$\rho c_p \frac{\partial T}{\partial t} + L \frac{\partial \phi}{\partial t} + \nabla \cdot (-\lambda \nabla T + \rho c_p T \mathbf{u}) = S_q, \quad (15)$$

where $L$ is the latent heat, $S_q$ is the source term corresponding to outward heat flux, $S_q = -\alpha(T - T_e)$, $\alpha$ is the heat transfer coefficient and $T_e$ is the temperature of the environment.

5.1. Simulation results

In this section some simulation results are presented that are obtained for various values of $\Delta T$. These simulations demonstrate that this method is useful for modeling non-equilibrium and equilibrium phase transitions as well. Consequently the equilibrium equation-of-state type model can be thought as a special case of the hysteresis model, by applying $\Delta T = 0$ K.

The transient behavior of the model system is analyzed by applying a space and time varying excitation. The outer wall of the tube is increasingly cooled to the middle of the tube and then the temperature difference is gradually decreased to the end of the tube. This effect can be achieved for example with a heat transfer coefficient $\alpha_0(z) = \alpha_{max}(t) \sin(\pi z/L)$, $z$ is the tangential space coordinate, $\alpha_{max}(t)$ is the maximum value of the heat transfer coefficient. The time dependent variation of the maximum heat transfer coefficient $\alpha_{max}$ is shown in Fig. 13.

Equilibrium and non-equilibrium phase transitions are allowed to occur in the different test cases. Therefore the results obtained by a simple equation-of-state model (first test case) can be compared to models of hysteresis phase transformations. In this study two examples of hysteresis are presented. In the second test case only a narrow hysteresis band is introduced, $\Delta T = 4$ K. This example can be thought as an increased version of the equation-of-state model, in which the hysteresis is used so as not to allow considerable condensation or evaporation to occur before the saturation temperature is reached. In this way effects arising from the symmetrically smoothed jump function that are not thermodynamically justified, can be prevented. The third test case shows an example for the supersaturation-superheating process with hysteresis calculated from saturation temperature according to (13) with $\Delta T = 10$ K. Transient simulation has been performed in the same time intervals, $t = 0, \ldots, 300$ s, for all test cases.

![Fig. 13](image-url) The time dependent variation of the maximum heat transfer coefficient $\alpha_{max}$
The time evolution of the temperature and the mass fraction near the wall at the cross-section of $z = 3.5D$ are shown in Fig. 14. The coordinates of radial locations are given in the figure legends. It can be seen that in the equilibrium approximation case, after the saturation conditions are reached, the temperature remains almost constant during the increasing - decreasing cycles of the excitation but the values of vapor mass fraction decrease continuously. The largest is the hysteresis loop; the largest are the temperature variations and less are the condensation rates during same time intervals.

Fig. 14. Time evolution of the temperature and the order parameter close to the wall, at the axial location $z = 3.5D$, radial locations $r = 0.09, \ldots, 0.1 m$, with
a) - b) $\Delta T = 0 K$; c) - d) $\Delta T = 4 K$ and e) - f) $\Delta T = 10 K$. 

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Minor hysteresis loops near the wall at axial location of \( z = 3.5D \) are shown in Fig. 15. The radial distances are signed in the figure legends. The hysteresis loops in the left hand side of the figure represent the variation of the order parameter with temperature, and the corresponding volume-averaged density variations are shown in the right hand side. It can be seen that by providing intensive cooling-heating across the wall, the minor loops become larger near the wall.

### Fig. 15

Minor hysteresis loops corresponding to the time-evolution of the mass fraction as order parameter, close to the wall, at the axial coordinate \( z = 3.5D \). The average density variation follows the hysteresis of the mass fraction, a) - b) \( \Delta T = 4 \text{ K} \) and c) - d) \( \Delta T = 10 \text{ K} \)

Inside the diffuse interface a pressure ‘hump’ may be expected. The hump is a manifestation of the capillary stress between the phases due to surface tension [6]. Really, the pressure humps are observable in the pressure fields near the wall, which are well presented in the cross-sections profiles in Fig. 16 as well. If the two phases were fluids, this pressure hump would act to keep the fluids from mixing.

Increasing differences between densities on the two sides of the interface increases the magnitude of the hump, indicating that in the presence of a normal flow, a hump would be present even in the absence of surface tension [6]. The smoothness of the pressure humps depends on the slope of the diffuse interface, therefore the sharpest pressure humps are provided by the case study of \( \Delta T = 4 \text{ K} \).

The time evolution of the diffuse interface between the two phases can be characterized by the evolution of the liquid volume fraction \((1 - \xi)\), which can be seen in left column of Fig. 16. The sharpest interfaces have been provided by simulation with \( \Delta T = 4 \text{ K} \). The highest values of liquid volume fractions comparing to the other two simulations correspond to the better phase separation observed in this model simulation.
Fig. 16. Liquid volume fractions and pressure profiles at the cross-section z=2.5D, time t = 50, 100, 150, 200, 250 and 300.
Top: without hysteresis, middle: \(\Delta T=4\) K, bottom: \(\Delta T=10\) K

6. Conclusion
In this paper the investigation and phenomenological approach of modeling of non-equilibrium vapor–liquid phase transition has been introduced in order to implement it on a transient non-isothermal two-phase flow model with phase change. The PDE based vapor-liquid phase transition model means improvement to the equation-of-state type phase transition models and can be more easily implemented for engineering applications than the kinetic type models. The vapor-liquid phase transitions have been treated on the macro-scale without the definition of the free energy functions of phases in advance. A saturation temperature dependent upper limit of the allowable supersaturation has been proposed to avoid the occurrence of unstable states. The model presented is based on
theoretical considerations. For modeling a real system, the PDF of the hysteresis model has to be supported by experimental data. This is a crucial question because the supersaturation limit could be strongly system dependent.

Introducing a hysteresis model of the vapor-liquid phase transition can improve other macroscale heat transfer models as well, that are associated with boiling and condensation phenomena and have been treated until now as virtually isothermal heat transfer processes.

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