

## A MODEL OF TWO-PHASE FLOW WITH RELAXATIONAL-GRADIENT MICROSTRUCTURE

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### 1. Introduction

The essential feature of two-phase liquid-vapour flow is its nonequilibrium nature, a fact proved experimentally [1]. The process of vapour creation is not initiated at the point where the saturation pressure is reached but its inception is displaced far downstream where the saturation pressure substantially exceeds the actual pressure of the water. This phenomenon manifests itself by a metastable state of the parent phase which reveals some 'resistance' against the change of state of aggregation. This is a direct reason for which the phase transition is a nonequilibrium process and has a crucial influence on its further course.

Rapid evaporation of water is an example of heterogeneous phase transition distinct by virtue of a large number of interfacial surfaces. As Landau and Lifszyc [2] say, the process of heterogeneous phase change should be accompanied by a metastable state, because, in reality, at least three reasons oppose the equilibrium process of, for example, evaporation. They are: surface tension and capillary effects in the region of phase separation, some time required for heat and mass exchange between a parent and a new phase and a finite rate of growth of nuclei. Thus, apart from inertial thermal effects, also mechanical effects have a contribution to the phase transition and play an important role in the process of growth of the new phase.

The main purpose of our work is to present the phenomenological approach to modelling of interfacial surfaces in nonequilibrium liquid-vapour flows. A modification to the classical relaxation equation [3], accomplished on the basis of the Ginzburg-Landau, is proposed. This modified equation allows the description of capillary effects in the homogeneous model of a two-phase mixture.

### 2. Non-convex extension of internal energy

According to the Joule hypothesis the internal energy of perfect fluid depends in a special way on the specific volume and specific entropy - it is a convex function of both these parameters. The Helmholtz potential  $\psi(v, T)$  corresponding to the internal energy is a convex function of the specific volume and a concave function of the temperature.

To describe a phase change proceeding in the fluid, the internal energy must be represented not only by two independent quantities - the specific volume  $v$  and specific entropy  $s$ , but also by a new additional parameter. This parameter describes a kind of order created at a point of continuum [4]. The internal energy, interpreted phenomenologically, becomes then a function of three parameters and their derivatives:

$$\varepsilon = \varepsilon(v, s, x, \partial_t x, \nabla x, \dots). \quad (1)$$

The order parameter  $x$  provides information about the degree of advancement of the phase transition. On the phenomenological level it is a scalar quantity.

Although the phase change takes place in perfect fluid, it is no longer a reversible non-dissipative process. The occurrence of metastable or unstable states underlies the fact that the process is nonequilibrium and the phase transition proceeds partly irreversibly. Due to the metastable states of the fluid the phase change is heterogeneous (in Gibbs' interpretation) and is distinct by virtue of a great amount of interfaces. The interfacial surfaces have their own energy which contributes to the total energy of the mixture, which can be written as a sum of the internal energy of the particular phases and the internal energy of the interfaces:

$$\varepsilon = x\varepsilon_{vapour} + (1-x)\varepsilon_{liquid} + \varepsilon_{surface}(x, \nabla x). \quad (2)$$

This energy (2) simulates the non-convex extension of the internal energy on the metastable and unstable regions first proposed by van der Waals [5], and allows the modelling of nonequilibrium phase transformations.

However, it is difficult to evaluate the contribution of the interfacial energy. This follows from the fact that the internal energy of the transition layer is not only a function of the surface entropy and the surface stretch, but also depends on the state of both phases and the geometry of the interface as well as its velocity.

Another important factor, on which  $\varepsilon_{surface}$  depends and which is difficult to estimate is the interfacial area density. It depends mainly on the rate of growth of new nuclei.

Since the existence of the interfaces in a small control volume means the presence of a gradient  $\nabla_n x$  perpendicular to the surface, then one can assume that the spatial gradient of  $x$  is a vectorial measure reflecting energetic fraction of the interfacial surfaces. This measure, supplemented by the measure of scale representing the amount of interfaces, would represent energetic contribution coming from capillary effects. We will expect that the bigger is the gradient  $\nabla_n x$  the bigger should be the surface tension. In other words, the scalar quantity  $x$  is a measure of how much internal microstructure the fluid contains, whereas the spatial gradient  $\nabla x$  represents capillary properties and the rate of 'building' of the microstructure.

Therefore, the internal energy of a heterogeneous two-phase mixture can be written in the simplified form:

$$\varepsilon = x\varepsilon_{vapour}(v, s) + (1-x)\varepsilon_{liquid}(v, s) + \varepsilon_{surface}(x, \nabla x). \quad (3)$$

### 3. Evolution equation of dryness fraction

A basis for our analysis is the so-called Ginzburg-Landau equation [6] describing the kinetics of the evolution of the order parameter - in our case the nonequilibrium dryness fraction  $x$ . This equation was formulated in the following form:

$$\dot{x} = -\Gamma \frac{\delta\psi}{\delta x} \quad (4)$$

where  $\Gamma$  is a positive frictional coefficient associated with dissipative effects during relaxation,  $\psi(T, v)$  is the specific Helmholtz free energy and  $\delta$  is the Volterra variational derivative.

The above formulation takes into account the fact that, in general, the Helmholtz free energy is not only a function of  $x$ , but also of its spatial derivatives. The inclusion of the gradients  $\nabla x$  in the equation for the free energy of the two-phase mixture has a physical significance: when a nonequilibrium phase change proceeds nonuniformly in the bulk of the liquid subjected to the uniform pressure and temperature field, there are no reasons for the creation of the gradients  $\nabla x$ . However, when the fluid undergoes heterogeneous phase transition (for example flashing), a large amount of interfaces appears, what gives rise to the creation of the dryness fraction gradients. In this case the Helmholtz free energy can be expressed as the sum of two contributions [7]:

$$\Psi = \Psi_0 + \Psi_{grad}. \quad (5)$$

In this expression  $\Psi_0$  is the free energy of the uniform system and is a function of the local value of  $x$

$$\Psi_0 = \Psi_0(x, x^2, x^3, \dots) \quad (6)$$

whereas  $\Psi_{grad}$  is a 'gradient energy' and can be expressed as a linear function of first and higher gradients of the order parameter  $x$ :

$$\begin{aligned} \Psi_{grad} = & \Psi_{grad}(\nabla x, (\nabla x)^2, (\nabla x)^3, \dots, \\ & \nabla^2 x, (\nabla^2 x)^2, (\nabla^2 x)^3, \dots, \\ & \nabla^3 x, (\nabla^3 x)^2, (\nabla^3 x)^3, \dots) \end{aligned} \quad (7)$$

Expanding the Helmholtz potential in a Taylor series about the uniform solution  $\Psi_0$  and making use of symmetry properties of isotropic medium we obtain:

$$\begin{aligned} \psi(x, \nabla x, \nabla^2 x, \dots) = \\ \Psi_0(x) + k_1 \nabla^2 x + k_2 (\nabla x)^2 + \dots \end{aligned} \quad (8)$$

where  $k_1$  and  $k_2$  are tensors reflecting the fluid symmetry.

Integrating our function  $\Psi$  over a macroscopically large volume  $V$  we obtain:

$$\Psi = \int_V \rho (\psi_0(x) + k(\nabla x)^2 + \dots) dV. \quad (9)$$

Employing the described reasoning we can write:

$$\frac{\delta \Psi}{\delta x} = \frac{\partial \psi_0}{\partial x} - 2k \nabla^2 x. \quad (10)$$

The first term in this relation is a function of the order parameter  $x$  only and is relevant to the energy of a uniform system. Considering a two-phase medium this expression is thought to have the meaning of free energy of the homogeneous mixture of ideally mixed phases, with no interfaces and no gradients of the order parameter  $x$ . The second term is only a function of derivatives of  $x$  and describes the so-called gradient energy. This energy is associated with a nonuniform field of the order parameter and is identified with the energy of the interfaces, which must occur in a real mixtures.

An expansion of the Helmholtz potential for the uniform system was suggested by Ginzburg and Landau [8] in the form:

$$\psi_0 = Ax^2 + Cx^4, \quad (11)$$

what leads to the final form of the evolution equation (4):

$$\dot{x} = \frac{2k}{\Gamma} \nabla^2 (x - \bar{x}) - \frac{2A}{\Gamma} (x - \bar{x}) - \frac{4C}{\Gamma} (x - \bar{x})^3. \quad (12)$$

Substituting the free constants in Eq. (12) we can obtain in a one dimensional approach that:

$$\dot{x} = -\frac{x - \bar{x}}{\beta} - \frac{(x - \bar{x})^3}{\gamma} + \kappa \frac{\partial^2}{\partial z^2} (x - \bar{x}). \quad (13)$$

Eq. (13) will be called the Ginzburg-Landau equation for the evolution of the order parameter  $x$ . This equation is the key feature of our model of two-phase water-vapour flow and describes relaxational-gradient microstructure.

#### 4. Mathematical model

A basis for the nonequilibrium model, called now the Ginzburg-Landau model, are conservation equations for mass, momentum and energy of the mixture and an evolution equation for the nonequilibrium dryness fraction. This model is homogeneous, that is assumes properties of a two-phase mixture as a mean value of particular phases - we simply average appropriate specific extensive quantities. The model assumes that the vapour remains under saturation conditions and the liquid is in a metastable state. Moreover, it assumes that the velocity difference between the phases is negligible and their pressures are equal.

Besides thermal disequilibrium associated with the temperature difference between the two phases, we additionally postulate chemical disequilibrium. This type of nonequilibrium is described by a difference between the equilibrium and nonequilibrium dryness fraction and appears in our model as the evolution equation for the order parameter  $x$ .

The model consists then of four equations written in the so-called quasi-one-dimensional approximation which takes into account variation of the cross-section area  $dS/dz$  [9]:

- mass conservation for the mixture

$$w \frac{\partial \rho}{\partial z} + \rho \frac{\partial w}{\partial z} = -\rho w \frac{1}{S} \frac{dS}{dz} \quad (14)$$

- momentum conservation for the mixture

$$\rho w \frac{\partial w}{\partial z} + \frac{\partial p}{\partial z} = -\tau_{TP} - \rho g \quad (15)$$

- energy conservation for the mixture

$$\rho \frac{\partial h}{\partial z} - \frac{\partial p}{\partial z} = \tau_{TP} \quad (16)$$

- the Ginzburg-Landau equation (13)

$$w \frac{\partial x}{\partial z} = -\frac{x - \bar{x}}{\beta} - \frac{(x - \bar{x})^3}{\gamma} + \kappa \frac{\partial^2}{\partial z^2} (x - \bar{x}) \quad (17)$$

The state vector contains  $\sigma = \{w, p, h, x\}$ , while the channel coordinate  $z$  is an independent variable. Terms on the right-hand sides of the conservation equations describe dissipative processes and reflect their irreversibility. They are as follows: the friction force  $\tau_{TP}$  and associated with it momentum and energy dissipation, the gravity force  $g$  and the relaxational vapour production. Free parameters of the model are three constants:  $\beta$ ,  $\gamma$  and  $\kappa$ . A relationship for the linear relaxation time  $\beta$  is taken in the form [9]:

$$\beta = \frac{T_c - T_0}{T_c - T_{sat}} \text{ [ s ]} \quad (18)$$

where  $T_0$  is the inlet temperature of the liquid,  $T_c$  - the critical temperature,  $T_{sat}$  - the saturation temperature. The remaining two constants of the model will be evaluated on the basis of numerical calculations and comparisons with experiments.

A solution of the system of conservation equations requires closure equations. Therefore, we employ equations of state, which give relations between thermodynamic quantities, and constitutive equations describing source terms.

The specific volume of the two-phase mixture is determined from the equation of state [10]:

$$v = \frac{1}{\rho} = xv_v + (1-x)v_l + v_{surface} \quad (19)$$

where  $v_v = v_{v,sat}(p)$  - the specific volume of the vapour is taken from the vapour-pressure line  $x=1$ , whereas  $v_l = v_{l,met}(p, h_{l,met})$  is the specific volume of the liquid calculated in the metastable region. The last term  $v_{surface}$  is omitted here.

The specific enthalpy of the two-phase mixture is given by [9]:

$$h = xh_v + (1-x)h_l + k(\nabla x)^2 \quad (20)$$

where  $h_v = h_{v,sat}(p)$  is the specific enthalpy of the vapour taken from the vapour-pressure line of saturation  $x=1$ , while  $h_l = h_{l,met}(p, v)$  is the specific enthalpy of the liquid calculated in the metastable region. These functions have been calculated on the basis of thermodynamic functions for water and vapour in the metastable region [11].

The friction pressure drop in two-phase flows can be calculated from the following formula [12]:

$$\tau_{TP} = \Phi^2 \tau_l \quad (21)$$

where  $\Phi^2$  is a two-phase multiplier,  $\tau_l$  denotes the single-phase shearing-like stress on the wall during the flow at the same mass flow rate. The coefficient  $\Phi^2$  takes into account the increased flow resistance due to the occurrence of vapour bubbles.

The friction pressure drop in a single-phase flow can be calculated from the classical formula:

$$\tau_l = \frac{1}{2} \frac{D}{S} f \rho_l w_l^2 \quad (22)$$

where  $D$  denotes the channel perimeter,  $S$  - the cross-section area,  $f$  - the friction factor dependent on the Reynolds number,  $\rho_l$  and  $w_l$  are the density and velocity of the liquid, respectively.

The friction coefficient in a single-phase flow can be calculated from the classical Blasius formula [13] derived for smooth pipes:

$$f = 0.0791 \text{Re}_l^{-0.25}, \quad (23)$$

where  $\text{Re}_l$  is the liquid Reynolds number.

The two-phase multiplier  $\Phi^2$  is a function of flow structure and according to Beattie should be calculated on the basis of the following formulas [13]:

for  $\alpha < 0.3$

$$\Phi^2 = \left[ 1 + x \left( \frac{\rho_l}{\rho_v} - 1 \right) \right]^{0.8} \left[ 1 + x \left( \frac{(3.5\mu_v + 2\mu_l)\rho_l}{(\mu_v - \mu_l)\rho_v} - 1 \right) \right]^{0.2} \quad (24)$$

for  $0.3 \leq \alpha < 0.8$

$$\Phi^2 = \left[ 1 + x \left( \frac{\rho_l}{\rho_v} - 1 \right) \right]^{0.8} \left[ 1 + x \left( \frac{3.5\rho_l}{\rho_v} - 1 \right) \right]^{0.2} \quad (24)$$

for  $0.8 \leq \alpha < 0.95$ ,

$$\Phi^2 = \left[ 1 + x \left( \frac{\rho_l}{\rho_v} - 1 \right) \right]^{0.8} \left[ 1 + x \left( \frac{\mu_v \rho_l}{\mu_l \rho_v} - 1 \right) \right]^{0.2} \quad (25)$$

for  $\alpha \geq 0.95$

$$\Phi^2 = \left[ \frac{\mu_v}{\mu_l} \right]^{0.2} \left[ \frac{\rho_v}{\rho_l} \right]^{0.8} \left[ 1 + x \left( \frac{\rho_l}{\rho_v} - 1 \right) \right]^{1.8} \quad (26)$$

In these expressions  $\mu_v$  and  $\mu_l$  denote viscosities,  $\rho_v$  and  $\rho_l$  - densities of the vapour and water, respectively, while  $x$  is the actual dryness fraction.

## 5. Numerical simulation and comparison with experiment

The numerical calculations were carried out in order to validate the proposed model (14)-(17). As a fundamental criterion to evaluate the correctness of the model, we assumed the inlet mass flow rate for a given pressure drop. The mass flow rate at the inlet, being an integral characteristic of a model, is very important from an engineering point of view and determines the usefulness of the model in the evaluation of critical mass flow rates at choking.

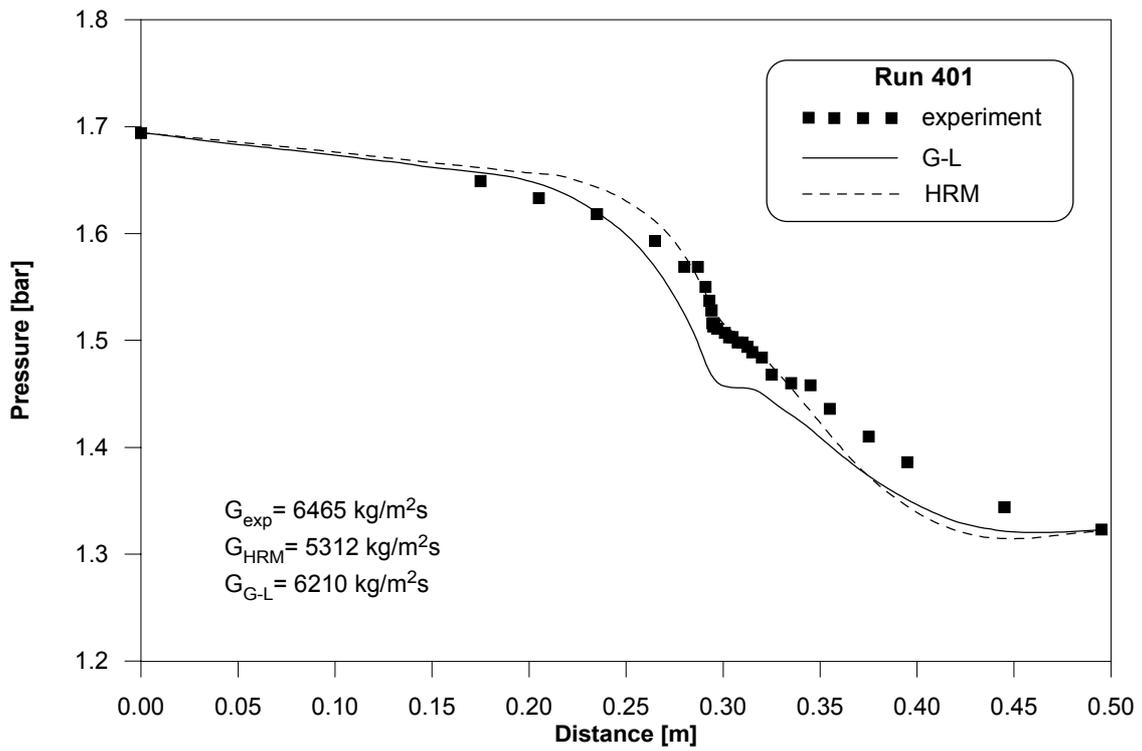
For the sake of evaluation of unknown coefficients in the Ginzburg-Landau equation, a numerical analysis was necessary. The coefficient of linear relaxation  $\beta$  (which will be called the linear relaxation time) was assumed according to Eq. (18). This formula, having theoretical background and including some features of the relaxation time in the relaxation model, turned out to be proper in our calculations.

On the basis of the performed calculations we selected the appropriate values for the unknown coefficients as follows:

$$\gamma = 3.35 \cdot 10^{-6} \text{ [ s ]}, \quad \kappa = 0.8 \text{ [ m}^2\text{/s ]}.$$

These values ensure the best results within the entire range of the parameters of the model Moby Dick and BNL experiments. This refers both to the calculated pressure and void fraction profiles and to the inlet mass flow rates. The complete results of the performed calculations for different runs are presented in Figs. 1-2. These graphs show numerically calculated pressure (Figs. 1a and 2a) and void fraction (Figs. 1b and 2b) profiles obtained by means of the Ginzburg-Landau model. For the sake of comparison with the measurements numerical curves obtained by means of the homogeneous relaxation model HRM are plotted against experimental points (cf. [1] and [14]). The pressure graphs also exhibit values of the inlet mass flow rate calculated on the basis of the above mentioned models and show the mass flow rates measured in the real flow. This quantity has been assumed as a criterion for the evaluation of our model. The optimization of this parameter has been the main purpose of our investigations.

a)



b)

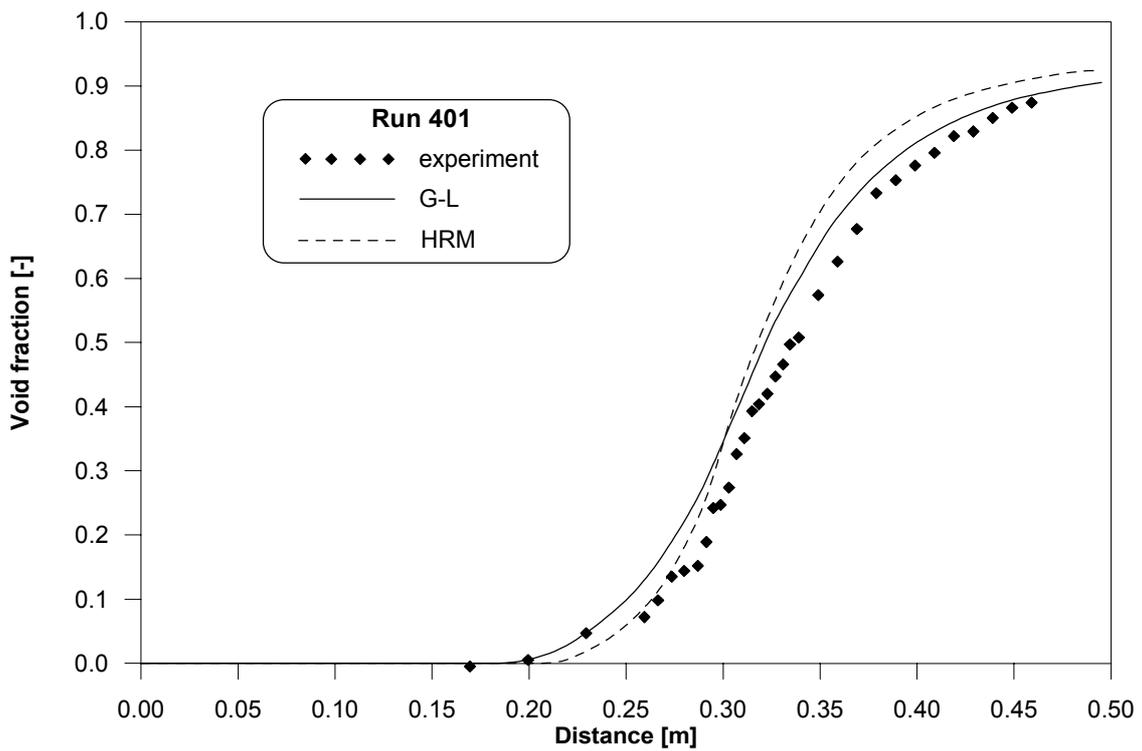


Fig.1. Pressure (a) and void fraction (b) profiles in the Moby Dick channel for run 401 calculated by means of the relaxation and Ginzburg-Landau models.

a)

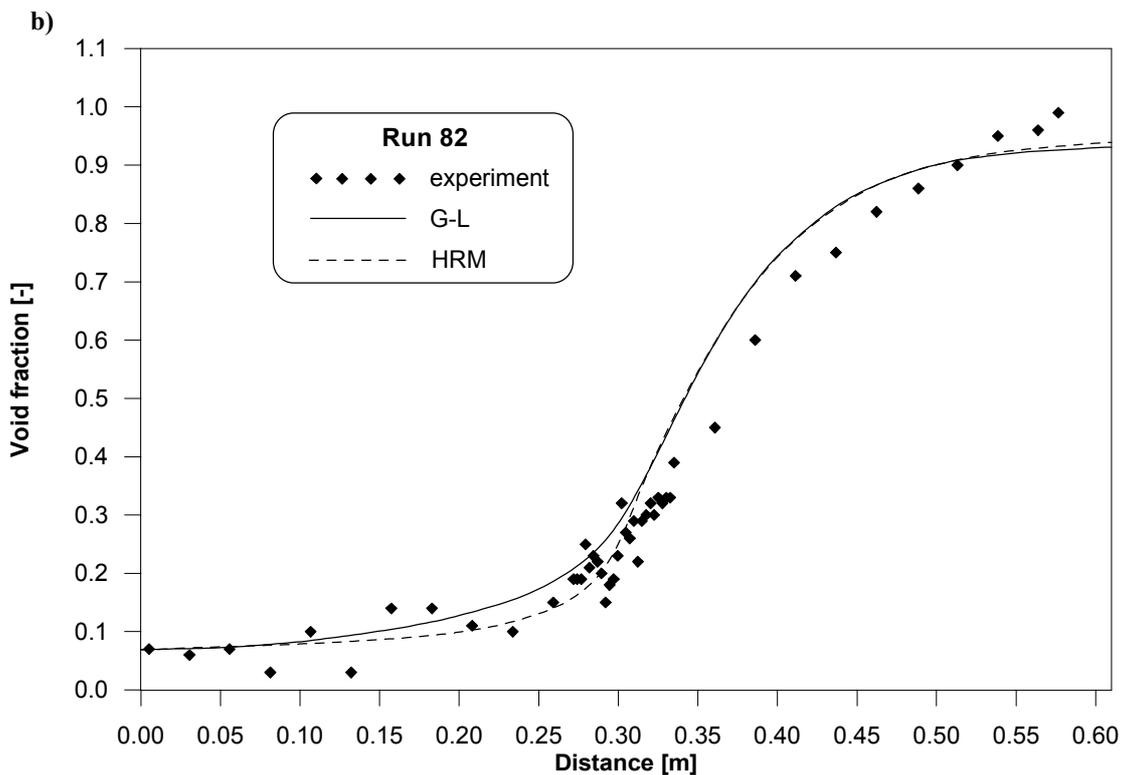
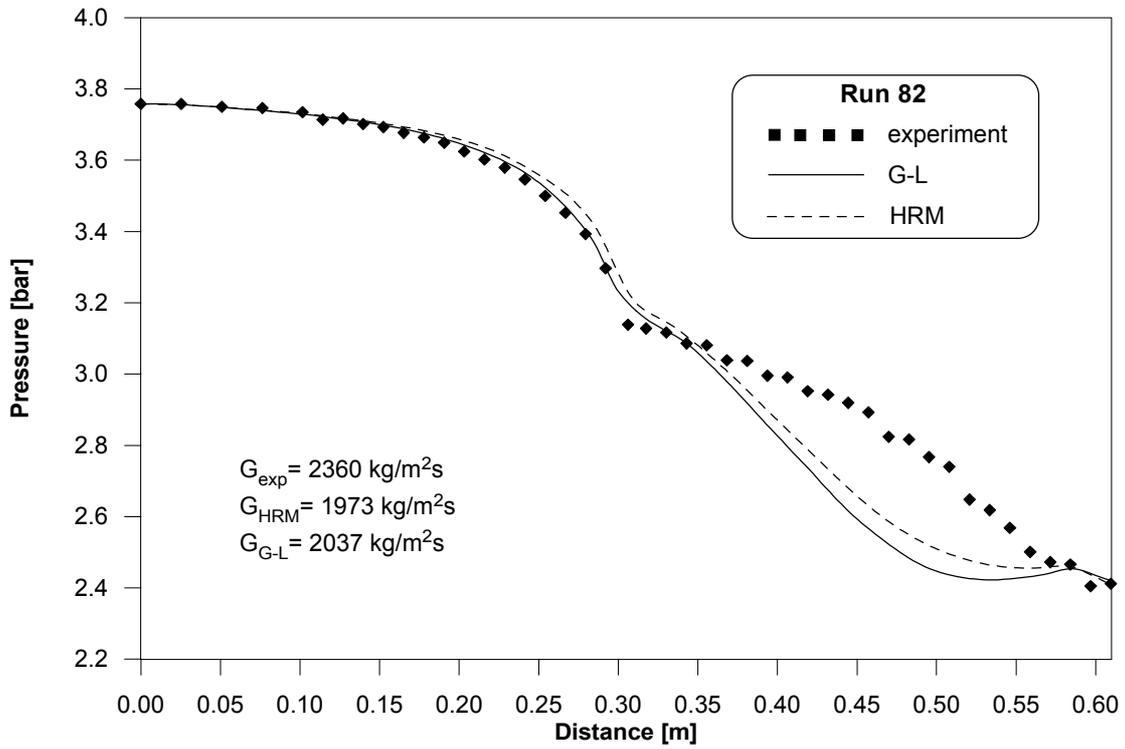


Fig.2. Pressure (a) and void fraction (b) profiles in the BNL channel for run 82 calculated by means of the relaxation and Ginzburg-Landau models.

It is clearly seen from the void fraction profiles that the proposed model better describes the vapour generation process within smaller void fractions of about 0.1 (see Figs. 1b and 2b). We suspect here an indubitable influence of the gradient term which models the phenomenon of surface tension. This phenomenon is particularly important in bubbly flow where the dispersed phase exists in the form of small vapour bubbles and the 'amount of gradients' (interfacial surfaces) is the largest. The biggest differences appear within the range of medium void fractions but one should notice that this is accompanied also by pressure discrepancies. In general,

we find that both the relaxation model and that of Ginzburg-Landau result in approximately the same pressure and void fraction profiles. This fact speaks for full equivalence of these models.

Nevertheless, the application of a new evolution equation results in more accurate values of the mass flux. At the same pressure and void fraction distributions, a substantial increase of the mass velocity was achieved, particularly for the Moby Dick experiments. The differences between numerical and measured values do not exceed 3%, what becomes more important due to the fact that all these flows are pseudo-critical. A similar trend is observed in the BNL experiments where also better values were obtained for the G-L model. In this case the discrepancies were larger than for the Moby Dick, but did not exceed 16%. Then, the Ginzburg-Landau model promises to predict better critical mass fluxes than HRM.

## 6. Summary

The proposed modification to the classical relaxation model (HRM) follows from the necessity of modelling the influence of interfacial surfaces in nonequilibrium water-vapour flows. The mathematical approach to modelling of the interfacial layer, consisting in the description of its internal energy by means of dryness fraction gradients, has been adopted from the theory of first order phase transitions.

Taking into account the interfacial energy in the energy of the two-phase mixture gives an additional gradient term in the evolution equation for the dryness fraction  $x$ . This term describes the so-called gradient energy and models the contribution of the interfacial area.

To sum up, the proposed modification to the relaxation model, having clear physical motivation by taking into account capillary effects, yields satisfactory results. The similarity of the pressure and void fraction profiles speaks for full equivalence of the relaxation equation, closed by a correlation for the relaxation time, and the Ginzburg-Landau equation with three free parameters. The latter in application to two-phase flows brings a substantial increase of the mass flow rate. This fact promises well for better predictions of critical mass flow rates in choked flashing flows.

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