GRADIENT THEORY FOR THE DESCRIPTION OF INTERFACIAL PHENOMENA IN FLASHING WATER FLOWS

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Abstract: The present work concerns the description of phenomena taking place within interfacial regions during a flow of water which is accompanied by heterogeneous flashing. The main aim of the work is to present a unified approach to first order phase transitions with the inclusion of capillary effects and to built on this basis a mathematical model describing nonequilibrium two-phase flows, in which the properties of the mixture include capillary components.

The analysis of the problem was started with a discussion of physical aspects of flashing, which are the contents of Chapter 2. On the basis of the experimental data analysis a physical model of the phenomenon was formulated.

In Chapter 3 a gradient description of first order heterogeneous phase transitions was given. The analysis was begun with a discussion of the properties and structure of interfacial areas. On the basis of the analysis constitutive equations for reversible stress tensor and free energy of a two-phase system treated as a homogeneous medium were formulated. The constitutive equations include capillary components modelled by means of the dryness fraction gradients and resulting from the nonuniformity of the system caused by the existence of two phases and interfacial surfaces.

On the basis of the proposed theory a homogeneous model of two-phase flow with capillary effects was derived, which is a subject of Chapter 4. Taking into consideration the assumptions of the homogeneous model, one-dimensional balance equations for mass, momentum and energy of the mixture and mass of vapour were derived. A constitutive equation for the source term appearing in the last equation was obtained on the basis of the theory of internal parameters with the usage of the proposed form of free energy including a gradient term known from the second gradient theory. The remaining constitutive equations for the density of the two-phase system, wall shearing stresses and capillary pressure were also given.

The proposed mathematical model was investigated from the point of view of wave properties, which were discussed in Chapter 5. The analysis of small disturbances was conducted, as a result of which a dispersion equation was obtained giving a relation between the velocity of disturbances, attenuation coefficient and frequency. This dispersive model was then applied for the prediction of critical mass flux in a channel flow using *PIF* method. On the basis of the comparison of the model predictions with experimental measurements a reasonably good agreement was found.

In Chapter 6 the results of numerical calculations of flashing flow in channel were presented. Since the proposed mathematical model contains several phenomenological coefficients, a parametric analysis was performed in order to determine their value and the influence on solutions. For the sake of the analysis the classical benchmark experiment known as the *Moby Dick* was used. After fitting the solution of the model into the experimental measurements new calculations for other runs and other experiments were carried out. As a result of the analysis a good agreement of the model with reality was found, as well as its usefulness for the calculations of pressure and void fraction distributions in channels and for the determination of mass flow rate of two-phase systems. It constitutes a confirmation of the correctness of the proposed model as well as the theory on the basis of which it was built.

Keywords: capillarity, flashing flow, thermodynamic nonequilibrium

Nomenclature

Latin symbols

a	—	parameter
A	—	affinity, cross-sectional area
$\mathbf{A}$	—	matrix of unsteadiness coefficients
b	—	body force vector
B	—	frequency of molecules collision
$\mathbf{B}$	—	matrix of nonuniformity coefficients
c	—	specific heat, speed (of sound, perturbations)
c	—	viscosity coefficients tensor
C	—	perimeter
C	—	algebraic sources vector
d	—	thermal diffusivity
D	—	diameter
D	—	deformation rate tensor, matrix of differential sources
$\mathbf{E}$	—	matrix of differential sources
f	—	specific free energy (Helmholtz potential), friction factor, function, frequency
F	—	force, total free energy
$\mathbf{F}$	—	matrix of differential sources
g	—	specific free enthalpy (Gibbs potential), gravitational acceleration
G	—	mass velocity (mass flux)
$\mathbf{G}$	—	matrix
h	—	specific enthalpy
i	—	variable
I	—	unit tensor
J	—	nucleation intensity

k	—	mechanical coefficient of capillarity, wave number
l	—	coefficient
L	—	length
$\boldsymbol{L}$	—	tensor
n	—	natural number, number
N	—	number, population
O	—	order
p	—	pressure
$\boldsymbol{P}$	—	pressure tensor
q	—	heat flux density
Q	—	heat flux
r	—	radius, radial co-ordinate
s	—	specific entropy
S	—	dummy variable of integration, total entropy
t	—	time
T	—	temperature
$\boldsymbol{T}$	—	stress tensor
u	—	specific internal energy
U	—	total internal energy
v	—	specific volume
V	—	total volume
w	—	velocity
W	—	work
x	—	dryness fraction, order parameter
$\bar{x}$	—	equilibrium dryness fraction
y	—	mass fraction of interfaces
z	—	co-ordinate

Greek symbols

α	—	void fraction
β	—	constant, linear relaxation time
χ	—	angle of channel inclination
δ	—	increase
ϕ	—	multiplier (two-phase, heterogeneity, pressure)
γ	—	non-linear relaxation time
η	—	dynamic viscosity (first viscosity, molecular viscosity), coefficient
κ	—	energetistic coefficient of capillarity
λ	—	thermal conductivity
μ	—	chemical potential
θ	—	relaxation time
ρ	—	density
σ	—	surface tension
$\boldsymbol{\sigma}$	—	state vector

τ	—	parameter, friction force
ω	—	frequency
ξ	—	interface thickness
ϑ	—	wetting angle
ζ	—	second viscosity (volumetric viscosity)
Δ	—	determinant, jump, difference
Γ	—	generation rate, source
Σ	—	decompression rate

Indices

b	—	bubble
B	—	bulk
c	—	critical
cal	—	calculated
d	—	droplet
e	—	equilibrium
exp	—	experimental
ext	—	external
fl	—	flashing
h	—	homogeneous, at constant enthalpy
hyd	—	hydraulic
het	—	heterogeneous
hom	—	homogeneous
imp	—	impossible
in	—	inlet
int	—	interfacial, surface
k	—	capillary
liq	—	liquid
lv	—	phase change
n	—	normal
ns	—	nucleation site
p	—	at constant pressure
ph	—	phase
pos	—	possible
r	—	reduced
s	—	slug
sat	—	saturation
st	—	static
sup	—	superheating
t	—	tangential
TP	—	two-phase
v	—	viscous

vap	—	vapour
w	—	wall
x	—	at constant dryness fraction
z	—	hollow
0	—	initial

1. Introduction

Water is a substance which occurs most commonly in nature and can exist in different states of aggregation. The change of state takes place through a phase transition, when the packing and the structure of H_2O molecules changes. Phase transformations taking place in water are a subject of our everyday experience. They happen spontaneously or are initiated by a man in a various kinds of machines and devices. In both cases the mechanism of phase transition is the same, just as thermal effects accompanying the process.

For study and application reasons a particularly interesting flow of water is the one accompanied by evaporation in adiabatic conditions, the so-called flashing. In this case we deal with a phenomenon in which, without thermal influence on the flow of liquid, conditions causing phase transition arise within the fluid. The factor initiating evaporation is adiabatic throttling accompanying the flow. The process of vapour generation is, in this case, spontaneous since in two-phase flow an increased pressure drop is observed, a factor which generates water *superheating* – a necessary condition for vaporisation.

The occurrence, due to flashing, of the two-phase flow results in a great *complication* of the physical situation. First, the process of evaporation proceeds in *the conditions* of thermodynamic nonequilibrium, and therefore a nonequilibrium *description* must be applied. The course of the process greatly influences the flow *situation*, which depends on the scale of nonequilibrium, and *vice versa*. Secondly, a two-phase mixture is not a simple sum of two homogeneous phases since interfacial areas – material regions of different physical properties and strong gradients of density, stresses, *etc.* – additionally appear. Within these interfaces nonequilibrium processes of mass, momentum and energy transfer take place due to these gradients. The intensity of the transfer processes depends on a configuration of interfaces, that is on the structure of the flow. The interfacial regions are also strongly turbulized and exhibit anisotropy of physical properties, which certainly influences the properties of two-phase systems. Thirdly, in a two-phase water-vapour flow completely new phenomena, not observed in single-phase flows, may occur, such as pseudocriticality, dispersed shock waves, pressure drop in a diverging channel in subcritical conditions. Any correct mathematical model should take into account the mentioned above properties of flashing flow and exactly describe the phenomena taking place in such flows. It can be achieved on the basis of the analysis of experimental data and the processes taking place in microscale – within interfacial regions and their surroundings.

2. Physics of flashing

2.1. Characteristic of the phenomenon

The phenomenon of flashing consists in rapid evaporation of a liquid in consequence of pressure drop below the saturation pressure corresponding to the current temperature of the liquid [1]. Therefore, it is a stress induced phase transition brought about by the mechanism of local tension of the fluid. Since the rapid pressure decrease is usually not accompanied by heat exchange with the surroundings, thus flashing can be treated as an adiabatic expansion of a fluid caused by decompression or outflow. The transformation of water into steam is accompanied by a change in specific volume (latent deformation) and in specific enthalpy (latent heat), and that is why flashing is rated among first order phase transitions.

Flashing water flows have been known for more than a hundred years. First experimental studies were carried out in the 19th century by Sauvage [2], while at the beginning of the present century by Rateau [3], Bottomley [4], Benjamin and Miller [5, 6] and Burnell [7]. At present, numerous examples of practical realisation of flashing flows can be found in industrial equipment and installations. These flows occur, among other things, in power industry, chemical engineering and refrigeration technology, both during normal operation of a device, when decompression is geometrically controlled, and in emergency situations, where depressurisation is uncontrolled. Flashing can occur in channels of constant cross-section, like in pipes, in regions of variable geometry, like in valves, or in pipeline breaks. During a hypothetical loss-of-coolant accident (*LOCA*) in a nuclear reactor a two-phase flow occurs in the place of break as a result of flashing. Such a type of situation is pictorially illustrated in Figure 2.1. A two-phase flow can also occur during normal operation of capillary tubes, reducers, measuring orifices and nozzles serving for the minimisation of flow resistance used as connections of pipelines of different diameters.

The most important feature of flashing is the existence of thermodynamic nonequilibrium in the fluid. This fact is experimentally confirmed and presents the largest difficulty in modelling since it requires the application of the laws of thermodynamics of nonequilibrium processes. The thermodynamic nonequilibrium results from a dynamic character of phase transition, which decelerates evaporation and causes the entry of the liquid into the region of metastable [8] or even unstable equilibrium. In single-phase flow it manifests itself in liquid superheating $T_{sup} = T_{liq} - T_{sat}(p_{liq})$, while in two-phase flow additionally in smaller amount of vapour compared with the appropriate amount in equilibrium state. For example, motionless water subjected to ambient pressure can exist in superheated state reaching 300°C. It comes from the fact that the nucleation of a new phase in first order phase transitions requires overcoming a certain energetic barrier. In practice, these barriers are often reduced due to the existence of ready nuclei of a new phase in the form of impurities, inclusions, ions, *etc*. Then, the required superheating is smaller and the process of nucleation is earlier initiated.
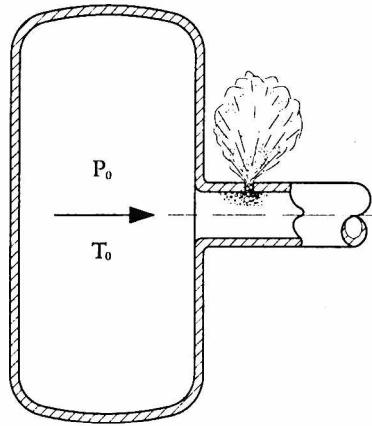
Figure 2.1. *Flashing in a pipe*

Not all bubbles created as a result of nucleation are stable and can grow. From thermodynamic considerations follows [9] that liquid superheating is necessary to satisfy the condition of equilibrium between the liquid and the arising vapour bubble. Water does not begin to evaporate at the boiling point corresponding to the equality of external pressure and the saturated vapour pressure, but at somewhat lower pressure which results from the initially small dimensions of the vapour bubble. It means that at a given temperature and pressure of water only bubbles of a given radius r can exist in thermodynamic equilibrium. For the vapour bubbles of radius grater than critical the external pressure is too low and they try to increase it by absorbing water, which next makes them even greater. However, for the bubbles smaller than critical the external pressure is too high and because of this they condense and become smaller and smaller, and eventually disappear. As a result of this, as the dimension of all bubbles is not equal and equal to critical size (which practically is impossible), the average radius of the vapour bubbles will increase, which will bring about global evaporation of the liquid and pressure increase. The process is self-sustaining and the growth of vapour bubbles and their coalescence will cause the creation of uniform bulk of vapour of the pressure equal to the equilibrium pressure of the liquid water. The critical radius decreases along with the increase of superheating and because of this the existence of bubbles of greater and greater radius is more probable. When the external pressure becomes so low that the critical radius is in the order of magnitude of the molecule radius, the existence of greater bubbles becomes certain by reason of random collisions of molecules.

2.2. Physical model of flashing flow

A correct description of flashing flow in a channel requires inclusion in the model the properties of real fluids. Owing to a large degree of complication of the phenomena taking place in such flows there arises a necessity of simultaneous

modelling of several thermodynamic and hydrodynamic processes that control the flow and become especially important in critical conditions. The most important of them are [17]:

- flashing of superheated liquid;
- the relation between void fraction α and dryness fraction x;
- local pressure losses caused by a rapid change of geometry;
- pressure drop brought about by acceleration and wall friction;
- heat exchange with the surroundings.

Thus, the crucial role is played by a correct description of the processes of mass, momentum and energy exchange between individual phases and interactions with the surroundings. The significance of transport processes modelling was emphasised by Bouré [18], in whose opinion the development of the theory of two-phase flows depends on the investigations on the phenomena governing the interfacial forces as well as the rate of heat and mass transfer. The latter problem is neglected in equilibrium models that assume infinitely fast interfacial heat and mass transfer and do not require additional theoretical models for the description of these processes. As practice shows [19], the modelling of transfer processes is extremely crucial in the description of water-steam flows in long pipes and nozzles ($L/D > 40$) since both the rate of steam generation and frictional losses determine the creation of choked flow.

Equilibrium models do not allow even a qualitative description of flashing water flows [20]. It results from the existence of the lack of thermodynamic equilibrium in such flows, which was confirmed in many experiments. It turns out that in real flows thermodynamic nonequilibrium between phases always exists, only its degree and time of existence in a flow varie. In the non-steady state experiments of Edwards and O'Brien [21], Gallagher [22], Zaker and Wiedermann [23], Fauske [24] and Sozzi and Sutherland [25] the time of duration of nonequilibrium states did not exceed 1 ms, but in Lienhard, Alamgir and Trela [14] and Bartak [26] the time of duration of nonequilibrium pressure ranged from several to a few dozen of milliseconds. As far as steady-state flows are concerned, the recorded water superheatings in flashing inception T_{sup}, being a measure of thermal nonequilibrium, ranged from $2 \div 3°C$ in the experiments of Reocreux [27] and Rousseau [28] to $5°C$ in the Jones [19] measurements. At lower pressures it gives local differences between the current pressure and the saturation pressure corresponding to the temperature of water in the order of a few dozen of kilopascals and significant displacement of the point of flashing inception downstream in comparison with equilibrium phase change. The results of such an inertial course of flashing are even qualitatively different distributions of fluid-flow and thermodynamic parameters measured in experiments and resulting from equilibrium theories. Examples of pressure distributions and the corresponding void fraction profiles in nonequilibrium
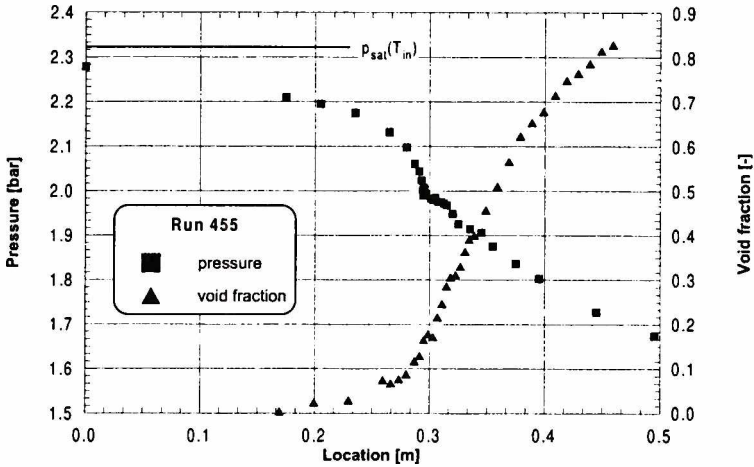
Figure 2.2. *Example of pressure and void fraction distributions in the Reocreux [27] pipe*
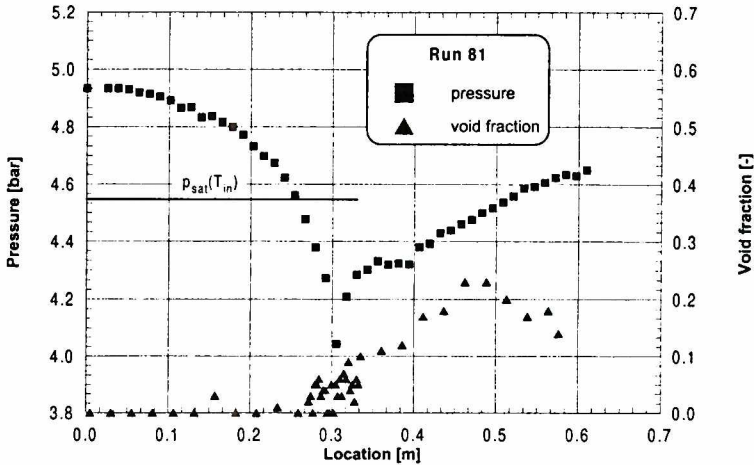

Figure 2.3. *Example of pressure and void fraction distributions in the Jones [19] nozzle*

flashing flows recorded by Reocreux [27] and Jones [19] are presented in Figures 2.2 and 2.3. They illustrate a delay in flashing inception and the existence of metastable flow both in the pipe (Figure 2.2) and in the nozzle (Figure 2.3).

Apart from thermal nonequilibrium in one-component two-phase flows mechanical nonequilibrium also exists, which is indicated by a difference in velocities of individual phases [29]. The value of slip ratio is the largest in areas of the generation of vapour bubbles which are, as experimental studies show [19, 27, 28], generated on the channel walls and at the instant of nucleation have zero velocity. As the liquid velocity increases, also the vapour velocity does and at near-critical velocities the slip ratio approaches unity. Henry [30, 31] showed that in critical one-component flows at low dryness fraction $x < 0.01$ the value of slip ratio should be near one. Also Lackme [20] found that in choked flashing flow the value of dryness fraction is small and visual observations of the flow indicate its homogeneous
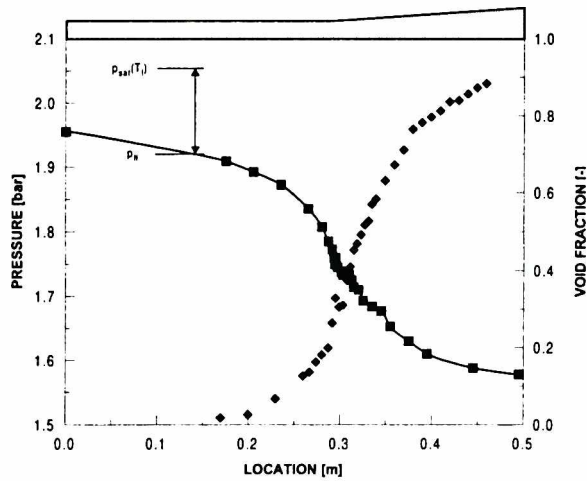
Figure 2.4. *Physical model of flashing flow based on the experimental measurements of Reocreux [27]*

structure at which it is difficult to find large velocity differences. They are in the order of $0.1 \div 1$ m/s, which, in the Nigmatulin and Soplenkov [32] opinion, has little importance at typical liquid velocities $10 \div 100$ m/s. That is why in near-critical flows with large velocities the neglect of relative velocity and the assumption on the lack of slip are justified, and the system can be treated as a homogeneous mixture in nonequilibrium state.

Considering adiabatic internal flows with large velocities in channels of slowly varying axisymmetric geometry, the influence of heat exchange with the surroundings and local pressure losses caused by a rapid change of geometry are neglected. In such flows the predominant phenomenon is nonequilibrium evaporation of a liquid, which is a result of a delay in water-steam phase transition and the finite rate of interfacial heat and mass transfer. Initially subcooled or saturated water is decompressed during the flow (Figure 2.4). Pressure drop in a vertical canal is brought about by friction (molecular and turbulent viscosity), gravitation force and acceleration. As a result of the losses the static pressure drops below the saturation pressure calculated for the inlet temperature of water T_{liq} and at the point where the pressure reaches p_{fl} the water starts to evaporate. The two-phase flashing flow is characterised by an increased pressure gradient and increase of void fraction. These quantities are macroscopic characteristics of two-phase flow and can be easily measured in experiment.

3. Gradient description of interfacial properties

3.1. Structure and properties of interfacial areas

3.1.1. Characteristics of an interfacial surface

A two-phase fluid as a mixture of liquid, vapour and dividing interfaces is, in fact, a heterogeneous system. Its physical properties are determined not only by the

properties of the component phases but also by the properties of the interfacial areas. The dividing surfaces can exist in various geometrical configurations which determine the topological structure of two-phase systems as well as the division of two-phase flows into bubbly, slug, churn, annular and droplet. In each case, the properties and dynamics of the two-phase system will be strongly dependent on the existing internal structure of the mixture. Also, the interfacial area possesses distinctive physical properties and its own dynamics but usually interactions with the surrounding homogeneous phases have a crucial influence on the behaviour of this region. This interfacial surface being formed under the influence of homogeneous phases simultaneously affects the state of the phases, behaves actively in relation to them and affects the formation of the neighbouring phases [80].

The concept of a dividing surface was introduced for the first time by Gibbs [81] in 1878. Considering a one-component two-phase system he treated the interfacial area as a physical interface which is characterised by a directed force of surface tension connected with pressure. The interfacial region is distinguished by the anisotropy of pressure caused by the nonuniformity of the interfacial region along its width. Physically, by a mathematical interface one should understand a three-dimensional material origination whose two dimensions are significantly greater than the third one – thickness. The thickness of the interfacial region is estimated at several molecular diameters and increases as approaching the critical point of the substance.

The behaviour of an interface is usually presented as analogous to the behaviour of an elastic membrane. But such a description neglects some significant physical differences which are based on the fact that a stretched interface increases its mass by introducing additional molecules from homogeneous regions at constant surface tension, whereas a stretched membrane conserves its mass and shows an increase of internal stress [82].

A stable existence of an interface is possible only when the thermodynamic potential of its creation assumes a positive value [38]. If its value were negative or equal zero, accidental fluctuations could spread the interfacial layer within the fluid, finally leading to a complete dispersion of one phase within another.

It should also be realised that this thin interfacial region is strongly turbulised [38]. In thermodynamic equilibrium between liquid and vapour, within the transitional zone a two-way traffic of molecules takes place – the molecules hit and condense on the interface from the vapour side and evaporate from the surface to the vapour phase. According to Adamson [38], for a saturated vapour at room temperature from each squared centimetre of water about $1.2 \cdot 10^{22}$ molecules per second arrive and go away. Through a surface equal to 10 Å^2 corresponding to the surface area of a single molecule of water, $1.2 \cdot 10^7$ molecules/s pass which gives deposition time of an individual molecule on the interface of the order of tenth of microsecond. In such a situation, also the exchange of molecules between the interfacial region and the adjacent liquid layers takes place. The coefficient of diffusivity of most liquids at room temperature is of the order of 10^{-5} cm^2/s. A molecule penetrates liquid on the
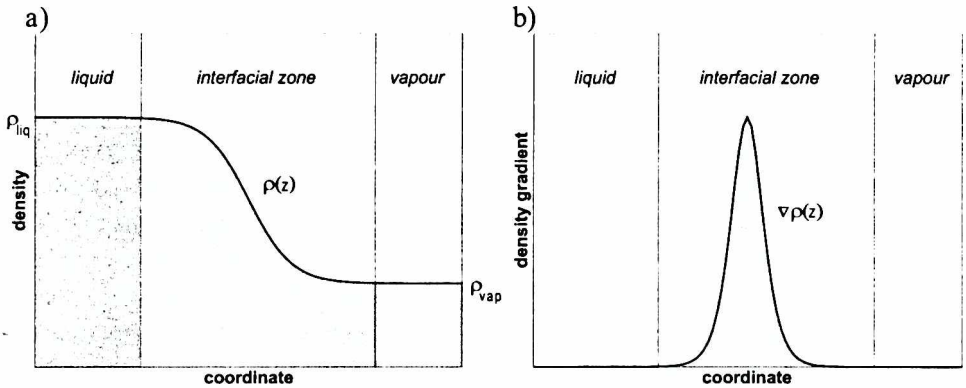
a)

| liquid | interfacial zone | vapour |

density

ρ_{liq}

$\rho(z)$

ρ_{vap}

coordinate

b)

density gradient

| liquid | interfacial zone | vapour |

$\nabla\rho(z)$

coordinate

Figure 3.1. *Pictorial character of variations of density (a) and its gradient (b) crosswise a surface dividing liquid and vapour*

depth of 10 nm already during 10^{-6} s. From the above data it follows that an equilibrium interface is on molecular level at a state of strong agitation and movement of single molecules penetrating the fluid from both sides of the interface. Average density represented on macroscopic level by the product of the mass of a molecule and their concentration [33] varies continuously from the density of the liquid to the density of the vapour. The intensity of the density variation is not constant along the thickness of the interface and, as it turns out, is the largest in the middle of the interfacial zone. Pictorial character of the variations of density and its gradient on crossing the interface dividing liquid and gas is shown in Figure 3.1.

A continuous variation of density of a two-phase liquid-vapour mixture is a result of variable distribution of fluid particles within the transitional zone. In a state of mechanical equilibrium intermolecular forces (van der Waals forces) determine spatial distribution of particles. When two molecules are sufficiently close to each other they interact via repulsive forces. On greater distances we deal only with attraction forces whose values smaller than those of repulsion. In a homogeneous phase of constant density the field of forces exerted by the surrounding molecules is symmetrical and the resultant force is equal zero. For particles situated within the interfacial region the resultant intermolecular force should also be zero. Otherwise, such a particle will be moved to a position in which this resultant force is equal to zero or will leave the liquid, which means evaporation. Evaporation is possible only for particles of the highest level of energy [83]. Thus, the structure of the transitional zone is such that interfacial distances vary continuously perpendicularly to this zone from the values in the homogeneous liquid phase to the values characteristic for the vapour. Variable distances between the molecules express, of course, their variable spatial packing manifesting itself by a variable concentration.

As it has been mentioned above, the increase of the area of an interface requires a displacement of some number of particles from the interior of the homogeneous phase to the interfacial region. Experience shows that this process requires some work resulting from the necessity of applying a force to compensate

the forces of molecular interactions. It turns out that for a given fluid the isothermal and reversible process of a unit increase of the interface area requires always the same amount of work. A macroscopic consequence of the existence of the intermolecular forces within the interfacial area is surface tension. It expresses a force exerted at all points of the interface, acting at the plane of the interfacial surface and directed in all the directions tangent to the surface. The value of this force for a unit length constitutes the mechanical definition of surface tension:

$$\sigma = \frac{dF}{dz}. \tag{3.1}$$

From an energetic point of view the surface tension can be defined as the amount of work required to increase the interfacial surface by a unit area:

$$\sigma = \frac{dW}{dA_{\text{int}}}. \tag{3.2}$$

Hence, systems showing the existence of surface tension tend to decrease their surface, which is a region richer in energy, realising in this way a natural tendency of energy minimisation. A characteristic feature of surface tension is its independence of surface area A_{int} and strong dependence on temperature T.

3.1.2. State of stress within an interfacial area

In a nondeformed system in which statistical dynamic equilibrium and the corresponding intermolecular structure were established, internal stresses do not exist [84]. The forces of molecular interactions are in mutual equilibrium appropriately to internal dynamic equilibrium.

The matter looks differently in a deformed system. In such a system, the internal structure corresponding to dynamic equilibrium is disturbed and as a result of this internal stresses caused by the intermolecular forces of very short range appear. These stresses manifest themselves in forces acting on arbitrary planes drawn in the deformed system and depend on spatial orientation of these planes as well as on their location. In the mechanics of continuous media the stress tensor T being a tensorial field quantity is used to describe stresses in a deformed system. Instead of the stress tensor, the so-called pressure tensor P is often used, especially in hydrodynamics. It is defined in the following way [33]:

$$P = -T. \tag{3.3}$$

In general, the pressure tensor can be decomposed into two additive parts [76]:

$$P = P^e + P^v. \tag{3.4}$$

The former part P^e is the equilibrium stress tensor and depends on the state of the system only. The components of this tensor express reversible thermodynamic pressure, that is a quantity defined in equilibrium. The latter part of the pressure tensor P^v is an irreversible part and depends on the rate of change of state as well

as on the gradients of the rate. Since viscous forces depend on the gradients thus this part is called the viscous pressure tensor. When a system is in equilibrium and does not exhibit any changes of state, then the pressure tensor is reduced to the first part. As it was noticed by Bilicki [42] Equation (3.4) is a physical assumption and means that the total momentum of a system is transported by two media. One is an elastic or compressible system, in which volumetric work is reversible, and the other is a dissipative system. A characteristic feature of this additive decomposition is that either way of momentum transport is independent of each other, that is each of them proceeds in such a way as if the second medium was absent.

The structure of the pressure tensor resulting from the character of intermolecular forces is different in homogeneous phase and in interfacial region. This refers both to the equilibrium and viscous part of the pressure tensor. Our discussion will be started with an analysis of the equilibrium stress P^e. As it is known, in a homogeneous system at rest only normal stresses appear. For the sake of symmetry of molecular interactions, the normal stresses acting in particular directions are assumed to be equal to each other which results in isotropic distribution. The state of stress in the system is then described by means of the isotropic pressure tensor [85]:

$$P^e = \begin{bmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{bmatrix},$$

(3.5)

where p is hydrostatic pressure equal as for absolute value and of negative sign to normal elastic stresses. The hydrostatic pressure is here identified with a reversible thermodynamic pressure occurring in the equations of state.

Within an interfacial region a different, anisotropic state of stress exists. It can be presented best by considering a horizontal flat interface dividing liquid and vapour in gravitation field. Neglecting the influence of gravity on the physical properties of the phases, its effect can be reduced only to the location of the vapour phase above the liquid. The condition of hydrostatic equilibrium is then expressed by the relation [86]:

$$\nabla \cdot P^e = 0.$$

(3.6)

In the conditions of the assumed planar geometry of the system it is obvious to assume that the pressure tensor, like density and phase fraction, depends only on the co-ordinate z perpendicular to the flat interfacial surface. Then, the condition (3.6) can be simplified and written in components:

$$\frac{dP^e_{zi}}{dz} = 0, \qquad i = x, y, z.$$

(3.7)

The condition of equilibrium (3.7) means that the pressures P^e_{zx}, P^e_{zy} and P^e_{zz} are constant and independent of the co-ordinate z. Within homogeneous phases the pressure tensor P^e is isotropic and equal to pI. Thus, from the condition of

hydrostatic equilibrium it follows that within flat interface the tangent pressures P^e_{zx} and P^e_{zy} are equal zero and the normal pressure P^e_{zz} is equal to p. On the basis of the symmetry of the pressure tensor in equilibrium one can further notice that $P^e_{xz} = P^e_{yz} = 0$, while tangent isotropy of the flat interface requires that $P^e_{xx} = P^e_{yy}$ and $P^e_{xy} = P^e_{yx} = 0$. To recapitulate, one can say that flat interface has two principal pressures: normal $P^e_n = P^e_{zz}$ and transverse $P^e_t = P^e_{xx}$, and does not exhibit tangent pressures. The normal pressure P^e_n is constant and equal to the hydrostatic pressure of uniform phases, but the transverse pressure P^e_t varies with the co-ordinate z and becomes equal to the normal pressure within the uniform phases. The pressure tensor is thus axisymmetric tensor of second order and according to tensor calculus has two independent components [87].

The origins of pressure anisotropy within an interfacial region are intermolecular forces since the kinetic part of the pressure tensor is isotropic [86]. The intermolecular forces strongly depend on the density of the fluid, that is on the molecular level on the concentration of particles. Since the number of molecules interacting with a considered reference molecule is different in different directions, thus the force of interactions in the direction normal to the interface will be different from that acting in the direction transverse to the interface. Thus, the pressures exerted in these two directions must be different.

At this point a third definition of surface tension can be quoted. Since the transverse pressure P^e_t within the interfacial region is different from that in the uniform phase where as it is known $P^e_t = P^e_n$, also the force acting in the transverse direction will vary and the reason of this variation is just the surface tension. The exact definition of the surface tension is given by the formula:

$$\sigma = \int_{-\infty}^{+\infty} \left(P^e_n - P^e_t \right) dz. \tag{3.8}$$

Integration of the pressure difference is extended from minus infinity to plus infinity since outside the interfacial region the difference is zero and does not contribute to the surface tension. As it is seen from relation (3.8) the surface tension σ can be interpreted as an integral of the excess of pressure exerted crosswise the interfacial area in relation to the pressure acting over the area. The value of this pressure excess is, of course, a function of position, and, as it turns out, at some point attains a maximum. According to Goodrich [87], for a typical value of the surface tension $\sigma = 0.05$ J/m² and the thickness of an interface $5 \cdot 10^{-9}$ m the pressure difference reaches 10 MPa. Similar differences between normal and transverse pressures are recorded by Carey, Scriven and Davis [88]. Assuming the value of the surface tension equal $\sigma = 0.02$ N/m and the thickness of an interface $2 \cdot 10^{-9}$ m they obtained the pressure excess equal to 10 MPa. For low normal pressures in the order of 1 bar it results in negative transverse pressure about -10 MPa. From an experimentally proved fact that the thickness of an interface at low pressures and high surface tensions is of the order of tens or hundreds of angstroms, Davis and Scriven [86]

draw a very important conclusion. It tells that within a part of the interfacial region the transverse pressure must be negative. There can exist regions of tension $P_n^e > P_t^e$, as well as those of compression $P_n^e < P_t^e$.

Generalising the analysis concerning the flat interface into arbitrary curved interfaces one should say that neither normal nor transverse component of the pressure tensor is constant. Apart from this, the transverse components are not equal to each other and despite the lack of movement tangent (shearing) pressures exist.

Having the complete knowledge of the state of stresses within static interface we can proceed to the analysis of a moving system containing dividing surfaces. In such a dynamic system, apart from reversible elastic stresses, some additional irreversible stresses connected with viscous forces appear. As it was mentioned above, these stresses depend on the rate of change of the state of the system and are described by viscous part of the pressure tensor $\boldsymbol{P}^v$. According to the Newton hypothesis the viscous stresses are a linear function of deformation rate and for most fluids it is a sufficiently precise approximation [33]. In this connection we can write:

$$\boldsymbol{P}^v = c\boldsymbol{D} , \tag{3.9}$$

where c is a fourth order tensor whose components are the coefficients of viscosity, while $\boldsymbol{D} = \dfrac{1}{2}(\nabla \otimes w + w \otimes \nabla)$ stands for deformation rate tensor. Within an uniform phase the tensor of viscosity coefficients is isotropic which results in the fact that as a fourth order tensor it has two independent components (Lame coefficients). In hydrodynamics they are known as the coefficients of first and second viscosity. On the basis of the anisotropy of a uniform system we can write:

$$P_{ii}^v = \zeta \sum_{j=1}^{3} D_{jj} + 2\eta D_{ii} , \tag{3.10}$$

$$P_{ij}^v = 2\eta D_{ij} , \quad \text{for} \quad i \neq j . \tag{3.11}$$

The former relation is an expression for viscous normal (main) stresses, while the latter describes viscous tangent (shear) stresses. The coefficient of first viscosity (molecular viscosity) is denoted here by η, while the coefficient of second viscosity (volumetric viscosity) – by ζ Expressions (3.10) and (3.11) are constitutive equations for isotropic Newtonian fluids.

Within an interfacial region the properties of the fluid are no longer isotropic. According to the theory of Goodrich [87] the tensor of viscosity coefficients is axisymmetric and possesses at most five independent components. For such a system one postulates the following components of viscous pressure tensor [87]:

$$P_{xx}^v = (\zeta' + 2\eta')D_{xx} + \zeta'D_{yy} + \zeta D_{zz} , \tag{3.12}$$

$$P_{yy}^v = \zeta' D_{xx} + (\zeta' + 2\eta') D_{yy} + \zeta D_{zz} ,$$

(3.13)

$$P_{zz}^v = \zeta D_{xx} + \zeta D_{yy} + (\zeta + 2\eta) D_{zz} ,$$

(3.14)

$$P_{xy}^v = P_{yx}^v = 2\eta' D_{xy} , \quad P_{xz}^v = P_{zx}^v = 2\eta'' D_{xz} , \quad P_{yz}^v = P_{zy}^v = 2\eta'' D_{yz} ,$$

(3.15)

Going from the interfacial area to the region occupied by a uniform system the pressures given be relations $(3.12 \div 3.15)$ converge to the values determined by $(3.10 \div 3.11)$. Five coefficients of viscosity ζ, ζ', η, η' and η'' describing transport properties of the axisymmetric interfacial region reach the limiting values of two coefficients of viscosity of uniform phases ζ and η. Physically, this means that in some directions there appear some excesses of viscous stresses as compared to the stresses acting in a uniform isotropic system. Thus, not only static (hydrostatic pressure) but also dynamic (viscosity) properties of the system exhibit anisotropy within the regions occupied by interfacial surfaces. These surfaces are characterised in some directions by some excess quantities whose value determines the intensity of anisotropy. The properties of a heterogeneous fluid do not vary discontinuously but in microscale exhibit a continuous variation.

3.2. Mechanical constitutive equation of a two-phase system

Now we proceed to phenomenological description of a two-phase system containing material interfacial areas. Our considerations will be carried out in terms of homogeneous model in which the properties of internally homogeneous medium are postulated for a heterogeneous two-phase system. These properties are a kind of averages of the properties of the component phases, and according to the author from definition should take into consideration also the properties of interfacial regions. Such a methodology of thermodynamic description of heterogeneous substances was proposed for the first time by Gibbs [81] who noticed that any extensive thermodynamic property describing a two-phase system should include, apart from the contribution of homogeneous phases, also some excess coming from dividing surfaces. From a phenomenological point of view, the description of molecular interactions and the dynamics of interfaces is possible after previous determination of local properties of the system and then transition on macroscopic level [35].

In order to obtain a constitutive equation describing stresses in a two-phase system with the inclusion of capillary stresses, the second gradient theory can be used. It is a general theory allowing description of capillary phenomena of a two-phase mixture assuming a continuous variation of thermodynamic parameters within the interfacial region. The bases of the theory were created by Dutch scientists already in the 19th century. The first thermodynamic considerations were presented by van der Waals [89] who proposed to introduce to the Helmholtz potential a term with density gradient modelling the energy of interfacial areas. Proceeding similarly, Korteweg [90] proposed a constitutive equation for capillary stress tensor in which

capillary stresses were described by density gradients. In both cases the density of the fluid plays a role of an order parameter distinguishing two fluids and dividing surfaces, and the gradients of density result from nonlocal molecular interactions within the interfacial zone [91].

Considering a nonequilibrium water-steam mixture we stated that the nonequilibrium dryness fraction x is the quantity which satisfies all the requirements imposed on internal variables. The nonequilibrium dryness fraction x expresses the actual fraction of vapour phase in the two-phase mixture and fulfils the function of order parameter very well. In water its value is 0, in steam 1, while within the interfacial region it continuously varies from 0 to 1. The gradient of the dryness fraction in homogeneous phases is zero and varies within interfacial areas only.

From the performed above considerations we have already learnt that the state of stresses in a nonuniform system depends not only on density at a given point but also on density in the nearest surroundings. In the case of a water-steam mixture described with the help of homogeneous model, the density varies as a result of the variation in vapour content expressed by the nonequilibrium dryness fraction x. In order to describe the nonlocal character of stresses one should express them in a function of the dryness fraction gradients. Having this in mind one can postulate a decomposition of the reversible stress tensor T^e into a part corresponding to the stresses in a uniform system T^h and a part T^k describing stresses caused by internal nonuniformity of the system which occurs within interfacial regions. The stresses in the uniform system without internal gradients are a function of the dryness fraction $T^h = T^h(x)$, while the capillary stresses additionally depend on its gradients $T^k = T^k(x, \nabla x, \nabla\nabla x, \ldots, \nabla \ldots \nabla x)$. Thus, we can express the stress tensor as a sum of two tensorial functions of second order [92]:

$$T^e = T^h(x) + T^k(x, \nabla x, \nabla\nabla x, \ldots, \nabla \cdots \nabla x). \qquad (3.16)$$

The dependence of stresses on dryness fraction describes in this case the action of short-range molecular forces (repulsion), while the dependence on the gradients of dryness fraction is related to the action of long-range forces of attraction between molecules. It is just the second part of the stress tensor, that is a source of the surface tension.

Gradient representation of the capillary stress tensor T^k is obtained by expanding the tensor T^e about a point at which all the gradients of the dryness fraction vanish. Like Aifantis and Serrin [92] we limit the expansion to the third order gradients and obtain:

$$T^e = T_0 + T_1\nabla x + T_2\nabla\nabla x + T_3\nabla x \otimes \nabla x + T_4\nabla\nabla\nabla x + T_5\nabla x \otimes \nabla x \otimes \nabla x, \qquad (3.17)$$

where the coefficients $T_0, \ldots, T_5$ are isotropic tensors depending on x, because they are determined by the properties of the system without gradients [86]. The coefficient T_1 as an isotropic tensor of third order is identically equal zero, like the isotropic tensors of fifth order T_4 and T_5. Then, relation (3.17) can be simplified to:

$$T^e = T_0 + T_2 \nabla \nabla x + T_3 \nabla x \otimes \nabla x. \tag{3.18}$$

On the right-hand side of Equation (3.18) we have a sum of three linear tensorial functions to which one can use the following representation of tensorial function [93]:

$$f T = l_0 (\text{tr} T) I + l_1 T. \tag{3.19}$$

As a result of this we obtain the following expressions:

$$T_0 = -pI, \tag{3.20}$$

$$T_2 \nabla \nabla x = l_2 \nabla^2 x I + l_3 \nabla \nabla x, \tag{3.21}$$

$$T_3 \nabla x \otimes \nabla x = l_4 (\nabla x)^2 I + l_5 \nabla x \otimes \nabla x, \tag{3.22}$$

in which p is pressure, and the coefficients $l_2, \ldots, l_5$ are, in general, functions of the dryness fraction x. Inserting relations (3.20÷3.22) into formula (3.18) we obtain the final formula for the equilibrium stress tensor of the two-phase system with internal microstructure:

$$T^e = -pI + l_2 \nabla^2 x I + l_3 \nabla \nabla x + l_4 (\nabla x)^2 I + l_5 \nabla x \otimes \nabla x. \tag{3.23}$$

The pressure p denotes here pressure in a uniform system without internal microstructure inducing anisotropy and being characterised by the gradients of the fluid properties. The contribution of interfaces is represented by the gradient terms. The influence of these additional stresses on the stress tensor is controlled by the four coefficients $l_2, \ldots, l_5$.

One should draw attention to the fact that a nonuniform system described by the stress tensor (3.23) apart from the anisotropy of normal stresses exhibits also tangent (shear) stresses. These are all elastic stresses, that are reversible in thermodynamic sense. Their origin resides in capillary forces. For capillary normal stresses we have:

$$T_{ii}^k = \left(l_2 \sum_{j=1}^3 \frac{\partial^2 x}{\partial z_j^2} + l_4 \sum_{j=1}^3 \left(\frac{\partial x}{\partial z_j} \right)^2 \right) \delta_{ii} + l_3 \frac{\partial^2 x}{\partial z_i^2} + l_5 \left(\frac{\partial x}{\partial z_i} \right)^2, \tag{3.24}$$

while for capillary tangent stresses we obtain:

$$T_{ij}^k = l_3 \frac{\partial}{\partial z_i} \left(\frac{\partial x}{\partial z_j} \right) + l_5 \frac{\partial x}{\partial z_i} \frac{\partial x}{\partial z_j}, \quad \text{for} \quad i \neq j. \tag{3.25}$$

Taking advantage of the constitutive equation for the stress tensor (3.23) one can calculate the surface tension for a flat interface within which the dryness fraction varies along z. The main normal and transverse stresses are then given by the relations:

$$T_{zz}^e = -p + (l_2 + l_3)\frac{d^2x}{dz^2} + (l_4 + l_5)\left(\frac{dx}{dz}\right)^2, \tag{3.26}$$

$$T_{xx}^e = T_{yy}^e = -p + l_2\frac{d^2x}{dz^2} + l_4\left(\frac{dx}{dz}\right)^2. \tag{3.27}$$

Making use of the definition of the surface tension given by relation (3.8) we can write:

$$\sigma = \int_{-\infty}^{+\infty}\left(T_{xx}^e - T_{zz}^e\right)dz = \int_{-\infty}^{+\infty}\left(-l_3\frac{d^2x}{dz^2} - l_5\left(\frac{dx}{dz}\right)^2\right)dz. \tag{3.28}$$

Integrating by parts the first term in the integral we obtain:

$$\int_{-\infty}^{+\infty}\left(-l_3\frac{d^2x}{dz^2}\right)dz = -l_3\frac{dx}{dz}\bigg|_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty}\left(\frac{dl_3}{dx}\left(\frac{dx}{dz}\right)^2\right)dz. \tag{3.29}$$

The first term on the right-hand side of expression (3.29) is identically equal zero since the dryness fraction is constant in infinity. Thus, we can write:

$$\sigma = \int_{-\infty}^{+\infty}k_1\left(\frac{dx}{dz}\right)^2 dz, \tag{3.30}$$

where the parameter k_1 is defined as follows:

$$k_1 = \frac{dl_3}{dx} - l_5. \tag{3.31}$$

3.3. The thermodynamic equation of state of a two-phase system

Now, we are going to discuss some thermodynamic aspects of the motion of a nonuniform two-phase system. In order to do this, a fundamental equation of state of the nonequilibrium water-steam mixture will be derived. Since the present work concerns flashing flows in which phase transition is induced by stress, thus from the possible fundamental equations the Helmholtz potential will be discussed. For such problems it is the most appropriate function since it is expressed in terms of temperature and specific volume. In adiabatic flows of water the temperature can be assumed constant, while the variation of the specific volume (or pressure) causes that the system becomes metastable or unstable, which in effect leads to phase change.

As it was noticed by Gibbs [81], any extensive thermodynamic quantity describing a two-phase system should also include, apart from the contribution of homogeneous phases, some excess coming from dividing surfaces. With reference to the Helmholtz potential it is postulated that the total free energy of the system is a sum of free energies of the component phases and the free energy of interfacial

areas. Even though the energies of the homogeneous phases are proportional to the number of molecules of a given phase and are a simple sum of the energies of single particles, this cannot be said about the energy of interfaces. This energy is equal to the difference between the energy of molecules being within the interfacial area and the energy which those molecules would have if they were within a uniform phase [80]. From classical thermodynamics it is known that energy of molecules increases with temperature, whereas the surface energy decreases along with temperature and at the critical point vanishes to zero.

The contribution of interfacial energy is extremely difficult to model. It results from the fact that the internal energy of an interfacial region is not only a function of surface entropy and surface stretching, but depends also on the state of both phases, geometry of the surface and the velocity of propagation in the fluid [16]. Other important factor on which the total interfacial energy depends is the interfacial area density.

In section 3.1 it was said that the reversible work required to increase the interfacial surface by a unit area is equal to the surface tension. In a reversible process proceeding at constant temperature and specific volume, the change of internal energy of the system is given by the relation [94]:

$$dU = dQ_{rev} + dW_{rev} = TdS + \sigma dA_{int} . \tag{3.32}$$

Hence, on the basis of definition, the change of free energy of the system can be written as [94]:

$$dF = -SdT + \sigma dA_{int} , \tag{3.33}$$

from which we obtain:

$$\sigma = \left(\frac{\partial F}{\partial A_{int}} \right)_{T,V} . \tag{3.34}$$

Relation (3.34) defines the surface tension as free energy of unit interfacial surface. The total free energy of the system is an integral from the unit energy:

$$F(T,V,A_{int}) = \sigma(T)A_{int} + F_B(T,V), \tag{3.35}$$

where $F_B(T, V)$ is a constant of integration and expresses the free energy of bulk phases. For a two-phase water-steam mixture relation (3.35) can be written in a different form:

$$F(T,V,A_{int}) = \sigma(T)A_{int} + F_{liq}(T,V_{liq}) + F_{vap}(T,V_{vap}). \tag{3.36}$$

In such a way we obtained a relation for the total free energy of the two-phase system, given as a sum of free energies of homogeneous phases and interfacial surfaces. While the contribution of liquid and vapour is easy to calculate, determination of the contribution of the interfacial free energy requires knowledge of the area of interfacial surfaces. This quantity is not constant but varies along with the variation of phase fraction and flow structure. Relating the total free energy of

the two-phase system to its mass we obtain the relation for the Helmholtz specific free energy in thermodynamic equilibrium:

$$f(T,v,a_{int}) = \sigma(T)a_{int}v_{int} + (1-\bar{x})f_{liq}(T,v_{liq}) + \bar{x}f_{vap}(T,v_{vap}), \qquad (3.37)$$

in which a_{int} [m²/m³] is the interfacial area density, v_{int} [m³/kg] – the specific volume of interfaces, while $\bar{x}$[-] – the equilibrium dryness fraction. The range of application of formula (3.37) is limited to the conditions of thermodynamic equilibrium since this formula was derived from the definition of surface tension – a quantity calculated on the basis of reversible work of the system.

In order to derive a fundamental equation for the free energy of a nonuniform system in the conditions of thermodynamic nonequilibrium we will take advantage of the second gradient theory. In the classical thermodynamics of nonequilibrium processes the definition of the energy of a system does not include contributions coming from the gradients of specific extensive properties. For a uniform system without gradients it does not matter at which point we calculate the energy of the system. In a situation of a nonuniform filed, for example density, concentration, phase fraction, the local definition of energy of the system is extended by nonlocal interactions resulting from the asymmetry of intermolecular forces. According to the second gradient theory presented in the works of van der Walls [89], Landau and Ginzburg [95] and Cahn and Hilliard [96] we will postulate that the specific free energy of a two-phase system depends on the local value of dryness fraction as well as on its value within the nearest surroundings. Therefore, the Helmholtz potential can be expressed as a sum of two contributions, which are functions of dryness fraction and its gradients, respectively:

$$f = f^h(T,v,x) + f^k(T,v,x,\nabla x,\nabla\nabla x,\ldots,\nabla\cdots\nabla x), \qquad (3.38)$$

where f^h is specific free energy of a uniform system of temperature T, specific volume v and dryness fraction x, while f^k denotes an additional contribution to free energy brought about by the nonuniformity of the field of dryness fraction. In the molecular theory of fluid interfaces given by Bongiorno, Scriven and Davis [97] the homogeneous term describes short-range interactions (repulsive forces), while the gradient term is responsible for long-range interactions (attractive forces). Since the presence of an interface in a small volume of averaging is connected to the occurrence of the gradient $\nabla_n x$ in the direction normal to the interface, then one can assume that the spatial gradient of x is a vectorial measure reflecting energetic contribution of interfacial surfaces. We will expect that the greater the gradient of dryness fraction is, the greater energy characterises the dividing surfaces. The scalar x is a measure of the amount of internal microstructure contained in our fluid, whereas the spatial gradient of x describes capillary properties of the system [16].

Gradient representation of the specific free energy can be obtained by expanding this function about a point in which all the gradients of the dryness fraction vanish. While doing this, it should be assumed that the dryness fraction and its gradient are mutually independent, and the free energy is a continuous function of its parameters. Proceeding as in the case of the stress tensor we obtain the relation:

$$f = L_0 + L_1 \nabla x + L_2 \nabla \nabla x + L_3 \nabla x \otimes \nabla x + L_4 \nabla \nabla \nabla x + L_5 \nabla x \otimes \nabla x \otimes \nabla x, \quad (3.39)$$

in which the coefficients $L_0, \ldots, L_5$ are isotropic tensors dependent on T, v and x, since they are determined by the properties of uniform and isotropic system. The coefficient L_0 is a tensor of zeroth order since energy is a scalar quantity, and it is equal to the specific free energy of a homogeneous system:

$$L_0 = f^h(T, v, x). \quad (3.40)$$

The isotropic tensor of first order L_1 is identically equal zero, like the isotropic tensors of third order L_4 and L_5. Relation (3.39) is then reduced to the following form:

$$f = f^h(T, v, x) + L_2 \nabla \nabla x + L_3 \nabla x \otimes \nabla x. \quad (3.41)$$

Since the coefficients L_2 and L_3 are isotropic tensors of second order, thus they can be expressed as:

$$L_2 = l_2^k I, \quad (3.42)$$

and

$$L_3 = l_3^k I. \quad (3.43)$$

The last two terms on the right-hand side of relation (3.41), as contributions to free energy, are of course scalars and in this connection must be represented by expressions independent of the gradient direction. Based on this physical property of energy we can simplify the last two terms in formula (3.41) and obtain:

$$f = f^h + l_2^k \nabla^2 x + l_3^k (\nabla x)^2. \quad (3.44)$$

A similar form of the specific free energy for two-component systems was obtained by Cahn and Hilliard [96]. From relation (3.44) the following form of the total free energy follows:

$$F = \int_V \left(f^h + l_2^k \nabla^2 x + l_3^k (\nabla x)^2 \right) \rho dV. \quad (3.45)$$

The integral from the second term one can transform in the following way [96]:

$$\int_V \left(\rho l_2^k \nabla^2 x \right) dV = -\int_V \left(\rho \frac{dl_2^k}{dx} (\nabla x)^2 \right) dV + \int_A \left(\rho l_3^k \nabla x \cdot n \right) dA, \quad (3.46)$$

and after the assumption that on the boundary of the region $\nabla x \cdot n = 0$, one can reduce the last term in relation (3.46) and obtain:

$$F = \int_V \left(f^h - \frac{dl_2^k}{dx} (\nabla x)^2 + l_3^k (\nabla x)^2 \right) \rho dV. \quad (3.47)$$

According to the theory of order parameters the term describing the free energy of a homogeneous system is, in the surroundings of equilibrium point, a quartic polynominal. In this connection we can write [16]:

$$f^h = l_1^h x^4 + l_2^h x^2.$$ (3.48)

On the basis of (3.47) and (3.48) the specific free energy f of the nonuniform system can be expressed in the following way:

$$f = l_1^h x^4 + l_2^h x^2 + l^k (\nabla x)^2,$$ (3.49)

where the coefficient controlling the contribution of gradient energy is defined as follows:

$$l^k = l_3^k - \frac{dl_2^k}{dx}.$$ (3.50)

The coefficient l^k is always positive, which means that there exists some energetic price connected with the creation of spatial nonuniformities of a field [98].

3.4. Equilibrium conditions

General definition of equilibrium tells us that in a state of thermodynamic equilibrium the considered system neither interacts with the surroundings nor admits any internal interactions between arbitrary subsystems [40]. With reference to a two-phase water-steam mixture, this definition includes the requirement of preservation of the equilibrium state in each phase as well as the requirement of preservation of equilibrium between individual phases. A homogeneous phase is in equilibrium when the gradients of intensive parameters of state causing temporal variation of extensive parameters do not occur [40]. Physically, this means that all internal transport processes taking place in the fluid ceased. To achieve interfacial equilibrium it is necessary for the interfacial transport of mass, momentum and energy to vanish.

Equilibrium phase transition takes place in a homogeneous way if the following conditions are satisfied [16]:

- equality of temperatures of both phases $T_{liq} = T_{vap}$;
- equality of pressures of both phases $p_{liq} = p_{vap}$;
- equality of the Gibbs free enthalpies of both phases $g_{liq} = g_{vap}$.

In heterogeneous phase transition, when two phases divided by an interface of complex structure are considered, the occurrence of capillary phenomena significantly influences the equilibrium conditions [82]. The influence is stronger at larger dispersion of a new phase, that is in evaporation at smaller dimensions of vapour bubbles. Taking into consideration the surface phenomena the conditions of thermodynamic equilibrium transform into, respectively [16]:

- difference of internal energies of both phases is equal to internal energy of the interface $u_{liq} - u_{vap} = u_{int}$;

- difference of momentum fluxes of both phases in direction perpendicular to the interface is equal to momentum of the interface $p_{liq} - p_{vap} = p_{int}$;

- difference of chemical potentials of both phases in direction perpendicular to the interface is equal to chemical potential of the interface $\mu_{liq} - \mu_{vap} = \mu_{int}$.

Some examples of the extension of equilibrium conditions by capillary effects can be found in the works of Gibbs [81] and Frenkel [99]. For a spherical vapour bubble the condition of mechanical equilibrium is expressed by the relation:

$$p_{liq} - p_{vap} = -\frac{2\sigma}{r},$$ (3.51)

while the condition of phase equilibrium is given as [99]:

$$\mu_{liq} - \mu_{vap} = \frac{2\sigma}{r} v_{vap}.$$ (3.52)

From relation (3.52) it follows that for equilibrium course of mass transfer between water and steam which is created in the form of bubbles, some difference of chemical potentials of both phases is necessary, and the chemical potential of the new phase must always be lower than that of the parent phase. This latter limitation results from the condition of thermodynamic stability since, as it is known, more stable is that phase which in given conditions has lower potential of energy and by the generation of the phase of lower potential the system realises the law of energy minimisation. In the conditions of phase disequilibrium the difference in chemical potentials is larger than in equilibrium and is the driving force (affinity) of mass exchange. For flashing, which proceeds in the conditions of pressure drop, the chemical potentials of water and steam vary along with pressure but until the saturation conditions are not achieved more stable is the liquid phase. After exceeding the saturation pressure the chemical potential of steam is lower than that of liquid water which in this region is in metastable state and sooner or later will become transformed into steam.

Definition of affinity A as a driving force of mass exchange can be obtained from the comparison of the Gibbs equation written for a two-phase system [40]:

$$du = \left(\frac{\partial u}{\partial s}\right)_{v,x} ds + \left(\frac{\partial u}{\partial v}\right)_{s,x} dv + \left(\frac{\partial u}{\partial x}\right)_{s,v} dx,$$ (3.53)

with the First and Second Law of Thermodynamics written for reversible sprocesses [40]:

$$du = Tds - pdv - Adx.$$ (3.54)

As a result of the comparison we obtain:

$$A = -\left(\frac{\partial u}{\partial x}\right)_{s,v}.$$ (3.55)

Equivalent definitions of A as a function of the remaining thermodynamic potentials can be obtained from the Gibbs equation after the application of the Legendere transformations:

$$A = \left(\frac{\partial h}{\partial x}\right)_{s,p} = \left(\frac{\partial f}{\partial x}\right)_{v,T} = \left(\frac{\partial g}{\partial x}\right)_{p,T},$$ (3.56)

where h is specific enthalpy, f – the Helmholtz specific free energy, while g – the Gibbs specific free enthalpy. In thermodynamic equilibrium we have:

$$A = 0,$$ (3.57)

and the equilibrium dryness fraction $\bar{x}$ is a function of the remaining two independent parameters defining thermodynamic state of the system:

$$\bar{x} = \bar{x}(s,v) = \bar{x}(s,p) = \bar{x}(v,T) = \bar{x}(p,T).$$ (3.58)

Now, we can identify the difference in chemical potentials of coexisting phases as a derivative of the Helmholtz thermodynamic potential with respect to the dryness fraction x:

$$A = \left(\frac{\partial f}{\partial x}\right)_{T,v} = \mu_{liq} - \mu_{vap}.$$ (3.59)

However, this definition does not take into account capillary phenomena and refers only to homogeneous systems without interfaces. The formula derived in the previous section for the Helmholtz free energy of heterogeneous systems (3.49) contains a term with the gradient of the dryness fraction. On this basis we extend the definition of the thermodynamic affinity (3.59) onto nonuniform systems and obtain the expression [16]:

$$A = \left(\frac{\delta f}{\delta x}\right)_{T,v},$$ (3.60)

where the Volterra variational derivative is defined in the following way [16]:

$$\frac{\delta f}{\delta x} = \frac{\partial f}{\partial x} - \nabla \cdot \left(\frac{\partial f}{\partial \nabla x}\right).$$ (3.61)

In phase equilibrium the thermodynamic affinity A is equal zero [100]. But it does not mean that the chemical potentials of both phases are equal to each other. In the light of definition (3.61) it is seen that their difference is equal to the chemical potential of the interface, which is represented by the gradient part. Since in the equilibrium state the amount of vapour is equal to its equilibrium value, the equilibrium value of the dryness fraction $\bar{x}$ can be determined from the condition of vanishing of the thermodynamic affinity [101]:

$$A = \left(\frac{\delta f}{\delta x}\right)_{T,v} = 0.$$ (3.62)
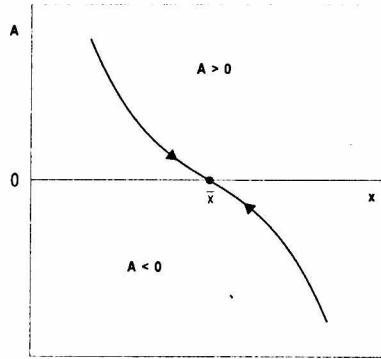
Figure 3.2. *Dependence of thermodynamic affinity on dryness fraction*

Condition (3.62) physically means that at equilibrium point the free energy reaches minimum at fixed other generalised deformations. Pictorial character of dependence of the thermodynamic affinity on the dryness fraction in the vicinity of equilibrium point is presented in Figure 3.2. At points where $x < \bar{x}$ we deal with nonequilibrium evaporation, while at points where $x > \bar{x}$ nonequilibrium condensation occurs.

4. Homogeneous model of flashing flow

4.1. Assumptions of one-dimensional homogeneous model

In the homogeneous approach a nonequilibrium model of two-phase flow consists of balance equations formulated for a two-phase mixture and the balance equation for vapour mass [102]. The latter describes the nonequilibrium character of evaporation in the flow and is postulated in the form of kinetic equation. The homogeneous approach assumes that the considered system is physically homogeneous and each element of the fluid volume contains a medium whose properties are a kind of average of the properties of component fluids. The influence of real heterogeneous structure of the two-phase system is modelled in constitutive equations postulated for the mixture of the two phases [103].

The most important assumptions taken in the proposed here one-dimensional homogeneous model are as follows [102]:

- velocity vector components perpendicular to the flow axis are neglected:

$$w_x = w_y = 0,$$

$$w_z = w;$$

- no slip between phases:

$$w_{liq} = w_{vap} = w;$$

- axial velocity gradients in directions perpendicular to the flow axis are omitted:

$$\frac{\partial w}{\partial x} = \frac{\partial w}{\partial y} = 0;$$

- thermal parameters gradients in directions perpendicular to the flow axis are omitted:

$$\frac{\partial T}{\partial x} = \frac{\partial T}{\partial y} = 0;$$

- heat conduction along the channel is negligible:

$$q_z = 0;$$

- pressure of the liquid is equal to that of the vapour:

$$p_{liq} = p_{vap} = p;$$

- liquid is metastable:

$$T_{liq} = T_{liq}\left(p, h_{liq}\right),$$

$$h_{liq} = h_{liq}\left(p, v_{liq}\right);$$

- vapour is saturated:

$$T_{vap} = T_{sat}\left(p\right),$$

$$h_{vap} = h_{vap}\left(p\right);$$

- flow is adiabatic:

$$q_{ext} = 0.$$

The model proposed in this work describes two-phase turbulent flows in annular channels with constant or slowly varying cross-sectional area. A two-phase flow in an axisymmetric channel with annular cross-section is, in general, a two-dimensional problem [72]. A confirmation of this is the possibility of creation in the divergent section of a nozzle the *jet* structure [27] and the existence of transverse profiles of void fraction [27, 31] and density [28]. But, both single and two-phase flows can be accurately described by means of one-dimensional balance equations closed by empirical constitutive relations. Nevertheless, nonuniform profiles of void fraction and velocity can influence the comparisons of one-dimensional models with experimental data [18]. For example, accelerational pressure drop is strongly

influenced by the existence of transverse profiles of void fraction and velocity. One-dimensional model of a two-phase flow treating the water-steam mixture as a nonequilibrium homogeneous system is the simplest model taking into account thermodynamic nonequilibrium between phases [47], accurately describes flashing flows in nozzles [104-107] and gives a possibility of the modelling of capillary phenomena. According to the classification given by Mikielewicz [103] it is thermomechanical model since it takes advantage of balance equation for mass, momentum and energy of the mixture. Such models are used when thermal effects are coupled with mechanical ones [103].

4.2. One-dimensional balance equations

4.2.1. Mass balance of the mixture

The principle of mass conservation tells that temporal change (substantial derivative) of mass in a fluid volume is equal zero [33]. It allows to formulate a differential form of the balance equation of mass of the two-phase mixture:

$$\frac{\partial \rho}{\partial t} + w \nabla \rho + \rho \nabla \cdot w = 0, \qquad (4.1)$$

from which one can obtain a conservative form:

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho w) = 0. \qquad (4.2)$$

This is the local formulation of the conservative property of matter. A one-dimensional equation of mass balance we obtain after integration and averaging of Equation (4.2) according to the procedure presented by Bilicki [108]. As a result we obtain:

$$A \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(A \rho w) = 0. \qquad (4.3)$$

Dependent variables appearing in this equation are quantities averaged over the cross-sectional of the channel. Performing differentiation and dividing by A we obtain the final form of one-dimensional balance equation for mass of the mixture:

$$\frac{\partial \rho}{\partial t} + w \frac{\partial \rho}{\partial z} + \rho \frac{\partial w}{\partial z} = -\frac{\rho w}{A} \frac{dA}{dz}. \qquad (4.4)$$

4.2.2. Momentum balance of the mixture

From the principle of momentum conservation it is known that temporal change of momentum in an arbitrary fluid volume is equal to the sum of body forces acting on this volume, and surface forces acting on the fluid surface [33]. On this basis one obtains a differential form of momentum balance of the two-phase mixture:

$$\rho\left(\frac{\partial w}{\partial t}+w\nabla w\right)=\rho b+\nabla\cdot T, \tag{4.5}$$

which, on the basis of the equation of mass balance (4.2), can be transformed to a conservative form:

$$\frac{\partial}{\partial t}(\rho w)+\nabla\cdot(\rho w\otimes w)-\nabla\cdot T=\rho b. \tag{4.6}$$

One dimensional equation of momentum balance is obtained after integration and averaging of Equation (4.6):

$$A\frac{\partial}{\partial t}(\rho w)+\frac{\partial}{\partial z}(A\rho w^2)+A\frac{\partial}{\partial z}(p+p^k+p^v)+C\tau=-A\rho g\cos\chi. \tag{4.7}$$

In this equation the body force was expressed by the product of density ρ and gravitational acceleration g, p^k denotes capillary pressure, p^v – viscous pressure, while χ – inclination angle of the channel. Shear stresses arising due to viscosity and capillarity forces are replaced by friction force τ on the channel wall.

So far our analysis was resolved to geometrical simplifications, that is to the reduction of the three-dimensional equation of momentum balance (4.6) to the one-dimensional Equation (4.7). In one-dimensional models normal shear stresses expressed by the gradient of velocity are usually neglected. Neglecting also the capillary shear stresses included in the friction force, Equation (4.7) can be written as:

$$\frac{\partial}{\partial t}(\rho w)+\frac{1}{A}\frac{\partial}{\partial z}(A\rho w^2)+\frac{\partial p}{\partial z}+\frac{\partial p^k}{\partial z}=-\rho g\cos\chi-\tau_{TP}. \tag{4.8}$$

Taking into account equation of mass balance (4.3) we obtain the final form of one-dimensional momentum balance:

$$\rho\frac{\partial w}{\partial t}+\rho w\frac{\partial w}{\partial z}+\frac{\partial p}{\partial z}+\frac{\partial p^k}{\partial z}=-\rho g\cos\chi-\tau_{TP}. \tag{4.9}$$

4.2.3. Energy balance of the mixture

The principle of energy conservation says that temporal change of total energy in a fluid volume is equal to the sum of the power of body forces, surface forces and the flux of energy supplied to the volume. From this the differential form of the equation of energy balance follows:

$$\rho\frac{\partial}{\partial t}\left(u+\frac{w^2}{2}\right)+\rho w\nabla\left(u+\frac{w^2}{2}\right)=\rho b\cdot w+\nabla\cdot(Tw)-\nabla\cdot q, \tag{4.10}$$

from which, having taken into account the equation of mass balance (4.2), the following conservative form follows:

$$\frac{\partial}{\partial t}\left(\rho u + \frac{\rho w^2}{2}\right) + \nabla \cdot \left(\rho w u + \rho w \frac{w^2}{2}\right) - \nabla \cdot (Tw) + \nabla \cdot q = \rho b \cdot w. \quad (4.11)$$

One-dimensional equation of total energy balance is obtained after integration and averaging of Equation (4.11):

$$A\frac{\partial}{\partial t}\left(\rho u + \frac{\rho w^2}{2}\right) + \frac{\partial}{\partial z}\left(A\rho w\left(u + \frac{w^2}{2}\right)\right) +$$
$$+ \frac{\partial}{\partial z}\left(Aw(p + p^k + p^v)\right)\frac{\partial}{\partial z}(Aq) = -A\rho g w \cos\chi. \quad (4.12)$$

Neglecting, as in momentum balance, the viscous normal pressure p^v and according to the model assumption the heat flux q, we obtain from Equation (4.12) the following relation:

$$A\frac{\partial}{\partial t}\left(\rho u + \frac{\rho w^2}{2}\right) + \frac{\partial}{\partial z}\left(A\rho w\left(u + \frac{w^2}{2}\right)\right) + \frac{\partial}{\partial z}\left(Aw(p + p^k)\right) = -A\rho g w \cos\chi. \quad (4.13)$$

Taking into consideration the identically satisfied equations of mass balance (4.3) and momentum balance (4.8) we obtain a one-dimensional equation of internal energy conservation:

$$A\rho\frac{\partial u}{\partial t} + A\rho w\frac{\partial u}{\partial z} + (p + p^k)\frac{\partial}{\partial z}(Aw) = A\tau_{TP}w. \quad (4.14)$$

Replacing internal energy by enthalpy we finally obtain equation of energy balance in the form of one-dimensional equation of enthalpy balance:

$$\rho\frac{\partial h}{\partial t} + \rho w\frac{\partial h}{\partial z} - \frac{\partial p}{\partial t} - w\frac{\partial p}{\partial z} - \frac{\partial p^k}{\partial t} - w\frac{\partial p^k}{\partial z} = \tau_{TP}w. \quad (4.15)$$

4.2.4. Mass balance of the vapour phase

The mass of vapour phase in a unit volume can be expressed as a product ρx. Balancing this quantity in a control volume V and taking into account internal sources one obtains after transformations a differential equation of balance of the vapour mass:

$$\frac{\partial}{\partial t}(\rho x) + \nabla \cdot (\rho x w) = \Gamma_{vap}. \quad (4.16)$$

Performing the procedure of averaging we obtain a one-dimensional equation of balance of the vapour phase:

$$A\frac{\partial}{\partial t}(\rho x) + \frac{\partial}{\partial z}(A\rho x w) = A\Gamma_{vap}, \quad (4.17)$$

from which we can eliminate the identically satisfied equation of mass balance (4.3) and dividing by ρ we obtain:

$$\frac{\partial x}{\partial t} + w\frac{\partial x}{\partial z} = \frac{\Gamma_{vap}}{\rho}. \tag{4.18}$$

4.3. Constitutive equations

4.3.1. The equation of state

As it is known form the classical thermodynamics of equilibrium processes (called by Truesdell thermostatics) the equation of state constitutes a functional relationship between one dependent variable and n independent variables in a state of thermodynamic equilibrium [109]. In a case of the fundamental equation of state for internal energy u we have the relation:

$$u = u(s, v), \tag{4.19}$$

in which s and v denote equilibrium specific entropy and specific volume of a system, respectively. These two quantities completely determine the thermodynamic state of the system and the knowledge of explicit form of the function of internal energy (4.19) allows to determine uniquely all thermodynamic parameters of the system [110].

Observation shows that systems with internal structure, as a water-steam mixture, possess an additional parameter (internal variable) entering the equation of state. For the water-steam mixture considered in this work, the dryness fraction x is such a parameter. However, there arises a question how to determine the properties of the two-phase system being in thermodynamic nonequilibrium?

An answer to this question can be found in internal variables theory, in which the so-called frozen equilibrium state corresponding to a given nonequilibrium state is defined [45]. The corresponding equilibrium state is reached from the nonequilibrium state in adiabatic way at constant specific volume v and constant dryness fraction x preserving the same flow velocity w. It follows from this that internal energies of both states are equal to each other. On the basis of the rule of local state [110] we know that intensive properties and entropy in a nonequilibrium state are the same as in the accompanying equilibrium state. Since in equilibrium the fundamental equation of state exists, then it must be also satisfied in the nonequilibrium state. Thus, for our nonequilibrium water-steam system we have [111]:

$$u = u(s, v, x), \tag{4.20}$$

where all the quantities appearing in this equation are nonequilibrium properties. Physically this means that in a nonequilibrium state an equation of state exists, that is the same relationship between thermodynamic parameters like in equilibrium. Having in mind that our considerations concern a nonuniform system and we postulate the inclusion of the dryness fraction gradients in the Helmholtz potential, the fundamental Equation (4.20) should be rather written in the following way:

$$u = u(s, v, x, \nabla x). \tag{4.21}$$

From the balance equations of our model it follows that a thermodynamic closure in the form of thermal equation of state for the density ρ of the two-phase mixture is required. As it is known, the density consists of densities of water, steam and interfacial surfaces. Therefore, the density of the two-phase system can be expressed by the relation:

$$\frac{1}{\rho} = v = x v_{vap} + (1 - x - y) v_{liq} + y v_{int}, \tag{4.22}$$

in which y stands for the mass fraction of interfacial areas.

According to the model assumption on thermodynamic equilibrium of the vapour phase, we can write the thermal equation of state for the vapour in the form:

$$v_{vap} = v_{vap}(p), \tag{4.23}$$

while for the superheated liquid we have the relation:

$$v_{liq} = v_{liq}(p, h_{liq}), \tag{4.24}$$

where the existence of an equation of state for liquid in the metastable state was assumed. As it is seen from relation (4.24), to calculate specific volume of the liquid we must know its pressure and enthalpy. The pressure, as a component of the state vector, is known from the balance equations, while the enthalpy of water can be calculated from the caloric equation of state of the two-phase system:

$$h = x h_{vap} + (1 - x - y) h_{liq} + y h_{int}. \tag{4.25}$$

The caloric equation of state of the vapour in equilibrium takes the form:

$$h_{vap} = h_{vap}(p). \tag{4.26}$$

In two-phase flow theory, the mass of interfacial regions is assumed to be negligible [35]. In this connection we can write:

$$y \approx 0, \tag{4.27}$$

and calculate the enthalpy of water on the basis of equation (4.25):

$$h_{liq} = \frac{h - x h_{vap}(p)}{1 - x}. \tag{4.28}$$

Finally, the thermal equation of state of the nonequilibrium two-phase system assumes the following form:

$$\frac{1}{\rho} = x v_{vap}(p) + (1 - x) v_{liq}(p, h_{liq}(p, h, x)). \tag{4.29}$$

It should be noticed that the capillary effects are not taken into consideration while calculating the thermodynamic properties of the system. The enthalpy of interfacial

surfaces, which, according to the theory presented in Chapter 3, should be described by the gradients of the dryness fraction, is neglected. Also the mass of interfaces is neglected due to their microscopic size. Values of the thermodynamic functions of water and steam in saturation and metastable region are calculated on the basis of steam tables worked out in the form of numerical procedures by Kardas and Bilicki [112].

4.3.2. Volumetric source of vapour mass

The process of nonequilibrium vapour generation, being an irreversible thermodynamic process, can be described by making use of the general rules of nonequilibrium thermodynamics. The thermodynamics of nonequilibrium processes considers irreversible phenomena taking place in homogeneous systems and describes them by phenomenological equations relating generalised fluxes with generalised thermodynamic forces [41]. Among such a class of phenomena the process of relaxation of an order parameter describing the thermodynamic state of a system can be numbered. The order parameter, entering the fundamental equation of state, must be a measurable quantity but cannot be controlled and take part in external work of the system. For evaporation, the nonequilibrium dryness fraction is such a parameter since it meets all the requirements laid down to order parameters [42].

The balance equation of vapour mass (4.18) is at the same time an evolution equation for the nonequilibrium dryness fraction x. The dryness fraction plays here a role of an order parameter (internal variable) and due to the occurrence of the source term on the right-hand side of Equation (4.18) it is a non-conserved order parameter. Description of the evolution of this parameter requires an additional constitutive equation which gives an explicit form of the source Γ_{vap}. Some instructions on the construction of such terms are provided by the internal variables theory [113]. In this method, the kinetics of the evolution of an order parameter is dependent on the thermodynamic components of the state vector and on generalised forces. Internal variables satisfy first order differential equations with respect to time, which can be written in the form [42]:

$$\dot{x} = f(T, v, x, \nabla T, \nabla v, \nabla x, \ldots).\qquad(4.30)$$

In various physical situations the general relationship (4.30) assumes the form of linear equation:

$$\dot{x} = f(T, v, x)A.\qquad(4.31)$$

In accordance with the presented theory the evolution equation for the nonequilibrium dryness fraction takes the form:

$$\frac{\partial x}{\partial t} = \frac{\Gamma_{vap}}{\rho},\qquad(4.32)$$

where ρ is density of a two-phase mixture, and Γ_{vap} – volumetric rate of vapour generation. Linear phenomenological equation for the rate of vapour generation is given as [41]:

$$\Gamma_{vap} = -l\frac{A}{T}, \tag{4.33}$$

where A denotes thermodynamic affinity, and l is a phenomenological coefficient. Hence Equation (4.32) assumes the form:

$$\frac{\partial x}{\partial t} = -\frac{lA}{\rho T}. \tag{4.34}$$

In the above equation the thermodynamic affinity A is this generalised force which drives the vapour generation. Physically, vapour production is a result of interfacial mass exchange controlled by the difference in chemical potentials of both phases. For this reason, the generalised thermodynamic force is equal to the difference in chemical potentials, and under definition (3.56) also to the derivative of the Helmholtz free energy over the dryness fraction. Since in the present work the nonlocal definition of the free energy is proposed, which is expressed with the help of the dryness fraction and its gradients, thus, consequently, one proposes a generalisation of the definition of the thermodynamic affinity:

$$A = \left(\frac{\delta f}{\delta x}\right)_{T,v}, \tag{4.35}$$

where $\delta/\delta x$ is Volterra variational derivative [16]:

$$\frac{\delta f}{\delta x} = \frac{\partial f}{\partial x} - \nabla \cdot \left(\frac{\partial f}{\partial \nabla x}\right). \tag{4.36}$$

Taking into account relation (4.35) we can write the source of vapour in the form of the Ginzburg-Landau equation [114]:

$$\Gamma_{vap} = -\frac{l}{T}\frac{\delta f}{\delta x}. \tag{4.37}$$

On the basis of formula (4.36) and from the relation for the Helmholtz free energy derived in Section 3.3 we conclude that its derivative in the surroundings of an equilibrium point is a function of the dryness fraction and its gradients, which can be generally expressed as follows:

$$\frac{\delta f}{\delta x} = f_1\left(x, x^2, x^3, \ldots, x^n\right) - \nabla \cdot f_2\left(\nabla x, (\nabla x)^2, (\nabla x)^3, \ldots, (\nabla x)^n,\right.$$
$$\left. \nabla^2 x, (\nabla^2 x)^2, (\nabla^2 x)^3, \ldots, (\nabla^2 x)^n, \ldots \nabla^m x, (\nabla^m x)^2, (\nabla^m x)^3, \ldots, (\nabla^m x)^n\right). \tag{4.38}$$

Here it was assumed, like in Section 3.3, that the dryness fraction and its gradient are independent variables. Expanding the function f_1 in the surroundings of the equilibrium point $x = \bar{x}$ we obtain:

$$f_1 = \frac{\partial f}{\partial x} = \frac{\partial f}{\partial x}\Big|_{v,T}^{e} + \frac{\partial^2 f}{\partial x^2}\Big|_{v,T}^{e}(x-\bar{x}) + \frac{\partial^3 f}{\partial x^3}\Big|_{v,T}^{e}(x-\bar{x})^2 + \frac{\partial^4 f}{\partial x^4}\Big|_{v,T}^{e}(x-\bar{x})^3 + \ldots$$

$$+ \frac{\partial^n f}{\partial x^n}\Big|(x-\bar{x})^{n-1} + \frac{\partial^{n+1} f}{\partial x^{n+1}}\Big|_{v,T}^{e}(x-\bar{x})^n .$$

(4.39)

In a state of phase equilibrium the nonequilibrium dryness fraction x attaines its equilibrium value $\bar{x}$ and the vapour generation is stopped. In this connection, the derivative of the Helmholtz potential over x must vanish. Since in expression (4.39) all the terms dependent on the difference $x - \bar{x}$ are equal to zero, then the free term must also vanish. Moreover, owing to the fact that the Helmholtz potential is described by a fourth order polynominal, all the derivatives of order higher than four are equal to zero and due to this all the terms in which these derivatives are factors vanish. One should also notice that all the terms appearing in expression (4.39) should depend on the sign of the difference $x - \bar{x}$, since for $x - \bar{x} < 0$ we have nonequilibrium evaporation and the amount of vapour must increase $\Gamma_{vap} > 0$, while for $x - \bar{x} > 0$ nonequilibrium condensation occurs and the amount of vapour decreases $\Gamma_{vap} < 0$. Owing to this, in formula (4.39) only terms containing even powers of the difference $x - \bar{x}$ can occur. Taking into account the above considerations of physical nature we can simplify formula (4.39) to the following form:

$$\frac{\partial f}{\partial x} = \frac{\partial^2 f}{\partial x^2}\Big|_{v,T}^{e}(x-\bar{x}) + \frac{\partial^4 f}{\partial x^4}\Big|_{v,T}^{e}(x-\bar{x})^3 .$$

(4.40)

Expanding similarly the function f_2 one obtains the relation:

$$f_2 = \frac{\partial f}{\partial \nabla x} = \frac{\partial f}{\partial \nabla x}\Big|_{v,T}^{e} + \frac{\partial^2 f}{\partial(\nabla x)^2}\Big|_{v,T}^{e}(\nabla x - \nabla \bar{x}) + \frac{\partial^3 f}{\partial(\nabla x)^3}\Big|_{v,T}^{e}(\nabla x - \nabla \bar{x})^2 + \ldots$$

$$+ \frac{\partial^{n+1} f}{\partial(\nabla x)^{n+1}}\Big|_{v,T}^{e}(\nabla x - \nabla \bar{x})^n + \frac{\partial f}{\partial \nabla^2 x}\Big|_{v,T}^{e} + \frac{\partial^2 f}{\partial(\nabla^2 x)^2}\Big|_{v,T}^{e}(\nabla^2 x - \nabla^2 \bar{x}) +$$

$$+ \frac{\partial^3 f}{\partial(\nabla^2 x)^3}\Big|_{v,T}^{e}(\nabla^2 x - \nabla^2 \bar{x})^2 + \ldots + \frac{\partial^{n+1} f}{\partial(\nabla^2 x)^{n+1}}\Big|_{v,T}^{e}(\nabla^2 x - \nabla^2 \bar{x})^n + \ldots$$

(4.41)

$$+ \frac{\partial^2 f}{\partial(\nabla^m x)^2}\Big|_{v,T}^{e}(\nabla^m x - \nabla^m \bar{x}) + \frac{\partial^3 f}{\partial(\nabla^m x)^3}\Big|_{v,T}^{e}(\nabla^m x - \nabla^m \bar{x})^2 + \ldots$$

$$+ \frac{\partial^{n+1} f}{\partial(\nabla^m x)^{n+1}}\Big|_{v,T}^{e}(\nabla^m x - \nabla^m \bar{x})^n ,$$

which, after performing the considerations given above, can be reduced to the following form:

$$\frac{\partial f}{\partial \nabla x} = \frac{\partial^2 f}{\partial (\nabla x)^2}\bigg|_{v,T}^{e} (\nabla x - \nabla \bar{x}).$$
(4.42)

Inserting expressions (4.40) and (4.42) into formula (4.38) we find:

$$\frac{\delta f}{\delta x} = \frac{\partial^2 f}{\partial x^2}\bigg|_{v,T}^{e}(x - \bar{x}) + \frac{\partial^4 f}{\partial x^4}\bigg|_{v,T}^{e}(x - \bar{x})^3 + \frac{\partial^2 f}{\partial (\nabla x)^2}\bigg|_{v,T}^{e}(\nabla \cdot \nabla x - \nabla \cdot \nabla \bar{x}).$$
(4.43)

Inserting the above relation to the Ginzburg-Landau Equation (4.37) and taking into account the assumption of one-dimensional flow, we obtain the searched formula for the volumetric vapour generation:

$$\Gamma_{vap} = -\frac{l}{T}\left(f_1^1(x - \bar{x}) + f_1^3(x - \bar{x})^3 - f_{22}^1 \frac{\partial^2(x - \bar{x})}{\partial z^2} \right),$$
(4.44)

where the following substitutions were done:

$$f_1^1 = \frac{\partial^2 f}{\partial x^2}\bigg|_{v,T}^{e},$$
(4.45)

$$f_1^3 = \frac{\partial^4 f}{\partial x^4}\bigg|_{v,T}^{e},$$
(4.46)

$$f_{22}^1 = \frac{\partial^2 f}{\partial (\nabla x)^2}\bigg|_{v,T}^{e}.$$
(4.47)

On the basis of formula (4.44) the change of the dryness fraction x can be expressed by the following equation [115]:

$$\frac{\Gamma_{vap}}{\rho} = -\frac{x - \bar{x}}{\beta} - \frac{(x - \bar{x})^3}{\gamma} + \kappa \frac{\partial^2(x - \bar{x})}{\partial z^2},$$
(4.48)

where:

$$\beta = \frac{\rho T}{l f_1^1},$$
(4.49)

$$\gamma = \frac{\rho T}{l f_1^3},$$
(4.50)

$$\kappa = \frac{l f_{22}^1}{\rho T}. \tag{4.51}$$

Equation (4.48) describes the source of mass of the vapour phase with the help of two relaxation terms with two relaxation times β and γ, as well as the gradient term with capillarity coefficient κ. Thus, we have strong (scalar) and weak (differential) interactions. The gradient term has its physical origin in nonuniformity of the field of the dryness fraction within the interfacial region and models an energy excess connected with capillary interactions. This excess energy is modelled, on macroscopic level, with the help of the derivative of the dryness fraction along the flow, while, on microscopic level, its origin is the variation of the dryness fraction across the interfacial region. The capillarity coefficient κ controls the contribution of the gradient energy and on this basis we can conclude that it depends on the surface tension. From a mathematical point of view the gradient term results from the nonlocal definition of the free energy of the two-phase system.

4.3.3. Shear stresses

Experiments show that for any mass flow rate in a channel of any geometry the frictional pressure drop in a two-phase mixture is larger than that in a single-phase flow of the same mass flow rate [18]. It results from an increase of the flow resistance due to the generation of vapour bubbles on the channel walls.

In friction model we assume that shear stresses in a two-phase flow are a linear function of stresses which would occur in a liquid flow with the same mass flow rate. This assumption can be written as follows [116]:

$$\tau_{TP} = \phi \tau_{liq}, \tag{4.52}$$

where a two-phase multiplier ϕ is a local drag coefficient of two-phase flow related with the increase of the flow resistance due to the appearance of vapour bubbles, τ_{TP} denotes shear stresses in tow-phase flow, while τ_{liq} stands for wall shear stresses in the liquid flow. It is classically assumed that the value of these stresses is proportional to the kinetic energy of the system and can be calculated from the following formula:

$$\tau_{liq} = \frac{1}{2} \frac{C}{A} f \rho_{liq} w_{liq}{}^2, \tag{4.53}$$

in which C denotes channel perimeter, f – the friction factor dependent on the Reynolds number, ρ_{liq} – liquid density, and w_{liq} – liquid velocity. Equation (4.53) defines the so-called volumetric friction force, and the multiplier C/A is a result of averaging of three-dimensional momentum equation. Taking advantage of the assumption of equal mass flow rates of liquid and liquid-vapour mixture we can write:

$$\rho w = \rho_{liq} w_{liq}, \tag{4.54}$$

from which we obtain a formula for liquid velocity:

$$w_{liq} = \frac{w\rho}{\rho_{liq}}.$$

(4.55)

Inserting the above relation into formula (4.53) we obtain a formula for the friction force in single-phase flow:

$$\tau_{liq} = \frac{1}{2}\frac{C}{A}f\frac{\rho^2 w^2}{\rho_{liq}}.$$

(4.56)

The friction factor f is calculated on the basis of the Blasius [117] formula derived for smooth pipes:

$$f = 0.0791\,\mathrm{Re}_{liq}^{-0.25},$$

(4.57)

where Re_{liq} is the liquid Reynolds number. The two-phase flow multiplier ϕ is a function of the flow structure and depends on the dryness fraction, density and viscosity of the system. Its value can be calculated using the Beattie [11] theory according to the following formulae:

bubbly flow $\alpha < 0.3$:

$$\phi = \left[1 + x\left(\frac{\rho_{liq}}{\rho_{vap}} - 1\right)\right]^{0.8}\left[1 + x\left(\frac{\left(3.5\rho_{vap} + 2\eta_{liq}\right)\rho_{liq}}{\left(\eta_{vap} - \eta_{liq}\right)\rho_{vap}} - 1\right)\right]^{0.2},$$

(4.58)

bubbly-slug flow $0.3 \le \alpha < 0.8$:

$$\phi = \left[1 + x\left(\frac{\rho_{liq}}{\rho_{vap}} - 1\right)\right]^{0.8}\left[1 + x\left(\frac{3.5\rho_{liq}}{\rho_{vap}} - 1\right)\right]^{0.2},$$

(4.59)

slug-droplet flow $0.8 \le \alpha < 0.95$:

$$\phi = \left[1 + x\left(\frac{\rho_{liq}}{\rho_{vap}} - 1\right)\right]^{0.8}\left[1 + x\left(\frac{\eta_{vap}\rho_{liq}}{\eta_{liq}\rho_{vap}} - 1\right)\right]^{0.2},$$

(4.60)

droplet flow $\alpha \ge 0.95$:

$$\phi = \left[\frac{\eta_{vap}}{\eta_{liq}}\right]^{0.2}\left[\frac{\rho_{vap}}{\rho_{liq}}\right]^{0.8}\left[1 + x\left(\frac{\rho_{liq}}{\rho_{vap}} - 1\right)\right]^{1.8}.$$

(4.61)

4.3.4. Capillary pressure

According to relation (3.24) normal capillary pressures can be defined as follows:

$$p_{ii}^{k} = -\left(l_2 \sum_{j=1}^{3} \frac{\partial^2 x}{\partial z_j^2} + l_4 \sum_{j=1}^{3} \left(\frac{\partial x}{\partial z_j} \right)^2 \right) \delta_{ii} - l_3 \frac{\partial^2 x}{\partial z_i^2} - l_5 \left(\frac{\partial x}{\partial z_i} \right)^2 . \tag{4.62}$$

From the above relation it can be seen that the capillary pressures are described by the terms with the dryness fraction gradients. Their contribution is controlled by capillarity coefficients which, as it was shown in Section 3.2, are closely related to the surface tension of a flat interface.

In order to describe capillary phenomena in one-dimensional approach, some simplifications are proposed. First of all, in such an approach the capillary pressure can be expressed by the derivatives of the dryness fraction in flow direction only. Since in one-dimensional approach the anisotropy of normal stresses is lost, thus, as it is done with pressure in isotropic systems, we propose to replace the spherical tensor of capillary pressures by the following isotropic tensor;

$$\boldsymbol{p}^k = p^k \boldsymbol{I} = \frac{1}{3} \left(p_{xx}^k + p_{yy}^k + p_{zz}^k \right) \boldsymbol{I} , \tag{4.63}$$

and to express the capillary pressure by squared derivative of the dryness fraction along flow direction:

$$p^k = -k \left(\frac{\partial x}{\partial z} \right)^2 . \tag{4.64}$$

Such a physical simplification allows to describe capillary effects with the use of a single phenomenological coefficient of capillarity k which controls the contribution of the surface tension forces to the stress tensor and possesses clear physical sense.

4.4. Free parameters of the model

The presented mathematical model of flashing flow has four free parameters. These are phenomenological coefficients of proportionality which model the properties of heterogeneous two-phase system on macroscopic level and originate from phenomena taking place on microscopic level.

Three free parameters appear in the expression for the volumetric source of vapour mass (4.48). These are the linear relaxation time β, the non-linear relaxation time γ and the energetic capillarity coefficient κ. The linear relaxation time β according to definition (4.49):

$$\beta = \frac{\rho T}{l f_1^1} ,$$

is a function of density, temperature, kinetic coefficient l describing dissipative effects of relaxation and a constant f_1^1 dependent on the coefficients appearing in

the expansion of the Helmholtz free energy of a uniform system in a Taylor series. This constant can be calculated from relation (4.45) after taking into consideration the expression for the free energy of a uniform system (3.49):

$$f_1^1 = 12 l_1^h x^2 \Big|_{v,T}^e + 2 l_2^h . \tag{4.65}$$

Thus, theoretical calculation of the relaxation time β requires the knowledge of three constants: l, l_1^h and l_2^h, which are difficult to determine. The constant l_2^h determines the contribution of the leading quadratic term in the expression for the Helmholtz potential. It can assume only positive values, since otherwise the parent phase would be unstable [114]. Such a situation takes place in the critical point where fluids change their state of aggregation under the influence of infinitesimal perturbations. Thus, while approaching the critical point the value of l_2^h should decrease to zero and above this point it should be negative. In the theory of phase transitions it is assumed that the coefficient l_2^h strongly depends on temperature [118], while the coefficient l_1^h – weakly. Thus, it is seen that the relaxation time β given by relation (4.49) strongly depends on temperature. For practical calculations the usage of the following empirical formula is proposed [16]:

$$\beta = \frac{T_c - T_0}{T_c - T_{sat}} [s], \tag{4.66}$$

which gives good results in calculations of two-phase water-steam flows.

The non-linear relaxation time γ, according to definition (4.50), can be expressed as follows:

$$\gamma = \frac{\rho T}{l f_1^3},$$

where the coefficient f_1^3 is calculated from the formula:

$$f_1^3 = 24 l_1^h \tag{4.67}$$

Similarly to this coefficient is a function of density, temperature, the coefficient and the constant l_1^h. This constant is usually assumed to depend on temperature weakly [118]. Since also the temperature itself varies slightly in the considered flows, we will assume that the non-linear relaxation time is constant and its value will be determined in parametric analysis.

The third free parameter in the constitutive equation for the source of vapour is the energetic coefficient of capillarity κ. It was defined by formula (4.51) as:

$$\kappa = \frac{l f_{22}^1}{\rho T},$$

from which it can be seen that it also depends on density, temperature, the relaxation coefficient and the constant f_{22}^1. This constant, according to definition (4.47) and the expression for the Helmholtz free energy, is defined in the following way:

$$f_{22}^1 = 2l^k, \tag{4.68}$$

from which it is evident that it depends on the coefficient l^k controlling the contribution of the gradient energy. Since we do not have any phenomenological theory allowing us to determine both l^k and l, we propose to determine the value of the whole coefficient κ by fitting numerical results to experimental profiles.

The last free parameter of our model is the mechanical coefficient of capillarity k. It appears in the momentum balance equation and controls the contribution of reversible capillary stresses in the stress tensor. According to relation (4.63) the capillary pressure can be written as follows:

$$p^k = \frac{1}{3}\left(p_{xx}^k + p_{yy}^k + p_{zz}^k\right), \tag{4.69}$$

from which, after taking into account formulae (4.62) and (4.64) as well as the assumption on one-dimensional flow, we have:

$$k = \frac{\left(l_2 + \frac{1}{3}l_3\right)\dfrac{\partial^2 x}{\partial z^2}}{\left(\dfrac{\partial x}{\partial z}\right)^2} + l_4 + \frac{1}{3}l_5 . \tag{4.70}$$

As in the case of previous coefficients, we have to determine the value of the coefficient k in terms of four unknown parameters $l_2,\ldots, l_5$, when lacking an appropriate theory for their determination. Also in this case the only solution is to determine the global value of k by comparisons with experiment.

4.5. List of the model equations

The proposed mathematical model of flashing flow is a homogeneous model, which takes into consideration the thermodynamic nonequilibrium between phases as well as the capillary effects resulting from a nonuniformity of the two-phase system. The capillary effects were taken into account above all in the equation describing nonequilibrium vapour generation, since despite the possibility of neglecting the thermodynamic properties of interfacial areas, one should take into consideration their influence on the course of phase transition [119]. Reversible capillary stresses were included in the stress tensor and the terms representing this kind of stresses occur in the balance equations for momentum and energy. Taking advantage of the generally accepted simplifying assumptions [35] we neglected mass, momentum and kinetic energy of interfaces. Those assumptions have physical justification in a negligible small mass of the interfacial areas.

The mathematical model consists of the following balance equations:

- mass of the mixture

$$\frac{\partial \rho}{\partial t} + w\frac{\partial \rho}{\partial z} + \rho\frac{\partial w}{\partial z} = -\frac{\rho w}{A}\frac{dA}{dz}; \tag{4.71}$$

- momentum of the mixture

$$\rho\frac{\partial w}{\partial t}+\rho w\frac{\partial w}{\partial z}+\frac{\partial p}{\partial z}+\frac{\partial p^{k}}{\partial z}=-\rho g\cos\chi-\tau_{TP}\ ; \tag{4.72}$$

- energy of the mixture

$$\rho\frac{\partial h}{\partial t}+\rho w\frac{\partial h}{\partial z}-\frac{\partial p}{\partial t}-w\frac{\partial p}{\partial z}-\frac{\partial p^{k}}{\partial t}-w\frac{\partial p^{k}}{\partial z}=\tau_{TP}w\ ; \tag{4.73}$$

- mass of vapour

$$\frac{\partial x}{\partial t}+w\frac{\partial x}{\partial z}=\frac{\Gamma_{vap}}{\rho}\ ; \tag{4.74}$$

and of constitutive equations providing relations for the following quantities:

- density of the two-phase mixture

$$\frac{1}{\rho}=xv_{vap}(p)+(1-x)v_{liq}\big(p,h_{liq}(p,h,x)\big); \tag{4.75}$$

- specific enthalpy of water

$$h_{liq}=\frac{h-xh_{vap}(p)}{1-x}\ ; \tag{4.76}$$

- source of vapour mass

$$\frac{\Gamma_{vap}}{\rho}=-\frac{x-\bar{x}}{\beta}-\frac{(x-\bar{x})^{3}}{\gamma}+\kappa\frac{\partial^{2}(x-\bar{x})}{\partial z^{2}}\ ; \tag{4.77}$$

- friction force

$$\tau_{TP}=\frac{1}{2}\frac{C}{A}\dot{\phi}f\frac{\rho^{2}w^{2}}{\rho_{liq}}\ ; \tag{4.78}$$

- capillary pressure

$$p^{k}=-k\left(\frac{\partial x}{\partial z}\right)^{2}. \tag{4.79}$$

The state vector comprises the following fluid-flow and thermodynamic parameters:

$$\sigma=\left\{\begin{array}{c}w\\p\\h\\x\end{array}\right\}. \tag{4.80}$$

5. Wave properties of the model

5.1. Wave phenomena in two-phase flows

In flows with large gradients of pressure and density, the essential role in the formation of the fields of these parameters is played by fluid compressibility [85]. The influence of compressibility manifests itself in the strongest way in gas flows with high velocities where we deal with wave phenomena. After exceeding the speed of sound, the processes occurring in the flow have qualitatively different character than in subsonic flows. Rapid jumps of the flow parameters (shock waves) can take place, zones of limited propagation of small disturbances (sound waves) occur, in divergent channels velocity increase is observed. All the above listed phenomena are well known and described in gasdynamics which deals with compressible flows with high velocities.

Similar effects of wave nature are observed in two-phase flows, where besides two phases - compressible vapour and incompressible liquid – material interfaces additionally occur. Within the interfaces, the processes of mass, momentum and energy exchange take place which essentially influence the wave properties of the two-phase mixture. Inertia of those interfacial transport processes is the reason for dispersion of the system which means that small disturbations being carriers of any information in such a system propagate with a velocity dependent on frequency of these disturbations. The velocity of propagation of small disturbances is additionally a function of the rate of these transport processes and the content of individual phases in the mixture.

Two-phase mixtures very easily attain transonic flow velocities [27, 120]. The generation within an incompressible liquid of a small amount of vapour causes the creation of a compressible two-phase mixture of lower density. In such a vapour-liquid two-phase system the velocity of propagation of small disturbances is very low as compared to that in pure liquid where the changes of pressure with density are very large. After exceeding the critical velocity by a fluid choking of the flow takes place and, as a consequence, a physical limitation of mass flux flowing through the canal for given stagnation conditions. Blockage of a channel with all its consequences can easily occur in a flow of a compressible two-phase medium, like the water-steam mixture. As it turns out [121], in the flow of water and its vapour the phenomenon can already occur at low dryness fractions $x < 0.01$. It results from the fact that the mixture of such a composition, despite a negligible mass content of the vapour, is characterised by large compressibility which owes up to a few hundred times greater specific volume of the compressible vapour phase as compared to the incompressible liquid. Studies on two-phase water-steam flows show [122] that the critical velocity in such systems is a few orders of magnitude lower than that in pure water or steam and depends on the volumetric content of individual phases. Taking into consideration the fact that the process of evaporation $dx > 0$ in a flow is usually accompanied by an increase of velocity brought about by

density decrease, as well as substantial lowering of the critical velocity, it is easily seen that choking conditions and shock waves can occur relatively early. Those undesirable wave phenomena are the reason for large losses of energy in the flow and often lead to dangerous breakdowns of industrial devices.

The connected with flow choking value of the critical mass flux of a two-phase system depends on several factors and the phenomenon of choking is far more complicated as compared to a single-phase flow, since rapid expansion of the fluid can bring about mechanical and thermal nonequilibrium [17]. Apart from inlet (stationary flows) or stagnation (unsteady flows) conditions, the value of the critical mass flux is influenced by such parameters like channel geometry, its length and diameter, liquid purity and frictional losses.

A completely new phenomenon of wave nature, not observed in single-phase flows, is pseudocriticality of the flow. It was discovered by Bouré [123], and its interpretation based on the theory of linear waves was given by Downar-Zapolski [49]. A flow is pseudocritical when large changes of backpressure cause not large and sometimes experimentally undetectable change of inlet conditions. In such a way, the increase of pressure drop in the channel does not bring about any increase of the mass flow rate, despite the fact that we are still in the regime of subcritical flow [124]. The phenomenon of pseudocriticality results from a strong damping of the wave forerunner, which is very long and precedes its front of high amplitude. Since the wave front propagates with the equilibrium velocity, at sufficiently large velocities of the flow, it is inaccessible for a part of the channel, while moving with the frozen velocity forerunner is so strongly damped that the energy of the wave moving upstream is very small. It results in an imperceptible variation of the mass flow rate, sometimes smaller than the applied measurement technique despite the existing subcritical conditions.

5.2. Analysis of small disturbations

5.2.1. Dispersion relation

In the analysis of wave properties of a model an important role is played by the method of small disturbations. It consists in superimposing on an *a priori* solution σ^0 of the model equations a small disturbation in the form [125]:

$$\sigma = \sigma^0 + \delta\sigma, \qquad (5.1)$$

where $\delta\sigma$ is a very small quantity smaller than unity. As a result of the analysis we obtain a dispersion equation which tells us whether the model is dispersive, at what velocity small disturbations propagate as well as if they are damped. The answer of the system of equations to such a disturbance determines stability of the model. When an infinitesimal disturbance is damped then the model is stable and correctly describes the considerable physical phenomenon. Otherwise, when the disturbance is amplified and during propagation its amplitude increases, then the model is unstable and results in non-physical solutions of really stable processes.

In order to perform the analysis of small disturbances the system of equations of the model presented in the previous chapter must be written in the symbolic form:

$$\mathbf{A}(\sigma)\frac{\partial \sigma}{\partial t}+\mathbf{B}(\sigma)\frac{\partial \sigma}{\partial z}=\mathbf{C}(\sigma,z)+\mathbf{D}(\sigma)\frac{\partial^2 \sigma}{\partial z^2}+\mathbf{E}(\sigma)\frac{\partial}{\partial z}\left(\frac{\partial \sigma}{\partial z}\right)^2+\mathbf{F}\frac{\partial}{\partial t}\left(\frac{\partial \sigma}{\partial z}\right)^2, \quad (5.2)$$

where the state vector σ (primitive variables) comprises:

$$\sigma=\begin{bmatrix} w \\ p \\ h \\ x \end{bmatrix}. \qquad (5.3)$$

The nonsymmetrical matrices of coefficients $\mathbf{A}$ and $\mathbf{B}$ in Equation (5.2) take the following form:

$$\mathbf{A}=\begin{bmatrix} 0 & v_p & v_h & v_x \\ 1 & 0 & 0 & 0 \\ 0 & -v & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad (5.4)$$

$$\mathbf{B}=\begin{bmatrix} -v & wv_p & wv_h & wv_x \\ w & v & 0 & 0 \\ 0 & -vw & w & 0 \\ 0 & 0 & 0 & w \end{bmatrix}. \qquad (5.5)$$

The source vector $\mathbf{C}$ has the form:

$$\mathbf{C}=\begin{bmatrix} \dfrac{vw}{A}\dfrac{dA}{dz} \\[2mm] -\dfrac{vC\tau}{A}-g\cos\chi \\[2mm] \dfrac{vC\tau w}{A} \\[2mm] -\dfrac{x-\bar{x}}{\beta}-\dfrac{(x-\bar{x})^3}{\gamma} \end{bmatrix}, \qquad (5.6)$$

while the source matrix $\mathbf{D}$ is given as:

$$\mathbf{D}=\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -\kappa\bar{x}_p & -\kappa\bar{x}_h & \kappa \end{bmatrix}, \qquad (5.7)$$

where: $v = \dfrac{1}{\rho}$, $v_p = \dfrac{\partial v}{\partial p}\bigg|_{h,x}$, $v_h = \dfrac{\partial v}{\partial h}\bigg|_{p,x}$, $v_x = \dfrac{\partial v}{\partial x}\bigg|_{p,h}$, $\bar{x}_p = \dfrac{\partial^2 \bar{x}}{\partial p^2}\bigg|_h$, and $x_h = \dfrac{\partial^2 x}{\partial h^2}\bigg|_p$.

The remaining two matrices in Equation (5.2) are defined as follows:

$$E = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -kv \\ 0 & 0 & 0 & wkv \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{5.8}$$

$$F = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & kv \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{5.9}$$

The method of small disturbations can be solely used to linear terms of the matrix Equation (5.2) [126]. Therefore, the last two terms of this equation will be neglected in further analysis. Proceeding according to the procedure of Ramshaw and Trapp [127] we obtain the following relation from Equation (5.2) [128]:

$$\mathbf{A}(\sigma^0 + \delta\sigma)\frac{\partial(\sigma^0 + \delta\sigma)}{\partial t} + \mathbf{B}(\sigma^0 + \delta\sigma)\frac{\partial(\sigma^0 + \delta\sigma)}{\partial z} =$$
$$= \mathbf{C}(\sigma^0 + \delta\sigma, z) + \mathbf{D}(\sigma^0 + \delta\sigma)\frac{\partial^2(\sigma^0 + \delta\sigma)}{\partial z^2} \tag{5.10}$$

Expanding the matrices **A**, **B** and **D** as well as the vector **C** in a Taylor series about the unperturbed solution σ^0 and limiting ourselves to linear terms of the expansion, from Equation (5.10) we obtain:

$$\left[\mathbf{A}(v^0) + \frac{\partial\mathbf{A}}{\partial\sigma^0}\delta\sigma\right]\left(\frac{\partial\sigma^0}{\partial t} + \frac{\partial\delta\sigma}{\partial t}\right) + \left[\mathbf{B}(\sigma^0) + \frac{\partial\mathbf{B}}{\partial\sigma^0}\delta\sigma\right]\left(\frac{\partial\sigma^0}{\partial z} + \frac{\partial\delta\sigma}{\partial z}\right) =$$
$$= \mathbf{C}(\sigma^0, z) + \frac{\partial\mathbf{C}}{\partial\sigma^0}\delta\sigma + \left[\mathbf{D}(\sigma^0) + \frac{\partial\mathbf{D}}{\partial\sigma^0}\delta\sigma\right]\left(\frac{\partial^2\sigma^0}{\partial z^2} + \frac{\partial^2\delta\sigma}{\partial z^2}\right). \tag{5.11}$$

Performing operations and taking into consideration the identically satisfied unperturbed Equation (5.2) as well as neglecting small terms of order $O(\delta^2)$ we finally obtain:

$$\mathbf{A}(\sigma^0)\frac{\partial\delta\sigma}{\partial t} + \frac{\partial\mathbf{A}}{\partial\sigma^0}\delta\sigma\frac{\partial\sigma^0}{\partial t} + \mathbf{B}(\sigma^0)\frac{\partial\delta\sigma}{\partial z} + \frac{\partial\mathbf{B}}{\partial\sigma^0}\delta\sigma\frac{\partial\sigma^0}{\partial z} =$$
$$= \frac{\partial\mathbf{C}}{\partial\sigma^0}\delta\sigma + \mathbf{D}(\sigma^0)\frac{\partial^2\delta\sigma}{\partial z^2} + \frac{\partial\mathbf{D}}{\partial\sigma^0}\delta\sigma\frac{\partial^2\sigma^0}{\partial z^2}. \tag{5.12}$$

This equation describes small disturbations about an unperturbed solution with local values σ^0, $\partial\sigma^0/\partial t$, $\partial\sigma^0/\partial z$, $\partial^2\sigma^0/\partial z^2$, which are treated here as fixed. Assuming further that the disturbation acting on the medium is harmonic, we assume it in the standard form:

$$\delta\sigma = \delta\sigma_0 \exp[i(kz - \omega t)], \tag{5.13}$$

which is a function of the wave number k and the frequency of disturbations ω. Inserting the harmonic disturbation (5.13) into Equation (5.12), after simplification we obtain:

$$-i\omega\mathbf{A}(\sigma^0)\delta\sigma_0 + \frac{\partial\mathbf{A}}{\partial\sigma^0}\frac{\partial\sigma^0}{\partial t}\delta\sigma_0 + ik\mathbf{B}(\sigma^0)\delta\sigma_0 + \frac{\partial\mathbf{B}}{\partial\sigma^0}\frac{\partial\sigma^0}{\partial z}\delta\sigma_0 =$$
$$\frac{\partial\mathbf{C}}{\partial\sigma^0}\delta\sigma_0 - k^2\mathbf{D}(\sigma^0)\delta\sigma_0 + \frac{\partial\mathbf{D}}{\partial\sigma^0}\frac{\partial^2\sigma^0}{\partial z^2}\delta\sigma_0 . \tag{5.14}$$

This equation can be next transformed into the form:

$$\left[-i\omega\mathbf{A}(\sigma^0) + ik\mathbf{B}(\sigma^0) + k^2\mathbf{D}(\sigma^0) - \frac{\partial\mathbf{C}}{\partial\sigma^0} + \mathbf{G}(\sigma^0, \partial_t\sigma^0, \partial_z\sigma^0, \partial_z^2\sigma^0)\right]\delta\sigma^0 = 0. \tag{5.15}$$

where we substituted:

$$\mathbf{G} = \frac{\partial\mathbf{A}}{\partial\sigma^0}\frac{\partial\sigma^0}{\partial t} + \frac{\partial\mathbf{B}}{\partial\sigma^0}\frac{\partial\sigma^0}{\partial z} - \frac{\partial\mathbf{D}}{\partial\sigma^0}\frac{\partial^2\sigma^0}{\partial z^2} . \tag{5.16}$$

This relation is a homogeneous linear equation with respect to $\delta\sigma^0$. It possesses nontrivial solutions only when the main determinant is equal to zero, that is when [129]:

$$\det\left[-i\omega\mathbf{A}(\sigma^0) + ik\mathbf{B}(\sigma^0) + k^2\mathbf{D}(\sigma^0) - \frac{\partial\mathbf{C}}{\partial\sigma^0} + \mathbf{G}(\sigma^0, \partial_t\sigma^0, \partial_z\sigma^0, \partial_z^2\sigma^0)\right] = 0. \tag{5.17}$$

The above formula is the dispersion equation determining a relation between the wave number k and the frequency ω. As it is seen from the above equation, the phase velocity determined by the relation $c_{ph}(\omega) = \omega/k(\omega)$ is a function of the frequency, which means that the model is dispersive. The dispersion of our model results from the fact that the algebraic source vector $\mathbf{C}$ is a function of the state vector σ as well as from the inclusion of differential sources expressed by the matrix $\mathbf{D}$. One can indicate one more source of dispersion in the model – it is matrix $\mathbf{E}$, which results from the fact that the model is described by means of the system of almost-linear partial differential equations in which the matrices of coefficients $\mathbf{A} = \mathbf{A}(\sigma)$, $\mathbf{B} = \mathbf{B}(\sigma)$ and $\mathbf{D} = \mathbf{D}(\sigma)$ depend on the state vector. That is why in the dispersion relation (5.17) the terms $(\partial\mathbf{A}/\partial\sigma^0)/(\partial\sigma^0/\partial t)$, $(\partial\mathbf{B}/\partial\sigma^0)/(\partial\sigma^0/\partial t)$, and $(\partial\mathbf{D}/\partial\sigma^0)/(\partial^2\sigma^0/\partial z^2)$ appear, which are a manifestation of nonlinearity of the model. Let us emphasize that the capillary properties enter through the equations of state both to the matrices $\mathbf{A}$ and $\mathbf{B}$, and to the vector $\mathbf{C}$, as well as through the constitutive equation to the matrix $\mathbf{D}$.

5.2.2. Disturbation velocity and attenuation coefficient

The dispersion relation (5.17) can be solved only after some simplifications [125]. Assuming a weak variation of the matrices **A**, **B** and **D** with the state vector as well as assuming that local unsteadiness $\partial\sigma^0/\partial t$ and gradients $\partial\sigma^0/\partial z$, $\partial^2\sigma^0/\partial z^2$ of the state vector are small, we can neglect the non-linear terms and assume $\mathbf{E} = 0$. Assuming moreover a small variation of the cross-sectional area of the channel $dA / dz = O(\delta)$, neglecting body forces and assuming $w = O(\delta)$, we reduce the vector **C** to a function depending only on thermodynamic nonequilibrium and obtain:

$$\frac{\partial C}{\partial \sigma^0} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \left(\frac{1}{\beta}+\frac{3(x-\bar{x})^2}{\gamma}\right)\bar{x}_p & \left(\frac{1}{\beta}+\frac{3(x-\bar{x})^2}{\gamma}\right)\bar{x}_h & -\frac{1}{\beta}-\frac{3(x-\bar{x})^2}{\gamma} \end{bmatrix}. \quad (5.18)$$

The regard to the assumptions in solving the dispersion Equation (5.17) leads to the following algebraic equation:

$$\left(if_1\right)k^4 + \left(\omega f_2 + i\left(f_3 + \omega^2 f_4\right)\right)k^2 + \left(\omega^3 f_5 + i\omega^2 f_6\right) = 0, \quad (5.19)$$

where:

$$f_1 = v^2\kappa,$$

$$f_2 = v^2,$$

$$f_3 = v^2\left(\frac{1}{\beta}+\frac{3(x-\bar{x})^2}{\gamma}\right),$$

$$f_4 = v_p\kappa + vv_h\kappa + vv_x\kappa\bar{x}_h + v_x\kappa\bar{x}_p,$$

$$f_5 = v_p + vv_h,$$

$$f_6 = \left(-vv_x\bar{x}_h - v_p - vv_h - v_x\bar{x}_p\right)\left(\frac{1}{\beta}+\frac{3(x-\bar{x})^2}{\gamma}\right),$$

This is a biquadratic equation with respect to the wave number k. It possesses four complex solutions k_1, k_2, k_3 and k_4, where the real parts of the roots k_1 and k_2 as well as k_3 and k_4 have the same absolute values and differ only in sign, while the imaginary parts are equal to each other. It results from the properties of the biquadratic equation which is invariant at transformation $k \to -k$. The wave number k being the number of waves falling on a unit length depends, as it results from Equation (5.19), on the frequency ω and on the values of parameters of the

thermodynamic state of the system which are taken into account in the coefficients $f_1 \ldots f_6$. Since k is a complex number, then we can write it in the form of a sum of real and imaginary part:

$$k = \text{Re}(k) + i\,\text{Im}(k).$$ (5.20)

The real part of the wave number k is a ratio of the frequency ω and the phase velocity c_{ph} [130]:

$$\text{Re}(k) = \frac{\omega}{c_{ph}},$$ (5.21)

while the imaginary part is interpreted as an attenuation coefficient [130]:

$$\text{Im}(k) = \eta.$$ (5.22)

Hence we have:

$$k = \frac{\omega}{c_{ph}} + i\eta.$$ (5.23)

The existence of four solutions which, as far as the absolute value of the real parts is concerned, constitute two different solutions means that the model possesses four velocities of propagation of small disturbations. Two of them have the same absolute value and differ only in sign, thus a disturbation propagates with the same velocity in two opposite directions. The same can be said about the remaining pair of velocities at which disturbations propagate upstream and downstream. Thus, in one direction small disturbations of any physical quantity can propagate at two different velocities. From the point of view of attaining the critical conditions, which is equivalent to the complete blockage for any kind of information generated downstream, the most important is the largest velocity. The fact that a flow exceeds the lower velocity of propagation of disturbations does not mean complete choking since those disturbations will always be able to move with a higher velocity and only after exceeding this velocity choking of the channel will occur.

Attenuation of a given velocity is the same in both directions since the imaginary parts of the solutions are equal to each other. As far as the value of attenuation at different velocities is concerned, it is different and, as it will be shown, higher for larger velocities and frequencies.

5.2.3. Numerical analysis of the dispersion equation

Numerical analysis was begun with calculations for the relaxation model in which the process of relaxation is described by means of two algebraic terms with constant relaxation times β and γ. Figure 5.1 presents the phase velocities for this model as a function of frequency of disturbations as well as the variation of this velocity with the nonlinear relaxation time γ is additionally shown. As it can be seen from the figure the velocity of disturbations increases along with the increase of
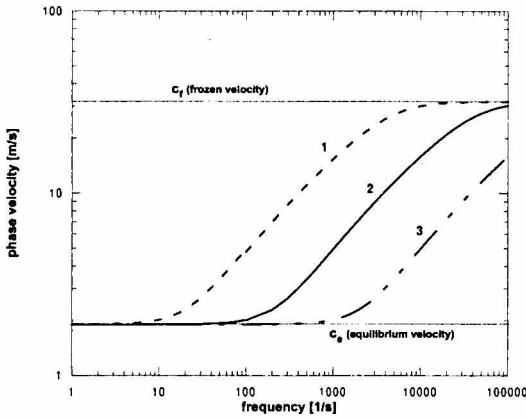
Figure 5.1. Phase velocity c_{ph} as a function of frequency (at different values of the coefficient of nonlinear relaxation γ : 1 – γ = 3.35e–5, 2 – γ = 3.35e–6, 3 – γ = 3.35e–7; p = 1.5 bar, α = 0.2
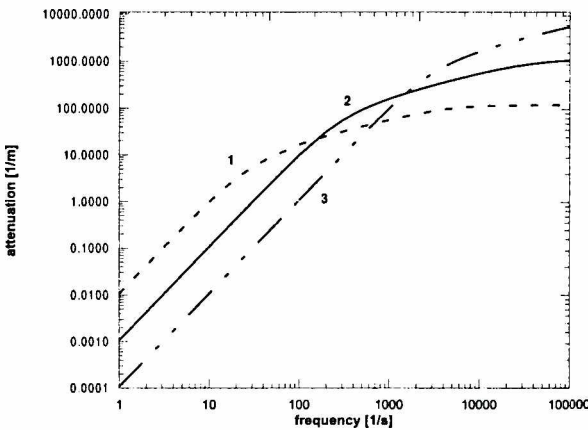

Figure 5.2. Attenuation coefficient Im(k) as a function of frequency (at different values of the coefficient of nonlinear relaxation γ: 1 – γ = 3.35e–5, 2 – γ = 3.35e–6, 3 – γ = 3.35e–7; p = 1.5 bar, α = 0.2

their frequency, and in the limit $\omega \rightarrow \infty$ attains the frozen velocity c_f. A lower limit of the phase velocity at $\omega \rightarrow 0$ is the so-called equilibrium velocity. The finite value of c_{ph} shows that the model is hyperbolic and possesses the properties of real two-phase flows in which the fluctuations of the state parameters propagate with a given velocity. This velocity depends on the rate of phase change which is characterised by the relaxation time. When the phenomenon proceeds very fast, *i.e.* is characterised by a low relaxation time, then the phase velocity in the whole range of frequencies is approximated by the equilibrium velocity which characterises the system in thermodynamic equilibrium and is independent of the frequency of disturbances. In such a system, the attainment of equilibrium takes place faster than the disturbances are generated and in this connection the next impulses propagate in equilibrium medium. Their velocity depends only on the values of parameters characterising the thermodynamic state of the system.
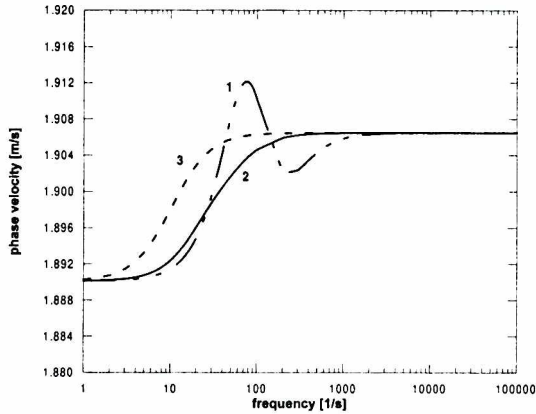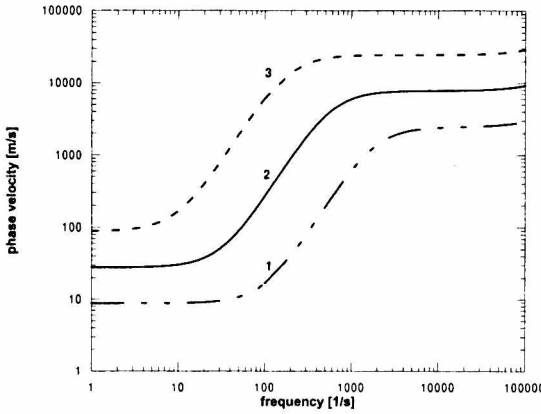
Figure 5.3. *Phase velocity c_{ph} as a function of frequency ω at different values of the coefficient of capillarity κ:* **1** *– κ = 0.08,* **2** *– κ = 0.8,* **3** *– κ = 8.0, γ = 3.35e–6; p = 1.5 bar, α = 0.2*

Figure 5.4. *Attenuation coefficient Im(k) as a function of frequency ω at different values of the coefficient of capillarity κ:* **1** *– κ = 0.08,* **2** *– κ = 0.8,* **3** *– κ = 8.0, γ = 3.35e–6; p = 1.5 bar, α = 0.2*

A graph of attenuation for the relaxation model is shown in Figure 5.2. It is clearly seen that signals of higher frequencies are damped stronger, that is the time of their action in the flow is shorter as compared to that for shorter waves. For all the times of nonlinear relaxation the coefficient of attenuation tends to zero in the limit of low frequencies at which equilibrium is reached in the two-phase mixture. At high frequencies of the generated signal its damping in the two-phase system is in practise constant and in infinity aims at a limited value. In faster processes, that is with shorter characteristic times, damping of the signal is, as it is seen, larger. For infinitely fast phenomena in which a new equilibrium state is attained immediately, also the disturbations are so strongly damped that they "die" at once.

The proposed model in which the energy of interfacial surfaces is described by the term with the second derivative of the nonequilibrium dryness fraction x has two velocities of propagation of small disturbations. The lower one is in the order of 2 m/s and is practically constant in the whole range of frequencies (Figure 5.3).

Figure 5.5. Phase velocity c_{ph} as a function of frequency ω at different values of the coefficient of capillarity κ: $1 - \kappa = 0.08$, $2 - \kappa = 0.8$, $3 - \kappa = 8.0$, $\gamma = 3.35e-6$; $p = 1.5$ bar, $\alpha = 0.2$

It does not exhibit significant variations with the variation of the capillarity coefficient κ which is responsible for the contribution of interfaces. Attenuation corresponding to this velocity is also constant in a wide range of frequencies, but exhibits a stronger dependence on the coefficient of capillarity (Figure 5.4).

However, from the point of view of attaining the critical conditions the most important is the highest velocity at which disturbations can propagate in a given model. Taking into consideration the second derivative causes that the quadratic form of the system of balance equations is undetermined and the system becomes parabolic which means that the velocity of propagation of small disturbations can be infinitely large. It is shown in Figure 5.5, when a relationship between the phase velocity and the frequency is drawn. The relation $c_{ph}(\omega)$ was calculated for different values of the coefficient of capillarity κ. It is clearly seen, especially for larger κ, that the higher the frequency of disturbations, the faster they propagate, tending to infinity. It is a characteristic feature of parabolic models. The change of the coefficient of capillarity acts so that its increase increases also the phase velocity. It is also worth noting that in comparison with the relaxation model, the order of magnitude of the velocity for the investigated range of frequency substantially rose. At $\gamma = 3.35e-6$, in the model without interfaces for $\omega = 1e+5$ s^{-1} this velocity is equal to 30 m/s, while in the model with interfaces its value reaches 9000 m/s. It is of course a non-physical value, not recorded in experiments. The reason for this may be the exceeding of the range of frequency for which a continuous model of two-phase flow can be used. The wavelength corresponding to frequency $1e+5$ is far smaller than the characteristic size of dispersed phase for which the diameter of a bubble $D = O(m^{-3})$ is of such a size. Therefore, the generation of disturbations of wavelengths shorter than a limiting value makes no sense as well as investigation of a model out of the range of its application.

An additional explanation of physical impossibility of effective propagation of disturbations with so large velocities is its stronger and stronger damping. A graph of the coefficient of attenuation as a function of frequency is shown in Figure 5.6, from
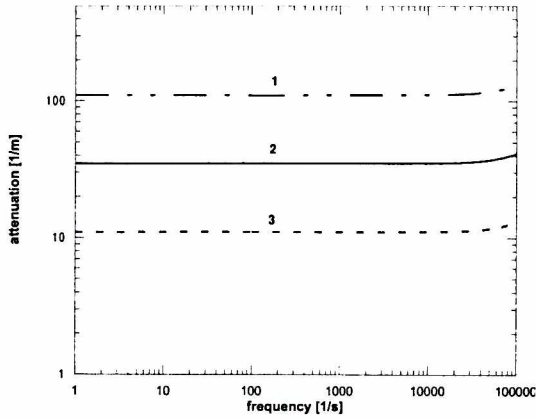
Figure 5.6. *Attenuation coefficient Im(k) as a function of frequency ω at different values of the coefficient of capillarity κ: 1 – κ = 0.08, 2 – κ = 0.8, 3 – κ = 8.0, γ = 3.35e–6; p = 1.5 bar, α = 0.2*

which it is seen that in the range of very large frequencies the larger the frequency of disturbations, the stronger they are damped. At infinitely short waves their damping is infinitely large, which means that such signals will be immediately "extinguished" and the range of their influence will be physically insensible. Also the tendency of variation with the change of the coefficient of capillarity is correct, since in the model without interfaces the attenuation was stronger than in the model with interfaces, and as it is seen from Figure 5.6 the larger their contribution, the weaker the attenuation and the slower variation with frequency. In the range of very low frequencies the velocity of disturbations is in the order of a dozen to a few dozen m/s and such values are recorded in real flows. Such disturbations are damped in the model with a constant strength.

5.3. Critical two-phase flows

5.3.1. Critical velocity and flow choking

The definition of critical velocity and connected with it choking of a flow is clear and precisely formulated for a single-phase compressible medium. In a one-dimensional flow of gas without heat transfer with the surroundings, one can neglect interactions with the surroundings and treat the adiabatic flow as isentropic without internal dissipative processes. The critical velocity in such a flow is the isentropic speed of sound (velocity of propagation of small disturbations) defined as follows [43]:

$$c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s}. \tag{5.24}$$

The critical velocity is always attained in a critical cross section which is the smallest section of the channel (geometrical throat) in case of a nozzle, or the outlet section in case of a pipe. The critical mass flow rate is calculated on the basis of fluid-flow and thermodynamic parameters attained in the critical section [43]:

$$\dot{m}_c = A_c \rho_c w_c. \tag{5.25}$$

For the considered isentropic flow of gas, the values of critical parameters are functions of stagnation parameters (stagnation pressure, stagnation density) and the thermodynamic properties of the system (specific heats ratio). In this connection the maximal possible flow rate is completely determined by the stagnation parameters, the equation of state and the minimal section.

Such approach to the problem and automatic transfer of definitions to the case of one-component two-phase flows can be misleading [124]. It results not only from a larger complication of the processes taking place in two-phase flows, caused by the existence of interfaces, nonequilibria of the phenomena and two-dimensional effects, but also from completely new phenomena not occurring in single-phase compressible media, as pseudocriticality or dispersed shock waves. Also the smallest cross-section of the channel usually associated with a place of extremum of physical parameters loses its importance [124]. Therefore, the condition of the flow criticality cannot be *a priori* postulated but should result from physical observations of the flow and the assumed theoretical model.

As it was shown by Bilicki and Kestin [131], the critical conditions are the same both for stationary and nonstationary form of balance equations. A conclusion follows that the phenomenon of choking can be studied, without a loss of generality, for steady-state flows.

One can distinguish three physical definitions of stationary choked flow [132]:

- flow is choked when it reaches the maximal mass flux in given stagnation conditions. An increase of the mass flow rate can only be realised by a change of stagnation conditions;

- choked flow is characterised by the fact that inlet conditions as well as those in a converging part are independent of outlet conditions while keeping stagnation conditions unchanged;

- choked flow reaches the speed of sound. This speed is reached inside the channel in case of nozzles, and at the outlet of the channel in case of pipes.

In nonstationary conditions, choking of a flow means that information generated downstream cannot propagate upstream beyond the section in which the critical flow occurs. Only the second definition directly characterises critical two-phase flow [17]. The remaining two definitions require some caution while using in two-phase flows. In reality, the speed of sound refers to a single phase and is different for water and steam. Moreover, any disturbation brings about a change of structure of the flow which can influence the critical conditions. The physical criterion of choking expressing the lack of influence of outlet on inlet parameters, mathematically means breaking of a continuous dependence between inlet and outlet boundary conditions [128]. This is the case when determinant of the system of ordinary differential equations describing the flow:

$$b_{ij}\frac{d\sigma_j}{dz} = c_i \tag{5.26}$$

is equal to zero [37]:

$$\Delta = \det b_{ij} = 0, \tag{5.27}$$

where b_{ij} is an element of the system matrix, c_i – is an element of the column vector of right-hand sides, while σ_j – is a component of the state vector.

A necessary condition for the occurrence of critical flow requires the existence of a singular point in critical section [134]. For this reason it is impossible to find an exact value of the critical mass flux by forward numerical integration since it requires crossing the singular point. Nevertheless, it is possible to approach the value of the critical flow rate by means of maximal possible G_{pos} and minimal impossible G_{imp} mass flux [135]. It is recognised that any mass flux smaller than critical corresponds to possible flow and numerical integration can be performed in the whole length of the channel L. However, a mass flux larger than critical corresponds to impossible flow since the critical flux is a maximal value in given inlet conditions and numerical integration cannot be carried out beyond the critical section. Thus, we have the following condition:

$$G_{pos} < G_c < G_{imp}, \tag{5.28}$$

and in a limiting case:

$$G_{pos} \approx G_c \approx G_{imp}. \tag{5.29}$$

In practice, one can control the difference between G_{pos} and G_{imp}, and approach the critical mass flux with a given accuracy. This is the essence of *PIF* method which is widely recommended for the determination of critical mass flow rates in nonequilibrium two-phase flows [124, 135].

5.3.2. Numerical calculations of critical mass velocity

The mathematical model of flashing flow described in Chapter 4 was tested in critical flows [136]. The results of numerical calculations obtained by means of the presented model were compared with the results of experimental measurements carried out in real critical flows of water and steam. As a point of reference we assumed two benchmark experiments: *Moby Dick* [27] and *BNL* [19]. The experimental studies were carried out at low and medium pressures ($1 \div 10$ bar) and medium temperatures ($100 \div 150°C$), at low values of the dryness fraction $x < 0.02$. The investigated medium was water of high purity, which during a vertical upward flow through a measuring section was decompressed and evaporated. The conditions of measurements and the geometries used are collected in Table 1. The reason for such a choice of experiments were the largest discrepancies between theoretical models and experimental data at low pressures and dryness fractions [18]. As Bouré [18] claims, the above discrepancies are caused by a crucial influence of nonequilibrium phenomena and the conditions of the generation of a new phase on the occurrence of critical flow. A critical section occurs the earlier, the smaller superheating in flashing inception and the smaller nonequilibrium during the phase change.

The aim of the numerical calculations was to determine by means of the *PIF* method critical mass velocities of the water-steam mixture and to compare the results of the calculations with the results of experimental studies. Boundary conditions at the inlet of the channel – pressure, temperature, void fraction – were assumed on the basis of the experimental data, while the velocity of the flow was selected in the *PIF* procedure in such a way as to attain conditions similar to critical at some section of the channel. Consequently, for each experimental run the value of critical mass flux was selected with a given accuracy. As a critical mass flux one assumed the arithmetic average of maximal possible and minimal impossible mass flux determined in the *PIF* procedure. The accuracy of the calculations can be determined from relation [135]:

$$Accuracy > \frac{G_{pos} - G_{imp}}{2G_c} = \frac{G_{pos} - G_{imp}}{G_{pos} + G_{imp}}. \tag{5.30}$$

Table 1. *Experimental data used for calculations*

Experiment	Geometry	P_{in} [bar]	T_{in} [°C]	G_{in} [kg/m²s]
Reocreux		$1.5 \div 2.1$	$116 \div 126$	$4150 \div 10300$
Jones		$1 \div 10$	$100 \div 150$	$1100 \div 7900$

The results of the calculations of critical mass velocity for 48 runs of the experiment of Reocreux [27] and 13 runs of that of Jones [19] are presented in Figures 5.7 and 5.8. Figure 5.7 presents numerically determined critical mass flux G_{cal} as a function of the experimentally measured critical flux G_{exp} for the conditions of the *Moby Dick* [27] and *BNL* [19] experiments, while Figure 5.8 shows the error of the theoretical model in determination of critical mass fluxes as a function of the calculated critical flux. As presented in the following figures, the mathematical
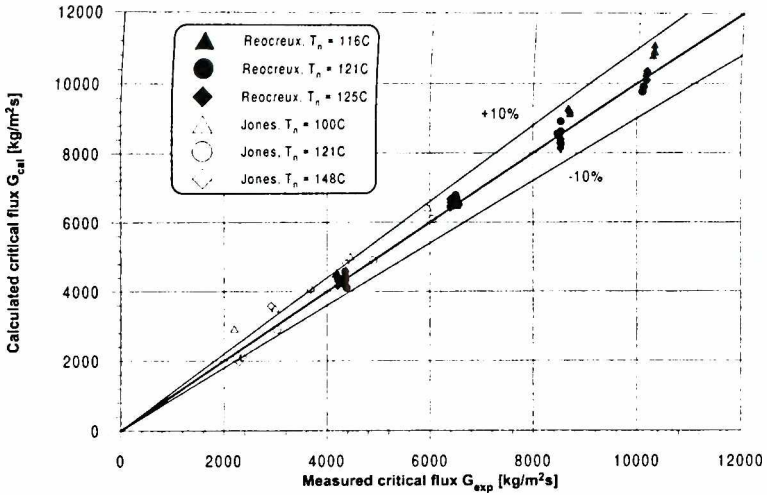
Figure 5.7. *Numerically determined critical mass flux G_{cal} as a function of experimentally measured value G_{exp} for the conditions of the Moby Dick and BNL experiments*
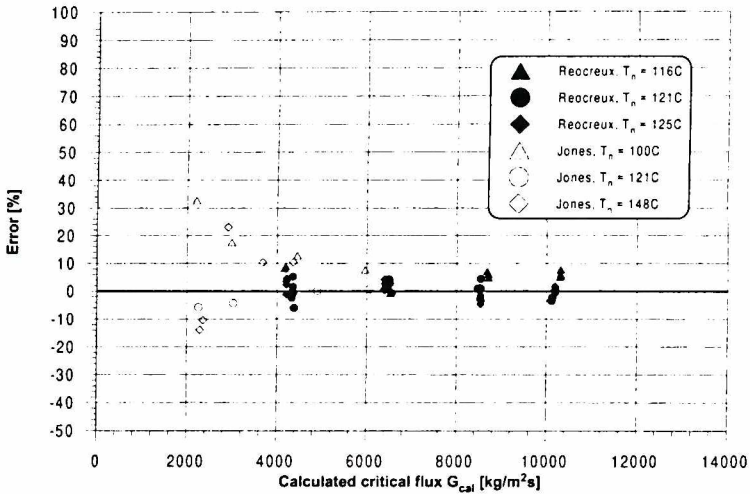

Figure 5.8. *Error of the theoretical model in determination of critical mass fluxes as a function of calculated critical flux G_{cal}*

model shows a reasonably good agreement with the measurement data. In case of the Reocreux [27] studies, the maximal error in the calculations of critical mass velocity does not exceed even 10%. For the Jones [19] investigations it ranges from 10 to 20%, except for a single run No. 56 in which the discrepancy 32% was recorded. A tendency of better agreement for increasing mass flux is worth noting. One can assume that in the limit of $G = 3000 \div 10000$ kg/m²s error of the model will not exceed 10% with a general tendency to overpredicting the mass flux. The average error of the predicted critical mass velocity for all the runs amounts to 5% which in nonequilibrium water-steam flows is a good result [137].

6. Flashing flow in channels

6.1. Parametric analysis of the model

The mathematical model of flashing flow presented in Chapter 4 includes free parameters which are phenomenological coefficients modelling the properties of a heterogeneous two-phase system on macroscopic level. Since we do not have any theories enabling us to calculate them on the basis of known microscale physical quantities, we propose to determine their values by fitting to experiment.

In order to preliminary verify the proposed model some numerical calculations were performed. The set of ordinary differential equations describing steady-state flow, together with closure equations and boundary conditions, constitutes a unique differential problem. The calculations were performed using the shoot method since the problem was formulated as a two-boundary problem in which boundary conditions were imposed at the inlet and the outlet of the channel. In the calculations we used the Runge-Kutta scheme of fourth order with automatic selection of integration step. At the inlet we imposed pressure, temperature and void fraction, while at the outlet – pressure. Al these quantities were taken from experimental measurements of real water-steam flows. The numerically obtained distributions of physical parameters were next compared with experimental profiles. For the comparisons we used the measurement data of the most reliable experiment on two-phase critical flows know as the *Moby Dick* [27].

As a basic criterion of assessment of the model the mass flow rate of the two-phase mixture for a given pressure drop in the channel was assumed. The value of the mass flow rate, being an integral characteristic of a model, is very important from an engineering point of view [103] and determines the usefulness of the model for the predictions of critical mass flow rates in choking.

In order to determine the unknown values of the coefficients in the Ginzburd-Landau equation a parametric analysis of the model was carried out. Based on the experimental data inlet conditions were imposed and the outlet velocity was selected so as to achieve agreement between the imposed outlet pressure and the values recorded in the experiment. Such calculations were carried out at constant values of the coefficients of linear and non-linear relaxation and the energetic coefficient of capillarity. The coefficient of linear relaxation β was assumed according to relation (4.66) proposed in Chapter 4 and during the calculations it was found that this formula gives good results. After finding this we finally decided to assume relation (4.66) for further calculations. The constant β as a coefficient of proportionality in the algebraic linear term $(x-\bar{x})/\beta$, has the greatest influence on the increase of the nonequilibrium dryness fraction and crucially influences the process of vapour generation. A reflection of this process is a distribution of the void fraction – the shape of the curve $\alpha(z)$ expresses the character of the evolution equation.

Therefore, assuming the established value of the linear relaxation time β we are standing in front of the problem of determination of the remaining two coefficients in Equation (4.48). Since we do not have any theory enabling their calculation, we
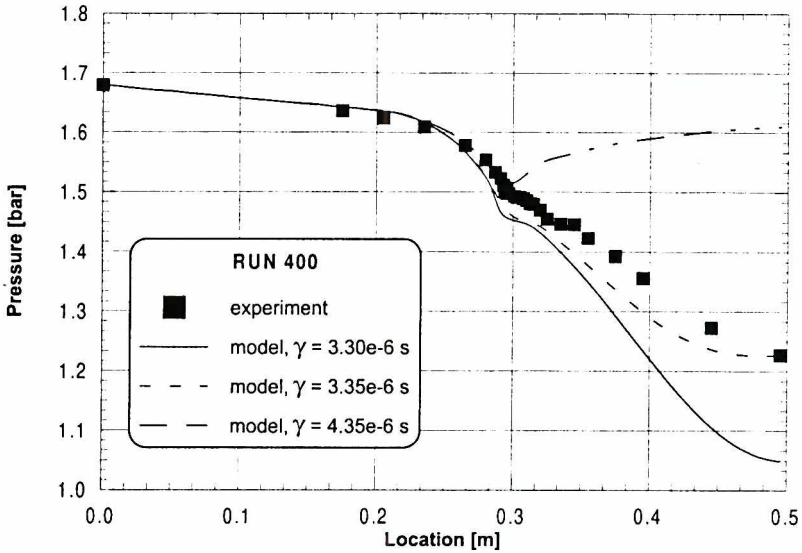
Figure 6.1. *Influence of variation of coefficient of non-linear relaxation γ on pressure distribution in channel for run No. 400 of the Moby Dick experiments, κ = const*
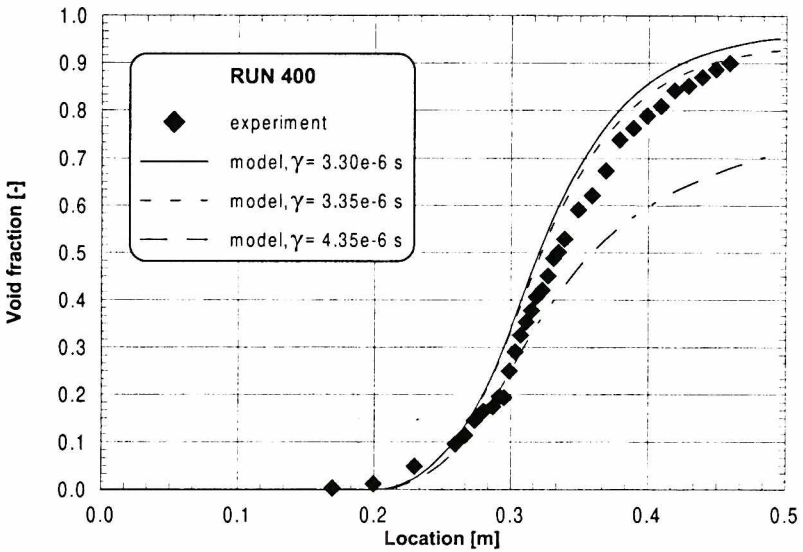

Figure 6.2. *Influence of variation of coefficient of non-linear relaxation γ on void fraction distribution in channel for run No. 400 of the Moby Dick experiments, κ = const*

propose to assume them as constants and to select their values so as to achieve as good agreement with experiment as possible. The value of the relaxation time γ was selected in run No. 400 of the experiment of Reocreux [27] and assumed equal to $3.35 \cdot 10^{-6}$ s. A hypothetical impact of a variation of this coefficient on the calculated pressure and void fraction profiles in the channel is shown in Figures 6.1÷6.2. These calculations were carried out for a fixed value of the energetic coefficient of capillarity κ as well as for a fixed mass flow rate. As it is seen the mathematical
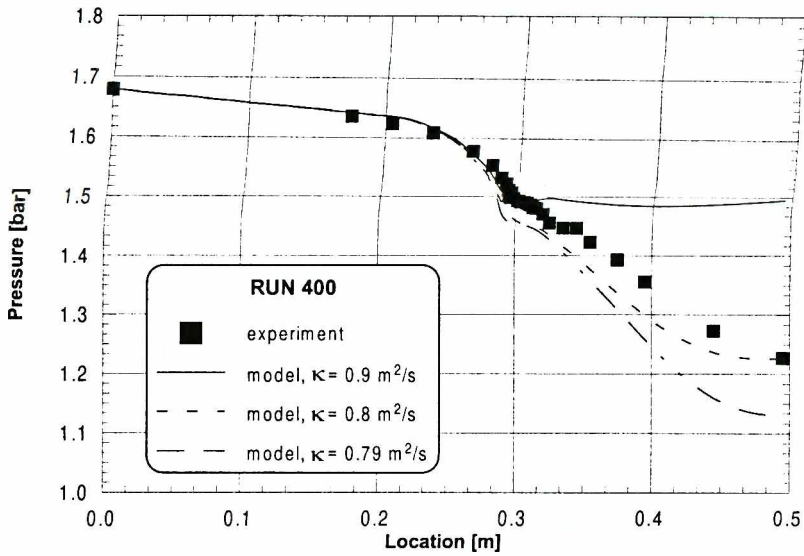
Figure 6.3. *Influence of variation of capillarity coefficient κ on pressure distribution in channel for run No. 400 of the Moby Dick experiments, γ = const*
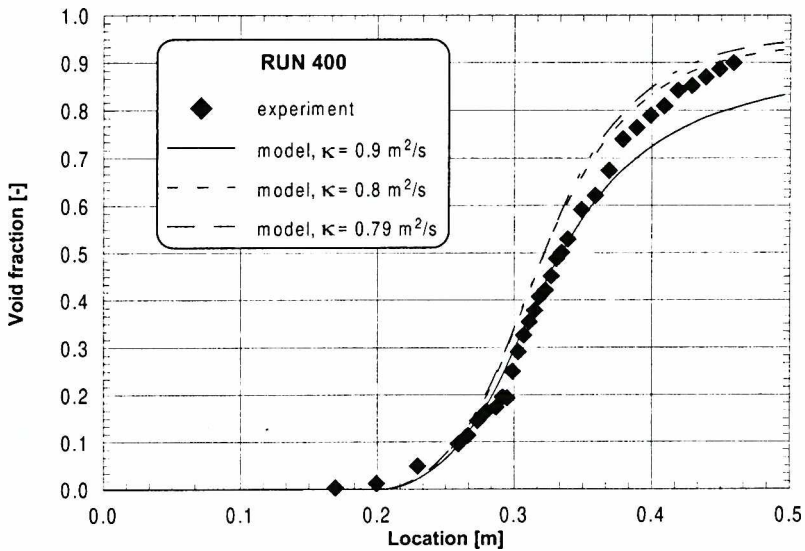
Figure 6.4. *Influence of variation of capillarity coefficient κ on void fraction distribution in channel for run No. 400 of the Moby Dick experiments, γ = const*

model is fairly sensitive to the variation of this time constant – not large changes of its value, of the order of several percents, result in visible differences in the profiles of pressure and void fraction. Deviations from the experimental profiles are particularly distinct in the divergent part of the nozzle. For a certain value of γ different about 30% from that giving the best agreement, the distribution of pressure in the divergent section of the channel has even qualitatively different character. In this case also the value of void fraction substantially differs from the experimental

value. In general, the increase in the value of the coefficient of non-linear relaxation γ causes vapour overproduction and results in too low values of pressure as compared with the experiment. Such a tendency can be explained by the fact that lower relaxation time brings flashing closer to equilibrium. A smaller time constant causes larger contribution of the cubic relaxation term and following more intensive increase of the nonequilibrium dryness fraction. In the case of γ resulting in the correct value of the outlet pressure a tendency to underpredict the calculated pressure as compared with the measured value can be noticed.

A similar parametric analysis was performed for a variation of the coefficient of capillarity κ. The results of the calculations are presented in Figures $6.3 \div 6.4$. The curves corresponding to $\kappa = 0.8$ m²/s are the profiles which fit the measurement points best. The pressure and void fraction distributions upstream from the throat are closest to the experimental profiles. In spite of the fact that as walking away from the throat of the channel the conformity of the pressure profiles is getting worse, at the exit of the nozzle the value equal to the measured one was obtained. As far as the amount of generated vapour is concerned, the onset and the end of flashing are the places of best conformity. The increase of κ by about 10% of the optimal value results in qualitatively different pressure distributions in the divergent section, the outlet pressure is larger than that recorded in the experiment, and the vapour generation is underpredicted starting from some point. But, the variations of κ decreasing its value even more substantially influence the pressure profiles, and at a change by 10% the flow in the channel is impossible since a turning point occurs in the model.

Such a parametric analysis was also performed for the mechanical coefficient of capillarity k, and as a result of the analysis its value was selected for $k = 10^6$ N. The results of the calculations carried out with the inclusion of the gradient term in the momentum equation are presented in the next section.

6.2. Numerical calculations of flashing flows in channels

The values established in the previous section of the free parameters are a closure of the mathematical model. Their values were determined by fitting numerical results to run No. 400 of the *Moby Dick* [27] experiments, known as the most reliable and benchmark experiment of nonequilibrium two-phase flows. One can presume that the selected here values of the free parameters will also be valid in the case of two- or three-dimensional models. It results from a character of three-dimensional equations describing the model that have the same number of free parameters as the simplified quasi-one-dimensional equations.

After fitting the values of the coefficients numerical calculations for other runs of the experiment were performed. In order to verify the model more completely we selected for numerical calculations runs of different pressures, temperatures and mass flow rates. Hypothetical profiles of basic physical parameters characterising the flow are shown in Figures $6.5 \div 6.9$. Both the pressure and void fraction profiles agree well with the experimental points. The zone of evaporation is accompanied by

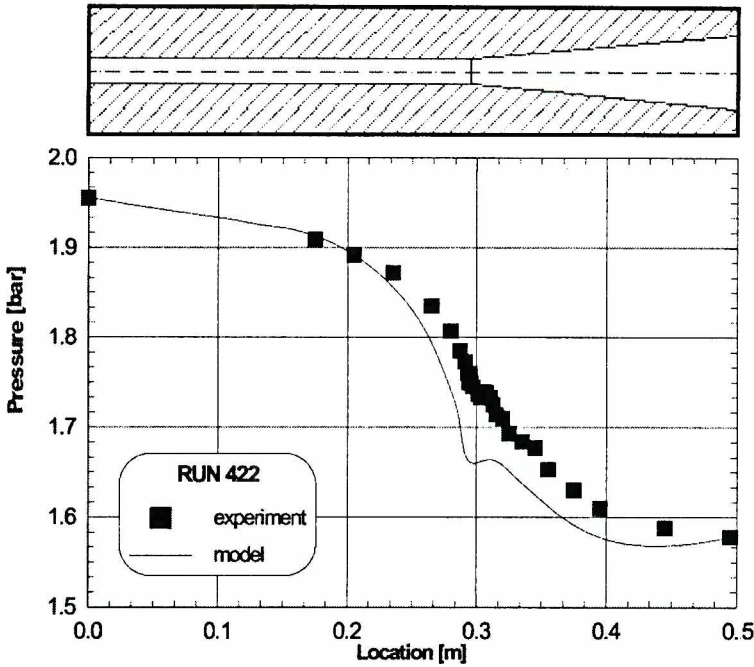**Figure 6.5.** *Experimental and theoretical pressure distribution along channel for run No. 422 of the Moby Dick experiments, T_{in} = 121.08 °C, p_{in} = 1.955 bar, G_{exp} = 6499.2 kg/m²s, G_{cal} = 6495 kg/m²s*
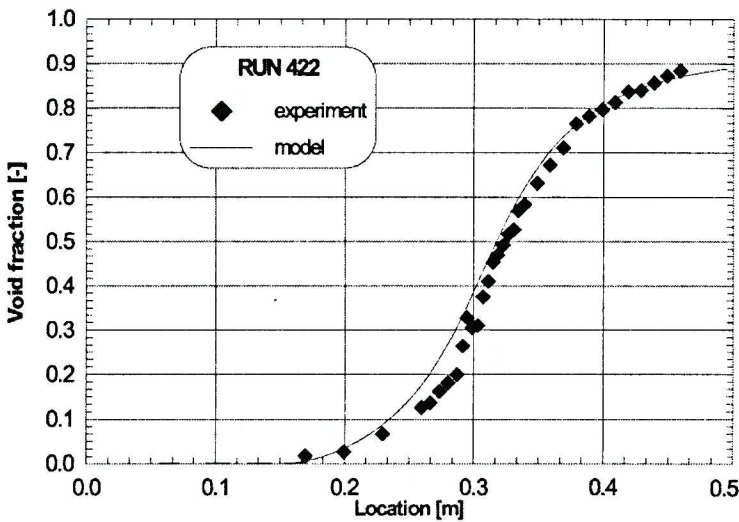

Figure 6.6. *Experimental and theoretical void fraction distribution along channel for run No. 422 of the Moby Dick experiments, T_{in} = 121.08 °C, p_{in} = 1.955 bar, G_{exp} = 6499.2 kg/m²s, G_{cal} = 6495 kg/m²s*

a characteristic increased pressure drop as compared with a single-phase flow caused by a momentum change due to the decrease of density of the fluid. A characteristic feature is the pressure underprediction despite the equality of the inlet
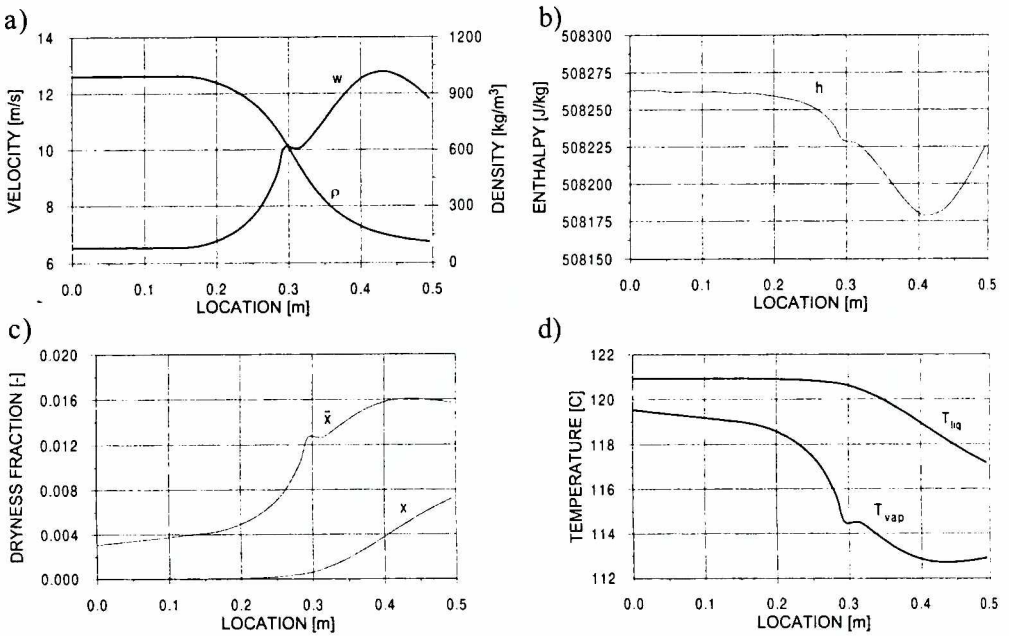
Figure 6.7. Distributions of physical parameters of flow along channel for run No. 422 of the Moby Dick experiments, T_{in} = 121.08 °C, p_{in} = 1.955 bar, G_{exp} = 6499.2 kg/m²s, G_{cal} = 6495 kg/m²s; a) velocity and density, b) enthalpy, c) dryness fraction, d) temperature

and outlet pressures to the experimental values. A similar trend is observed for run No. 459 performed for higher pressures, temperatures and mass velocities than in run No. 422. Discrepancy of the calculated mass flux is here of the order of several percents. From the distributions of temperature and dryness fraction the quantity of thermodynamic nonequilibrium prevailing in the fluid can be concluded. In a single-phase flow of metastable water the thermodynamic nonequilibrium increases as a result of pressure drop causing an increase of the equilibrium dryness fraction and decrease of the saturation temperature at simultaneously constant temperature of the water and constant real dryness fraction. When the two-phase flow occurs an interesting physical situation arises – the quantity of nonequilibrium at first increases, despite the evaporation which should lead the system towards equilibrium. But it does not proceed so since the state of equilibrium in the flow varies from point to point so intensively that the values of the equilibrium parameters evolve faster than the real quantities. In the vicinity of the throat of the channel the largest deviations from equilibrium are observed and afterwards the system relaxes towards equilibrium.

Similar calculations were carried out for the *BNL* [19] experiments. In this case the experimental measurements were performed in a convergent-divergent nozzle at substantially higher pressures ($p > 3$ bars) and temperatures ($T > 140$°C). The calculations were carried out for run No. 82 in which the pressure in the divergent section decreases, as well as for run No. 288 which is characterised by a pressure increase in the diverging section. In both cases not only qualitative but also
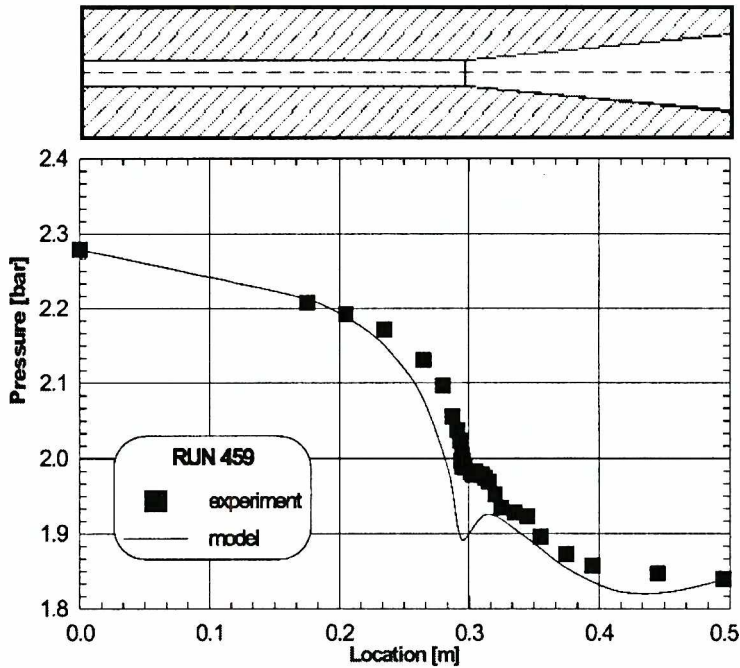
Figure 6.8. *Experimental and theoretical pressure distribution along channel for run No. 459 of the Moby Dick experiments, $T_{in} = 125.15\,°C$, $p_{in} = 2.279$ bar, $G_{exp} = 10181.8$ kg/m²s, $G_{cal} = 10347$ kg/m²s*
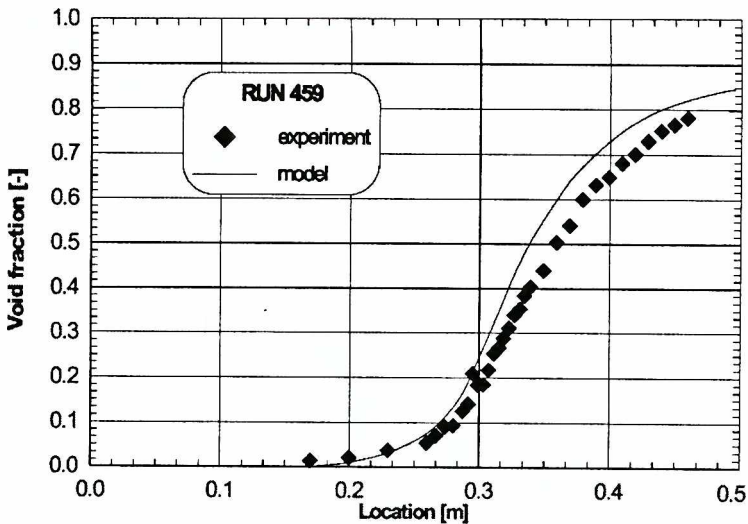

Figure 6.9. *Experimental and theoretical void fraction distribution along channel for run No. 459 of the Moby Dick experiments, $T_{in} = 125.15\,°C$, $p_{in} = 2.279$ bar, $G_{exp} = 10181.8$ kg/m²s, $G_{cal} = 10347$ kg/m²s*

quantitative agreement with the experiments was achieved, which is seen from Figures 6.10÷6.13. The agreement was achieved with the coefficients selected in another experiment carried out in different conditions and for different channel geometry. Also the obtained mass fluxes correspond well to the measured values.
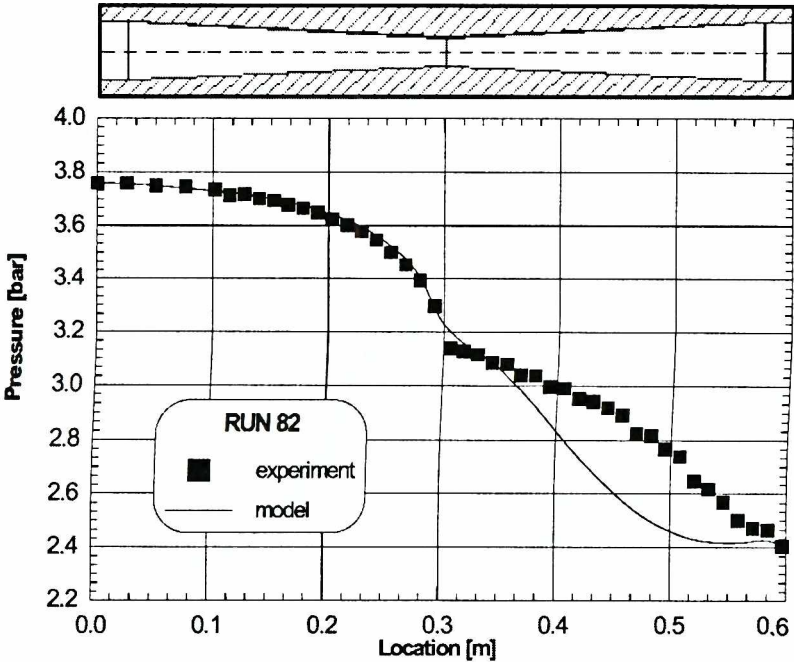
Figure 6.10. Experimental and theoretical pressure distribution along channel for run No. 82 of the BNL experiments, $T_{in} = 142.3\,°C$, $p_{in} = 3.758$ bar, $G_{exp} = 2360$ kg/m²s, $G_{cal} = 2084$ kg/m²s
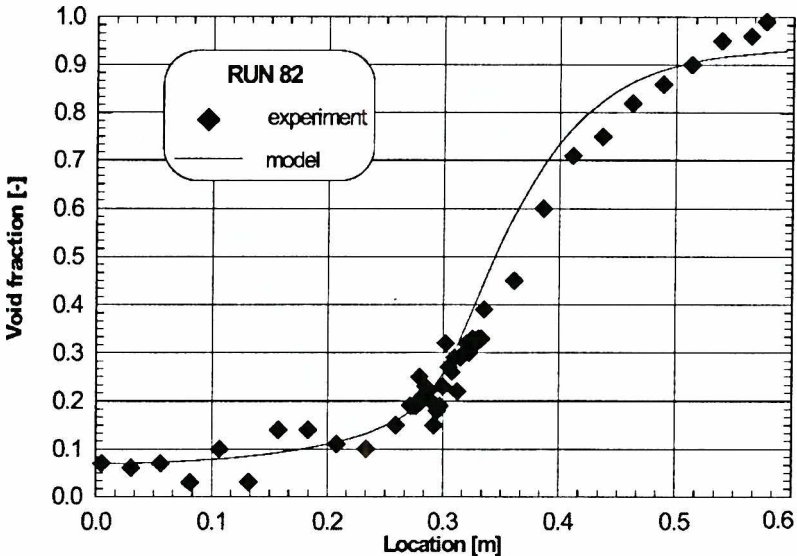

Fig 6.11. Experimental and theoretical void fraction distribution along channel for run No. 82 of the BNL experiments, $T_{in} = 142.3\,°C$, $p_{in} = 3.758$ bar, $G_{exp} = 2360$ kg/m²s, $G_{cal} = 2084$ kg/m²s

Verification of the model was also performed in conditions radically different from the considered above. Experimental data were taken from the Russian experiments of Karasev *et al.* [138] which were carried out in a microscale nozzle at pressures in the order of a few dozen of bars and temperatures about 300 °C.
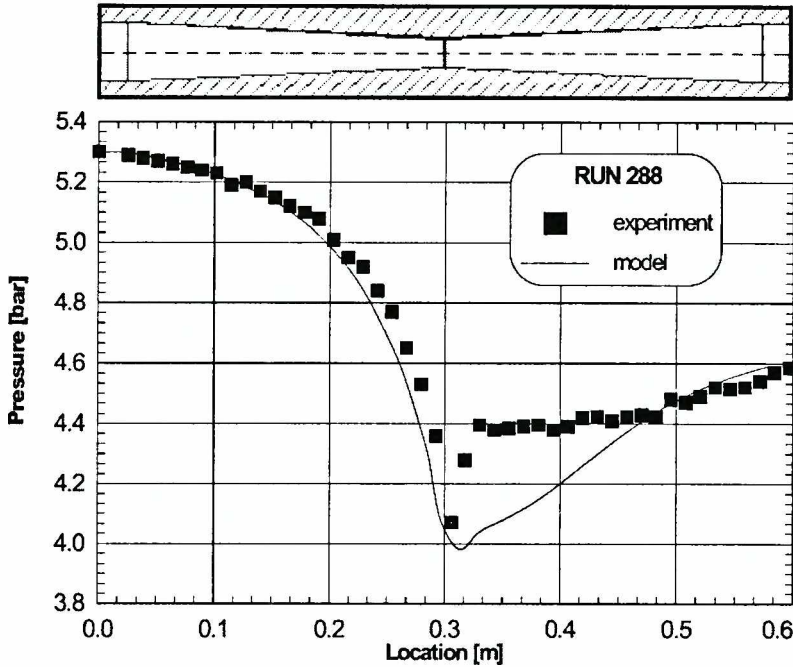
Figure 6.12. *Experimental and theoretical pressure distribution along channel for run No. 288 of the BNL experiments,* $T_{in} = 149.1\,°C$, $p_{in} = 5.3$ *bar,* $G_{exp} = 3580$ *kg/m²s,* $G_{cal} = 4010$ *kg/m²s*
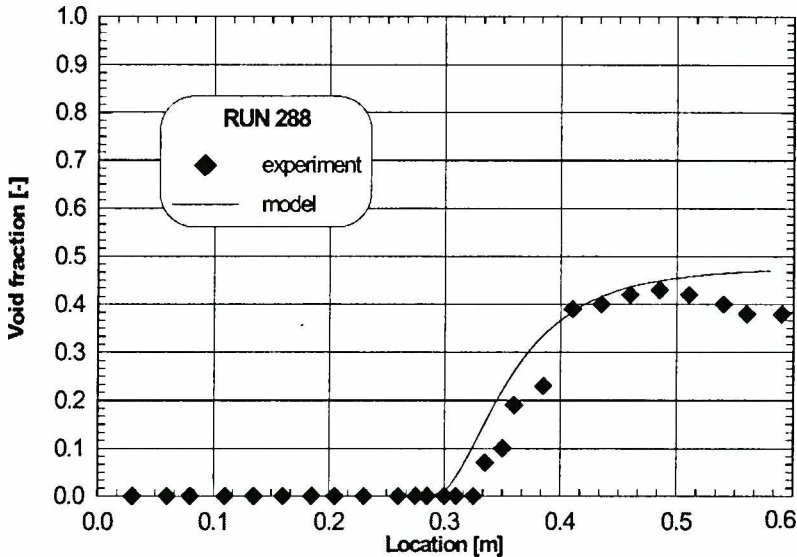

Figure 6.13. *Experimental and theoretical void fraction distribution along channel for run No. 288 of the BNL experiments,* $T_{in} = 149.1\,°C$, $p_{in} = 5.3$ *bar,* $G_{exp} = 3580$ *kg/m²s,* $G_{cal} = 4010$ *kg/m²s*

The results of numerical calculations are shown in Figures 6.14÷6.15. The comparison of the numerical results with the experimental data was done only for pressure since measurements of void fraction were not performed. As it is seen, the pressure reveals a reasonably good agreement with the experimental measurements.
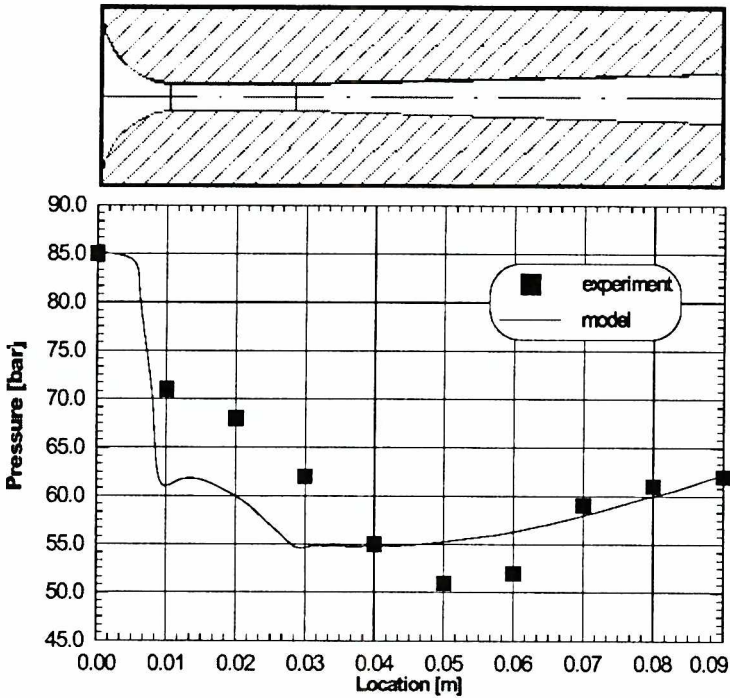
Figure 6.14. *Experimental and theoretical pressure distribution along channel for the Karasev experiments,* $T_{in} = 299\,^{\circ}C$, $p_{in} = 85$ *bar*
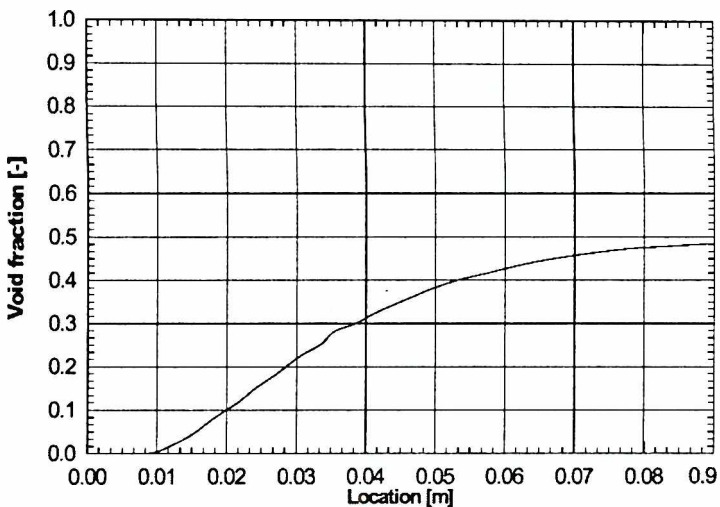
Figure 6.15. *Theoretical void fraction distribution along channel for the Karasev experiments,* $T_{in} = 299\,^{\circ}C$, $p_{in} = 85$ *bar*

Despite its increase in the diverging section, an increase of void fraction is observed, which shows that evaporation takes place in this region of increasing pressure.

The performed calculations for different geometries of channels and at different physical conditions reveal not only satisfactory agreement of the model with the

experiments but also the experimentally observed phenomenon of pressure decrease in a divergent channel in subcritical conditions. This is a characteristic feature of pseudo-critical two-phase flows which differentiates them from single-phase flows.

In the summary of the numerical calculations one can say the present model can be used for the predictions of pressure drops and the calculations of mass flow rates in the whole range of the dryness fraction $0 < x < 1$. These quantities are integral characteristics of a model and are very important in engineering calculations. One can calculate both two-phase flows in the whole channel and flows of water with evaporation started inside the modelled channel. At the inlet of a canal one can assume subcooled, saturated or superheated water as well as a mixture of saturated steam and subcooled, saturated or superheated water. In terms of the presented model one can obtain distributions of basic thermodynamic and fluid-flow parameters, like pressure, velocity, temperature of water and steam, void fraction, dryness fraction, density, mass and volumetric flow rate, enthalpy, internal energy, kinetic energy of a mixture, water and steam. Also additional, specific for the model characteristics, like friction force, capillary stresses, intensity of vapour generation, *etc*. are available.

7. Summary

The aim of the present paper was to describe phenomena taking place on interfacial surfaces during nonequilibrium flashing water flow. An attempt was made to build a mathematical model describing two-phase flows within the framework of homogeneous approach and taking into account heterogeneous structure of the system.

The above purposes were accomplished by formulating a theory of heterogeneous phase transitions of first order enabling us to describe capillary effects explicitly. The main aspects of the proposed theory concern constitutive equations for a stress tensor and free energy of the two-phase water-steam medium. On the basis of the second gradient theory and the theory of internal parameters, a relation for reversible stresses in a system with internal microstructure was derived. In this relation, a stress tensor of homogeneous system and a capillary stress tensor describing stresses induced by internal nonuniformity of the system were distinguished. Capillary stresses have their origin in the gradients of the dryness fraction within interfacial areas and on phenomenological level were modelled just with the help of these gradients. That is why the constitutive relation for the stress tensor of two-phase system includes gradient terms which are a representation of the capillary stresses.

The same theories were used to derive a formula for the free energy of the two-phase fluid. As in the case of the stress tensor, in this formula a part representing the free energy of homogeneous system was distinguished from an additional contribution coming from interfacial surfaces. The energy of interfaces was expressed by the gradients of the dryness fraction modelling nonlocal molecular interactions and the energy connected with them.

The main aspect of the work is the formulation on the basis of the proposed theory of a nonequilibrium mathematical model describing two-phase water-vapour flows. One-dimensional balance equations for mass, momentum and energy of the mixture and balance equation for the mass of vapour were derived. The momentum and energy equations include gradient terms modelling the capillary stresses, which were obtained on the basis of the proposed form of the stress tensor. From the postulated form of the free energy, a constitutive equation for the volumetric source of vapour was derived. This is a relaxation equation and is an extension of the classical relaxation equation successfully describing nonequilibrium vapour generation. This new, in the field of two-phase flows, equation includes two relaxation terms and a gradient one which is responsible for the contribution of interfacial energy.

The performed analysis of wave properties of the model revealed that it is dispersive with respect to small disturbations. This means that small exponential disturbations propagate with a velocity dependent on their frequency. It turned out that the velocity of disturbations increases along with the frequency to infinity, at a simultaneous increase of the coefficient of attenuation. Physically this means that information in such a system can propagate with very large velocities, but owing to their strong damping the spatial range of propagation is significantly limited. Thus, the model is dispersive and dissipative. A consequence of this is a limited mass flux in channel flows, which was confirmed by the numerical calculations of critical mass flux of the two-phase medium. A series of calculations performed for the conditions of critical flow revealed a good quantitative agreement of the theoretical model and the experimental measurements which suggest the practical usefulness of the model.

Apart from a theoretical significance consisting in showing a way of modelling of capillary phenomena within the framework of homogeneous approach, the present work is also of practical importance. The presented here one-dimensional model of flashing flow, besides calculations of critical flows, can also be used in the determination of pressure and void fraction profiles in channels. Its usefulness in such an analysis was confirmed by the calculations carried out for the *Moby Dick* and *BNL* experiments. The comparison of the results of numerical calculations to the measurement data revealed not only qualitative but also quantitative agreement between them. Pressure drop in a channel, mass flow rate of liquid and vapour, maximal flow rate of a two-phase mixture are important, from an engineering point of view, integral characteristics of two-phase flows, which depend on various local parameters describing the flow. That is why the conformity of these characteristics with reality is a strong confirmation of physical correctness of the model and its mathematical representation.

A way of determination of the coefficients appearing in the constitutive equations for the stresses and free energy of the two-phase system was not proposed. We limited ourselves only to an estimation of the values of the constants appearing in the one-dimensional equations by fitting calculations into experiments.

A further step in the development of the presented model could be theoretical determination of the unknown phenomenological coefficients with the aid of molecular theories.

The presented considerations on the state of stresses concern only reversible stresses, not connected with motion of luid. It is generally recognised that the existence of interfaces introduces anisotropy of physical properties, and the motion of the interfaces causes dissipation of momentum and energy, which should also be taken into account in a model of the system with internal dissipative microstructure. Some analogies can be also suspected in the behaviour of thermal properties of such systems. Hence, it is seen that the presented model can be developed in various directions, and the present work is only the first and the simplest step in the description of capillary effects with the help of homogeneous model, well checked and for many years developed in the field of two-phase flows.

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