A REVIEW OF THE RELAXATION MODELS FOR PHASE TRANSITION FLOWS CENTERED ON THE TOPOLOGICAL ASPECTS OF THE NONEQUILIBRIUM MASS TRANSFER MODELLING

Wojciech ANGIELCZYK*

*Faculty of Mechanical Engineering, Białystok University of Technology, ul. Wiejska 45C, 15-351 Białystok, Poland

w.angielczyk@pb.edu.pl

Abstract: The first part of this work is a brief (application-oriented) review of the different classes of multiphase flow models. The review starts with the most generic approaches and descends to the class of Homogeneous Relaxation Models (HRM) of two-phase flow. Subsequently, this work presents a detailed review of the developed relaxation equations describing nonequilibrium mass transfer in two-phase flows. Some of the reviewed equations (in particular, the closure equations of HRMs) have quite simple mathematical structures but there are indications that they should be, in a specific way, more complex. Consequently, the main aim of this article is to bring attention to this problem and expose its nature and practical importance. The analyses conducted in this study reveal that relaxation closure equations formulated as advection equations may disrupt the phase space structure of the model, whereas equations formulated as phasic mass conservation do not pose such an issue. This distinction arises from the presence of a greater number of gradients in the conservation equations (a minimum of two, compared to potentially just one in an advection equation), rendering the conservation equations mathematically more complex.

Key words: nonequilibrium mass transfer, relaxation equation, Homogeneous Relaxation Model, Delayed Equilibrium Model

1. INTRODUCTION

Over the past few decades, significant strides have been made in advancing the mathematical and numerical modelling of phase transition flows. These advancements have substantially enhanced our ability to describe intricate phenomena, particularly nonequilibrium processes occurring within and between flowing phases. A prevalent method for characterizing nonequilibrium involves treating it as a superposition of distinct disequilibrium processes [1]. These processes are incorporated into the model as relaxation terms within the mass, momentum, and energy conservation laws or via dedicated closure relaxation equations.

Each type of a multi-phase flow is a flow of separate fluids. There always are interfaces (or an interface) that distinguish one phase (fluid) from another [2]. Consequently, every multi-phase flow can be modelled using the Navier-Stokes equations providing that the boundary conditions for each of the phases and at the moving interfaces are specified (direct simulation) [3]. The computational cost of such an approach is enormous, and accounting for the nonequilibrium processes is problematic. Besides, practically important is the number and the surface area of these interfaces in the considered element of the flowing fluid. Taking the ratio of the mentioned quantities into consideration allows us to make appropriate simplifications concerning boundary conditions, fluid and flow variable averaging procedures and finally, the type and number of governing equations. Implementation of those simplifications in a mathematical form gives a flow model specialized for a given two-phase flow structure or range of structures. In this way a variety of specialized models were developed. One of the

most generic of them is the two-fluid model in which a system of conservation equations for mass, momentum, and energy is solved for each phase/fluid [3]. As a consequence of the space and/or time averaging of the phases' properties, the detailed structure of the interphase is lost. However, this six-equation model can account for the difference in pressures, temperatures, and velocities of the phases [4]. Moreover, source terms or closure equations describing interphase mass, momentum, and energy transfer can account for the nonequilibrium effects [4].

The other broad application range model is a seven-equation two-phase flow model of Baer and Nunziato (BN) [5] that can account for velocity, pressure, and temperature disequilibrium between the phases. Originally, the BN model was developed to describe a deflagration-to-detonation transition in granular explosive materials (thus, it is a two-phase solid-gas flow model). However, after certain modifications, it turned out to be capable of describing multiphase flows with ongoing phase transitions accompanied by various non-equilibrium effects [6].

The following multiphase and multidimensional version of the BN model is possibly the most generic:

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla(\alpha_k \rho_k u_k) = C_k, \qquad (1)$$

$$\frac{\partial(\alpha_k \rho_k u_k)}{\partial t} + \nabla(\alpha_k \rho_k u_k \otimes u_k + \alpha_k p_k \underline{I} - \alpha_k \underline{\tau}_k) = p_{k*} \nabla \alpha_k + M_k - \underline{\tau}_I \nabla \alpha_k + \alpha_k \rho_k g_k, \qquad (2)$$

$$\frac{\partial(\alpha_k \rho_k E_k)}{\partial t} + \nabla[\alpha_k(\rho_k E_k + p_k)u_k - u_k \alpha_k \underline{\tau}_k] = u_I p_{k*} \nabla \alpha_k - p_I F_k + \epsilon_k - u_I(\underline{\tau}_I \nabla \alpha_k) + q_k + J_k + \alpha_k \rho_k(u_k g_k), \qquad (3)$$

$$\frac{\partial \rho_k}{\partial t} + \nabla(\rho_k u_k) = -\frac{\rho_k}{\alpha_k} F_k, \tag{4}$$

where: α - the volume fraction, ϵ - the interphase energy transfer rate per infinitesimal volume (piv) [W/m3], ρ - the density [kg/m3], C – the interphase mass transfer rate piv [kg/(s m3)], E - the specific total energy [J/kg] (the potential energy is commonly neglected), F - the compaction rate (mimics the effects of microstructural forces) [1/s] [7], g - the acceleration vector caused by the net external body force [m/s2], J - the external heat transfer rate piv [W/m3], M – vector of the interphase momentum transfer rate piv [N/m3], p - the pressure [Pa], q – the conduction heat transfer rate piv [W/m3], t – time [s], $u = [u_x, u_y, u_z]^T$ - the velocity vector [m/s], $\underline{\tau}$- the viscous stress tensor (frequently calculated by the Newtonian approximation [4]) [Pa], $\underline{I}$- the identity tensor, k - subscript indicating the phase $(k = 1, ..., n)$, k* - subscript indicating the conjugate phase of the phase k [6], n - number of phases, I – subscript denoting interface quantity.

The blue terms in Eq. (1-4) are viscosity, heat conduction, and external energy source terms, respectively, recently added to the BN model by Zhang et al. [6]. However, the interphase mass transfer C_k was omitted in [6], consequently, the model can accurately describe flows without interphase mass exchange.

In the presented model formulation (Eq. 1-4) this limitation was removed (by addition of the first green term). Also, the terms for including external body forces effects (two last green terms) were added.

The presented partial differential equations express the conservation of mass (Eq. 1), momentum (Eq. 2), and energy (Eq. 3) and they must be formulated for each of n phases, while the compaction dynamics equation (Eq. 4) is required only for $(n - 1)$ phases [7].

Taking $n = 2$ and replacing the green and blue terms with zeros yields the multidimensional version of the original (seven-equations) BN model [7] wherein for k=1, k*=2 (or for k=2, k*=1), moreover:

$$C_2 = -C_1, \quad \epsilon_2 = -\epsilon_1, \quad M_2 = -M_1, \quad F_2 = -F_1. \tag{5}$$

Let us further assume that the mixture is a vapor-liquid system and admit k=1 for the vapor and k=2 for the liquid, and introduce $C = C_1 = |C_2|$, and $F = F_1 = |F_2|$, then the previously described compaction rate and the source terms can be expressed as follows [8]:

$$F = r_p(p_2 - p_1), \tag{6}$$

$$M = Cu_1 + r_u(u_1 - u_2), \tag{7}$$

$$\epsilon = C\left(e_2 + \frac{1}{2}u_2^2\right) + r_u u_2(u_1 - u_2) \\ + r_T(T_1 - T_2), \tag{8}$$

where: T denotes absolute temperature [K] and e stands for specific internal energy [J/kg]. More on the physical meaning of those source terms can be found in [8]. For the purpose of this work, it is only important to understand that those source terms characterize phase interactions and that some of their components (relaxation terms) decide how fast the difference in a given phasic variable decreases (relaxes) with time. In this meaning, one can say that the drag source $r_u(u_1 - u_2)$ present in the momentum (Eq. 2) and energy (Eq. 3) equations, equilibrates velocities. The heat transfer term $r_T(T_1 - T_2)$ in the energy equations (Eq. 3) equilibrates temperatures. Finally, the whole compaction dynamics equation (Eq. 4, with the relaxation term F)

is a relaxation law that drives the phases toward pressure equilibrium.

The relaxation rates r_p, r_u, r_T are all positive and the higher they are the faster a given variable equilibrates.

In contrast to the two-fluid model (dedicated mainly to fully separated flows), BN-type models assume that the flowing mixture is homogeneous enough to be treated as a continuum with phenomenologically appropriate parameters such as density, velocity, temperature, or sound speed.

1.1. Hierarchy of the BN-type relaxation models

A narrower-scope model can be derived from BN model (Eq. 1-4) by introducing infinite-rate relaxation for a selected property. In such a way a hierarchy of relaxation models can be established [9].

Applying an infinite relaxation rate of velocity reduces the model to the six-equation single-velocity model [9] that can account for pressure, temperature, and chemical potential disequilibrium between the phases. Thus, the resulting model is simpler (easier to be solved [9]) but unable to fully describe a possible mechanical disequilibrium in the flow (both phases still could have different pressures but must have the same velocity). This kind of model can accurately describe cavitating, flashing and condensing flows providing that one of the phases is quite uniformly distributed in the other phases (homogeneous flow). Moreover, it can be used for modelling of the interfacial flows as the same type equations apply to the direct numerical simulation of boiling flows at sub-bubble scale.

Subsequently, assuming instantaneous pressure relaxation the five-equation mechanical equilibrium model (single-velocity and single-pressure) is obtained [9]. The formulation of a such model was done by Kapila et al. (2001) [8] and then it was adjusted for cavitating flows by Saurel et al. (2008) [10] and Le Martelot et al. (2013) [11]. This class of models accurately describes flashing and condensing homogeneous flows. It can be used for predicting the cavitating flows in cases when the pressure difference between phases does not play a significant role [11].

In the limit of instantaneous mechanical and thermal relaxation we obtain a four-equation, single-velocity, single-pressure, and single-temperature two-phase flow model.

The first of such models relayed on the relaxation of the chemical potential [12]. The later model proposed simultaneous relaxation of three different fluid properties (including the Gibbs free energy) [13]. However, in the subsequent models [14], the interphase mass transfer is driven by a difference in only the Gibbs free energy of the phases. In [15], a fast solver for such models is proposed.

Considering the equality of pressures and temperatures of the phases, a non-zero difference in Gibbs free energy is possible due to the application of the van der Waals Equation of State (EOS) for each phase [16]. However, a physically consistent EOS leads to the same Gibbs free energy for vapor and liquid at the same temperature and pressure. In turn, an assumption that both phases are in metastable states introduces inequality of at least one of the mentioned intensive properties. For those reasons, this class of models can be treated as physically inconsistent.

Finally, in the limit of full instantaneous thermodynamic equilibrium, the three-equation Homogeneous Equilibrium Model (HEM) [17] is obtained. The HEM can accurately describe homogeneous two-phase flows without strong pressure changes and

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rater with subsonic velocities as it does not account for any of the nonequilibrium effects, and it underestimates the sound speed for flows characterized by low vapor mass fraction.

There is a four-equation (single-velocity, single-pressure) two-phase flow model that is often treated as a BN-type model however it cannot be obtained as the above-mentioned models. It is a Homogeneous Relaxation Model (HRM) [18] in which the interphase mass transfer is driven by a thermal disequilibrium between the metastable liquid and the saturated vapor. An evolution of vapor mass fraction in the HRM is described by a rate equation [19]. Introducing of a third phase into the HRM leads to the Delayed Equilibrium Model (DEM). This additional phase is a saturated liquid that has the same pressure p as the remaining phases and the same temperature as the saturated vapour $T_{sat}(p)$. The temperature of the metastable liquid T is higher than the temperature of the saturated phases.

1.2. General remarks and historical background on modelling of the relaxation phenomenon in fluids

Relaxation is a process of return of a disturbed system to equilibrium. Relaxation time θ characterizes the speed of the return. If the state of the system is characterized by the property ψ, then its relaxation changes are described as follows [20]:

$$\frac{D\psi}{Dt} = \frac{\partial\psi}{\partial t} + u\nabla\psi = -\frac{\psi - \psi_{eq}}{\theta}, \tag{9}$$

where ψ_{eq} is the value of the property ψ at equilibrium. The physical sense of the relaxation time θ is such that after it has elapsed the deviation from the equilibrium state $(\psi - \psi_{eq})$ decreases e times (e - the base of the natural logarithm).

The idea of relaxation time has been successfully used already by Einstein (1920) [21], to analyse sound propagation in partially dissociated gases, and Mandelshtam and Leontovich (1937) [22], in the analysis of sound absorption in liquids. Nevertheless, probably the first application in the field of two-phase flows is attributed to Bauer (1976) [23], who replaced ψ in Eq. (9) with the vapour mass fraction x to describe nonequilibrium mass transfer between phases of a gas-liquid mixture. Then, the concept presented by Eq. (9) was adopted in the seven-equation two-phase flow model of Baer and Nunziato (1986) [5]. However, it was not until 1990 that Bilicki et al. [18] analysed this equation in the background of the linear theory of irreversible processes (stating that it is fully consistent with the mentioned theory). They also showed that the theoretical expression for the relaxation time depends on the second-order derivative of specific Helmholtz free energy a. This suggests that in the concerned modification of Eq. (9), implicitly, apart from ∇x, a second gradient ∇a is involved. Also, the same article shows how to attach the concerned relaxation equation to the system of the conservation equations (of mass, momentum and energy) to formulate the HRM. Subsequently, the authors described the difference between the HEM and HRM, focusing on a study of dispersion, characteristics, choking, and shock waves. However, no closure equation for the relaxation time θ was proposed; instead, several constant values for this parameter were assumed in the calculations.

2. REVIEW OF NONEQUILIBRIUM MASS TRANSFER RELAXATION MODELLING FOR TWO-PHASE FLOWS

This review is supposed to present selected available literature approaches that, according to the author's knowledge, cover all developed consistent modelling techniques.

To make this review more useful, it was decided to provide the numbers of equations and tables that describe the presented equations in the Original Article (OA). Those numbers are given in angle brackets.

The equations, that can be found in the OA, generally differ visually from the presented versions since they have been transformed to match the form given by Eq. (11) or Eq. (12), and the nomenclature of this work.

2.1. Simple thermodynamic relations

Only equations with one relaxation source term are classified into this category. These relations are most often encountered in BN-type models in the form of the phasic mass conservation equation (Eq. 1). Otherwise, they have the form of an advection equation:

$$\frac{\partial \beth_k}{\partial t} + u_k \nabla \beth_k = K_k, \tag{10}$$

where $\beth_k$, in the case of the two-phase flow, is the volume fraction α, the vapour mass fraction x or the mass fraction of the saturated phases y (the saturation index). In all these cases:

$$K_k = r(\psi_k - \psi_{k*}), \tag{11}$$

or

$$K_k = r(\psi_k - \psi_{eq}), \tag{12}$$

where ψ_k denotes a thermodynamic property of the k phase, ψ_{eq} denotes a value of that property at equilibrium (for $\psi_k = y$, $\psi_{eq} = y_{eq} = 1$), and r is a relaxation rate. The relaxation rate is inversely proportional to the relaxation time θ of the considered thermodynamic property ψ.

The above description is a generalisation (of the various approaches found in the literature – Tab.1 and Tab. 2) made to emphasise the fundamental concept: the difference of a certain property between phases (or its value at the equilibrium state) is the driving force of the mass exchange process. However, it has the following limitations: It can only be used for properties that, at equilibrium, have the same value in all phases. Eq. (11) has no physical meaning for properties describing mixture composition (such as the volume fraction and the mass fraction).

A drawback of the considered approaches is predicting zero interphase mass transfer when $\psi_k = \psi_{k*} \neq \psi_{eq}$ (or, in other words, when $\psi_k = \psi_{k*}$ and $r \neq \pm\infty$). Thus, the model formulation in which such a situation is possible (e.g., a model with constant r) cannot describe the equilibrium mass transfer.

Tab. 1 summarises the approaches described by Eqs. (10 – 12). Tab. 2 is a synopsis of the approaches described by Eqs. (1,11,12) for which C = K. The last column of each of these tables shows the reference index of the article from which the given equation comes (Original Article Index, OAI). This column also exhibits the fluid type for which the equation was developed. If the fluid is not specified, the equation is supposed to hold for

every fluid. Some approaches presented in Tab. 2 are based on the conservation equation of the phasic mass (Eq. 1) in which the left-hand side uses x instead of α. In this case, (x) is added just after the model type description.

Tab. 1. Review of the selected simple thermodynamic relations for nonequilibrium mass transfer modelling with a form given by Eq. (10). Denotations and remarks: T - in the description of the model type, indicates that the model is transient; a lack of T implies a steady-state flow model, S_I - the specific exchange surface; c- the acoustic speed; $\varphi = [p_{sat}(T) - p][p_c - p_{sat}(T)]^{-1}$; $p_{sat}(T)$ – the saturation pressure at a temperature of the metastable liquid T; p_c – the fluid's critical pressure; A, P – the flow channel cross-section area and its perimeter, respectively; $(2y - y^2)_{eq} = 1$; u_{L0} - the liquid superficial velocity; $\varepsilon = 75.28(A_{div} - A_{conv})(A_{ref} - A_{conv})^{-1}$; A_{div}, A_{conv} – the convergence and divergence rates of the converging-diverging nozzle, respectively; A_{ref} – referential nozzle divergence rate

Form of K / Model type	$\beth, \psi$	Relaxation rate r	OAI / Fluid
Eq. (11) < Eq. 3.1a > / 3D T BN	α, p	$\dfrac{S_I}{c_1\rho_1 + c_2\rho_2}$ < Eq. 3.1h >	[10]
Eq. (11) < Eq. 6a / Eq. 1a > / 3D T BN	α, p	Constant / Unspecified < Eq. 2a > / ---	[9/11]
Eq. (11) < Eq. 1a > / 3D T BN	$\alpha, \rho c^2$	$\dfrac{\nabla u}{\rho_1 c_1{}^2\alpha_1{}^{-1} + \rho_2 c_2{}^2\alpha_2{}^{-1}}$ < Eq. 1a >	[11]
Eq. (12). < Eq. 3 > / 1D T HRM	x, x	$\left[3.84 \cdot 10^{-7} \cdot \alpha_1{}^{-0.5}\varphi^{-1.8}\right]^{-1}$ < Eq. 11 >	[19] / H₂O
Eq. (12) < Eq. 4 > / 1D T HRM	x, x	$\left[2.14 \cdot 10^{-7} \cdot \alpha_1{}^{-0.5}\varphi^{-1.8}\right]^{-1}$ < Eq. 21 >	[24] / CO₂
Eq. (12) < Eq. 9 > / 3D HRM	x, x	$\left[\theta(p) \cdot \alpha_1{}^{a(p)}\varphi^{b(p)}\right]^{-1}$ < Eq. 12, Tab. 3 >	[25] / CO₂
Eq. (12) < Eq. 25 > / 1D DEM	y, y	$-0.02\dfrac{P}{A}\varphi^{0.25}$ < Eq. 25 >	[26] / H₂O
Eq. (12) < Eq. 8 > / 1D DEM	$y, 2y - y^2$	$-0.01\dfrac{P}{A}\left(\dfrac{|u|}{|u_{L0}|}\right)^{0.1}\varphi^{0.25}$ < Eq. 8 >	[27] / H₂O
Eq. (12) < Eq. 59, Eq. 60 > / 1D T DEM	y, y	$-(0.0084\dfrac{P}{A} + 0.6337)\varphi^{0.228}$ < Eq. 59, Eq. 60 >	[28] / H₂O
Eq. (12) < Eq. 24, Eq. 25 > / 1D DEM	y, y	$-(38 + 1.3 \cdot 10^{-39}e^\varepsilon)\varphi^{-0.22}$ < Eq. 24, Eq. 25 >	[29] / CO₂
Eq. (12) < Eq. 2 > / 1D DEM	y, y	$-(0.1086\dfrac{P}{A} + 0.5958)\varphi^{0.228}$ < Eq. 2, Tab. 8 >	[30] / C₂H₂F₄

Tab. 2. Review of the selected simple thermodynamic relations for nonequilibrium mass transfer modelling with a form given by Eq. (1). Denotations and remarks: μ – the chemical potential; g – the specific Gibbs free energy; h - the specific enthalpy; ML – subscript denoting the metastable liquid; SL - subscript denoting the saturated vapor; SL – subscript denoting the saturated liquid; $(h_{ML}h_{SG})_{eq} = h_{SL}h_{SG}$; $\varkappa$ - isentropic exponent of the vapor

Form of C / Model type	ψ	Relaxation rate r	OAI / Fluid
Eq. (11) < Eq. 3.1.1 / Eq. 1b > / 1D/3D T BN	μ	Constant / Unspecified < Eq. 2c> / ---	[9/12]
Eq. (11) < Eq. 3, Eq. 47a / Eq. 3.1 > / 1D,3D T BN (x)	g	$\rho\, r_g(S_I, p, T)$ < Eq. 3, Eq. 47a / Eq. 3.1 >	[14/15]
Eq. (12) < Eq. 4a, Eq. 14 > / 1D T HRM (x)	$h_{ML}h_{SG}$	$\dfrac{\rho^2(x - x^2)(\varkappa - 1)}{\varkappa\, p\,(h_{SL} - h_{SG})\,\theta}$ < Eq. 4a, Eq. 14 >	[31] / H₂O
Eq. (12) < Eq. 6 > / 1D HRM (x)	x	$\dfrac{\rho}{2.15 \cdot 10^{-7} \cdot \alpha_1{}^{-0.54}\varphi^{-1.76}}$ < Eq. 10 >	[32] / CO₂

2.2. Empirical phenomenological relations

All equations described by the fourth and next rows of Tab. 1 and the equations from the two last rows of Tab. 2 can be classified as empirical phenomenological relations since their relaxation rates have been developed for specific fluids by adjusting the presented equations' constants so that the modelling would result with possibly best approximation of the experimental data.

2.3. More advanced thermodynamic approaches

This category gathers equations based on the idea presented in the previous section that have more than one relaxation source term. Additionally, approaches using more than one equation (from the set of all equations constituting the model) to describe non-equilibrium mass transport are also presented here. A notation that in each relaxation term, the difference in the property

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that is relaxed stands in the square brackets was used. Therefore, everything outside of these brackets, in a given relaxation term, is the relaxation rate of the considered property.

In [17], <Eq. 3.1.1>, an approach based on a 1D version of Eq. (1) is presented. In this equation the right-hand side is given in the following form <Eq. 3.1.8b>:

$$C = r[s_1 - s_2] + r\left[\frac{h_2}{T_2} - \frac{h_1}{T_1}\right] + r\left[\frac{L}{T_1} - \frac{L}{T_2}\right], \quad (13)$$

where s is the specific entropy, and $L = h_{SG} - h_{SL}$ is the specific latent heat. In this approach, there are three relaxation source terms that have a common relaxation rate r being a positive constant.

Another 1D equation is proposed in [33] in the following form <Eq. 43c>:

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial(\rho_2 u)}{\partial x} = r[f(\rho_2) - f(\rho_1)] + r\mu(\rho_2)[\rho_1 - \rho_2], \quad (14)$$

where f is the Helmholtz free energy per unit volume. The relaxation rate in the first relaxation source term is $r = \gamma^{-1}(\rho - \rho_1)(\rho - \rho_2)$, while for the second relaxation source term it is $r\mu(\rho_2)$. Finally, γ is a relaxation parameter that determines the rate at which the chemical potentials and pressures of the two phases reach equilibrium.

The approach presented in [13], among the five model equations, contains three equations responsible for non-equilibrium mass transfer modelling. The first of them <Eq. 1a > has a form of the volume fraction advection equation (Eq. 10, $\beth = \alpha$). Thus, it is necessary to present only its right-hand side:

$$K = \nabla\boldsymbol{u}\omega[\rho_2 c_2^2 - \rho_1 c_1^2] + \rho v\left(\frac{c_2^2}{\alpha_2} + \frac{c_1^2}{\alpha_1}\right)\omega[g_2 - g_1] +$$
$$H\left(\frac{\Gamma_2}{\alpha_2} + \frac{\Gamma_1}{\alpha_1}\right)\omega[T_2 - T_1], \quad (15)$$

where $\omega = (\rho_1 c_1^2\alpha_1^{-1} + \rho_2 c_2^2\alpha_2^{-1})^{-1}$, v and H are relaxation coefficients, Γ is the Grüneisen coefficient. The second and third equations <Eq. 1b, Eq. 1c> are the phasic mass conservation equation (Eq. 1). Thus, it is necessary to present only their right-hand sides:

$$C = \pm\rho v[g_2 - g_1]. \quad (16)$$

Another approach using three equations (out of the six model equations) for non-equilibrium mass transfer modelling is presented in [34] and extended in [35]. The first equation is the volume fraction advection equation <Eq. 63a>, whose right-hand side reads:

$$K = \zeta_p[p_1 - p_2] + \frac{\zeta_T\hbar A_{\text{int}}}{V}[T_1 - T_2] - \frac{\zeta_G A_{\text{int}}}{V}[g_1 - g_2], \quad (17)$$

where $\hbar$ is the heat transfer coefficient, A_{int} is the interface area (the area of the interphase heat transfer), V is the volume of the considered mixture element, $\zeta_p, \zeta_T, \zeta_G$ are relaxation coefficients. The second and third equations <Eq. 63b, Eq. 63c> are the phasic mass conservation equation. Thus, it is necessary to present only their right-hand sides:

$$C = \pm\frac{A_{\text{int}}}{V}[g_1 - g_2]. \quad (18)$$

It is worth noting that Eqs. (15-18) contain relaxation terms based on the difference between phasic specific Gibbs free energy.

2.4. Relations based on the statistical phase change analysis

The fundamental works in this domain determine the net rate of molecular interfacial transport j that can be a basis for the calculation of the interphase mass transfer rate C. However, translating the equations for j, into those describing C, would significantly complicate them and impede recognition of the relaxed properties and the relaxation rates. Thus, it was decided to avoid that and to introduce only the nomenclature corrections.

In each equation (presented in this and the next section), the difference in the property that is relaxed is enclosed in curly brackets. Therefore, everything outside these brackets is the relaxation rate of the considered property.

The net rate of molecular Interfacial transport of gas into the liquid phase is derived in [36], <Eq. 33>, in the following form:

$$j = -\frac{2 A_s}{C_{eq}}\frac{p_1'}{\sqrt{2\pi m_1 kT_2}}\{C - C_{eq}\}, \quad (19)$$

where A_s is the fraction of the area available for absorbing gas molecules when the liquid is in equilibrium with the gas, p_1' is the partial pressure of the gas above the liquid, m_1 is the molar mass of the absorbed gas, k is the Boltzmann constant, C is the concentration of the gas in the liquid (number of the molecules per unit volume).

In [37] net rate of molecular interfacial transport <Eq. 57> is described as dependent on difference in phasic chemical potentials:

$$j = \frac{2K}{kT}\{\mu_1 - \mu_2\}, \quad (20)$$

where K is the equilibrium molecular exchange rate between phases, T is the two-phase mixture temperature.

Quite complex relation for net rate of molecular interfacial transport is presented in [38], <Eq. 42, Eq. 45>:

$$j = \frac{\eta\, p_{sat}(T_2)}{\sqrt{2\pi mkT_2}}\langle exp\left[\frac{\mu_2}{T_2} - \frac{\mu_1}{T_1} + h_1\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right] - exp\left[-\frac{\mu_2}{T_2} + \frac{\mu_1}{T_1} - h_1\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]\rangle, \quad (21)$$

where $\eta = \exp\left(\frac{1}{\rho_2 kT_2}\left[p_{eq} - p_{sat}(T_2)\right]\right)$, m is the molar mass. However, it can be recognize as a relaxation equation only when transformed to the following form:

$$j = \frac{\eta\, p_{sat}(T_2)}{\sqrt{2\pi mkT_2}}\frac{1}{\dot\rho}\{\dot\rho^2 - 1\}, \quad (22)$$

where

$$\dot\rho = exp\left[\frac{\mu_2}{T_2} - \frac{\mu_1}{T_1} + h_1\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right].$$

In [39] an analysis of evaporation through the classical kinetic theory was conducted. The authors developed relation that reads:

$$j = \frac{\sigma}{1 - 0.5\sigma}(2\pi mkT_2)^{-0.5}\left\{\frac{p_{sat}(T_2)}{\sqrt{T_2}} - \frac{p_1}{\sqrt{T_1}}\right\}, \quad (23)$$

where σ is an empirical coefficient called the condensation coefficient.

2.5. Relations based on the nucleation theories and/or the kinetic theory of phase change

The equations presented here can also be included in the previous section because the kinetic theory of phase change and nucleation theories are closely related to the statistical phase change analysis. However, the rule here is that if the OA specifies the interphase mass transfer rate C instead of the net rate of molecular interfacial transport j, it qualifies for this section.

Of course, many equations for C derived within the theories considered here are not relaxation equations. Unfortunately, despite that some of them are used in the relaxation models. For example, in [40], an equation describing the evolution of the saturation index y, which does not have the features of a relaxation equation was introduced into the DEM. Consequently, the obtained model is not a relaxation model.

In [41], <Eq. 10>, an approach based on the steady-state version of Eq. (1) is presented (however, α is replaced by x). In this equation, the right-hand side is given in the following form, <Eq. 12>:

$$C = R_{boil} = \pm \left[\frac{\hat{\sigma}}{2-\hat{\sigma}}\right]\left(\frac{m\prime}{2\pi G_c T_{\text{sat}}}\right)^{1/2}\{p - p_{\text{sat}}\}, \tag{24}$$

where $\hat{\sigma}$ is the accommodation coefficient that represents the number of molecules passing during the phase change process (it is dependent on the flow conditions and the working fluid, thus, it needs to be adjusted according to the experimental data), G_c is the universal gas constant, m' is the molecular mass. In this approach, C is called the boiling source term R_{boil}.

The above approach is extended in [42] by enlarging the interphase mass transfer rate C by the so-called cavitation source R_{cav}:

$$C = R_{boil} + R_{cav} = R_{boil} \pm \frac{c_c\sqrt{K_T}}{\delta}\rho_1\rho_2(1-x)\left(\frac{2}{3}\frac{p_{\text{sat}}-p}{\rho_2}\right)^{0.5}, \tag{25}$$

where c_c is the cavitation constant, K_T is the turbulence kinetic energy, δ is the surface tension. It can be seen that since the last exponent on the right-hand side differs from one, R_{cav} is not strictly appropriate relaxation term.

3. TOPOLOGICAL ASPECTS OF RELAXATION MODELS

The topological analysis is crucial for understanding the elementary features of the considered models and applying the proper numerical procedures for determining the practically acceptable solutions. This analysis focuses on the steady-state version of the two-phase flow model and uses the theory of dynamical systems. It was conducted and described, in a rather detailed way, in [43] and (more recently) in [44]. Thus, solely elements of the theory that are critical for further investigation of the relaxation equations describing nonequilibrium interphase mass transfer are presented.

In case of doubts regarding the analysis, the reader is guided to the above-mentioned articles or the author's previous publications: A detailed description of the physical sense and mathematical formulation of relaxation models, as well as the Homogeneous Equilibrium Model is presented in [45], while procedures for determining the solutions are presented in [46]. Finally, practical applications of this two can be found in [47].

3.1. General form of the equation system and its transformations

Practically all known one-dimensional models of a steady-state flow can be presented in a form of the following nonlinear ordinary first order differential equation system [43]:

$$A(\sigma)\frac{d\sigma}{dz} = b(z, \sigma), \tag{26}$$

The size and elements of the matrix A and the vector σ depend on the model type. The vector σ consists of n quantities describing a thermodynamic state of the fluid, and if necessary, the velocity of the fluid. The elements of the matrix A depend only on σ's components, and b's elements additionally depend on the spatial coordinate z (specifying distance along the flow channel axis). The set of governing equations (26) supplied with the vector $\sigma_B=[\sigma_{1,B}, \sigma_{2,B}, \ldots, \sigma_{n,B}]$ (describing the flow inlet conditions, the inlet is located at z_B) creates an initial-value problem. A solution to the problem is a trajectory $\sigma(z)$ in $n + 1$ dimensional phase space Ω, which conventionally can be obtained by a numerical integration of the equation system (26).

The system of equations (26) can be solved with respect to the derivatives of σ's components by using Cramer's rule:

$$\frac{d\sigma_i}{dz} = \frac{N_i(z,\sigma)}{D(\sigma)}, \qquad i = 1,2,\ldots,n, \tag{27}$$

where, D denotes the determinant of A, and N_i are determinants, each of which is created by replacing the i-th column of A with b. The most practically useful form of the equation system is obtained by application of the dummy parameter t [43]:

$$\frac{dz}{dt} = D, \ \frac{d\sigma_i}{dt} = N_i. \tag{28}$$

It is worth to notice that in the above autonomous form the independent variable is not z but the dummy parameter t.

3.2. Topological Structure of The Phase Space

Each possible state of a system is represented as a point in the phase space Ω. Thus, for example, if in the mathematical model n=3 then σ consists of 3 components, say: the pressure p, the enthalpy h, the velocity w. Consequently, the state of the fluid and flow in any cross-section of the nozzle is determined by three values of those parameters and value of the spatial coordinate z. Thus, the phase space of this example is 4-dimensional.

However, in general, the phase space is $n + 1$ dimensional, thus for simplicity, the most interesting features of its structure are presented in the form of projections on a pressure p - spatial coordinate z plane depicted in Fig. 1. Accordingly, the black, green, and red curves present projections of $n + 1$ dimensional trajectories on $p - z$ plane. Each solid line is a projection of a solution to the initial-value problem mentioned in the previous subsection. The inlet conditions related to those flows differ only in the velocities. Consequently, all trajectories related to the solid lines start form the same values of the inlet pressure p_B, the inlet density ρ_B, and the inlet specific enthalpy h_B but they are related to different mass flow rates.

It is necessary to distinguish three classes of points in the phase space Ω:

- Regular points at which $D \neq 0$. At each of these points the systems (26), (27) and (28) are equivalent. Any numerical

forward-marching integration of system (26) that starts from the inlet conditions $B=[z_B, \sigma_{1,B}, \sigma_{2,B}, \ldots, \sigma_{n,B}]$ and passes towards the channel outlet, only through the regular points, gives a proper approximation to a physically acceptable analytic solution. The system (26) satisfies the existence and uniqueness requirements (only one trajectory passes through any regular point). A trajectory that consists of only regular points is fully subsonic or fully supersonic. Fig. 1 shows projections of three subsonic trajectories - the green curves that are called Possible Flow (PF) trajectories.

− Turning points at which $D = 0$ and and all $N_i \neq 0$ [18]. At those points the systems (26) and (27) are not equivalent. Numerical integration of (26), in the vicinity of the turning point, produces a systematically accumulating numerical error. As a result, the integration could become impossible even before reaching the turning point. This is because $|d\sigma_i/dz| \to \infty$ while $D \to 0$. However, the autonomous system (28) satisfies the existence and uniqueness requirements at those points. Hence, during its numerical integration, one can simply pass through a turning point and can obtain a proper approximation of a trajectory that, at the turning point, changes direction along the z-axis (the red curves in Fig. 1). The one-dimensional steady-state flow cannot change direction in the channel. Therefore, those trajectories are physically acceptable only if they pass through a point of inlet conditions B and the turning point is located at the end of the channel. Consequently, the solutions that pass through turning points localised inside of the channel are called Impossible Flow (IF) trajectories.
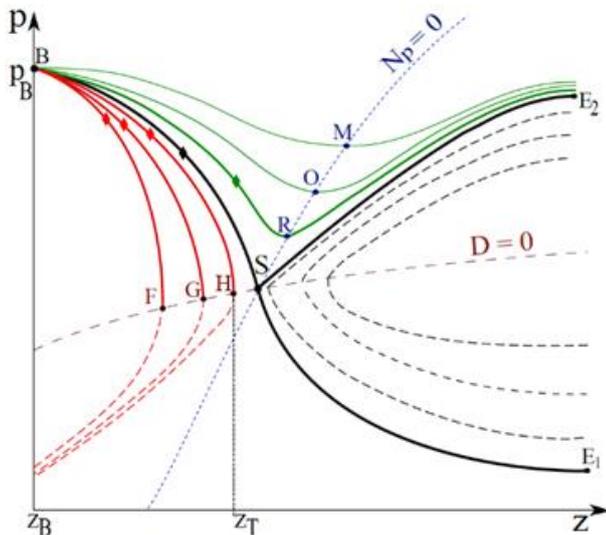

Fig. 1. Illustration of the structure of the considered phase space

In work [18] was shown that $D = 0$ occurring at the channel end is also a choking criterion (or critical flow condition) since $D = 0$ means that at this point the fluid's velocity reaches the local speed of sound, and as a result, the mass flow rate and the subsonic part of the trajectory are unchangeable even despite possible pressure drop occurring beyond the channel exit.

Fig. 1 shows projection of three IF trajectories (the red curves). They pass through the turning points F, G, H. Turning points determine the curve $D = 0$ (the projection of this curve is shown in Fig. 1 as the brown dashed line).

− Singular points at which $D = 0$ and all $N_i = 0$. Here are considered only nondegenerate singular saddle points like S at which $\text{rank}(A) = n - 1$ and through which exactly two trajectories pass. Namely, BSE_1 and BSE_2 in Fig. 1 (but only BSE_1 is "really" a transonic trajectory since on BSE_2 the velocity of the fluid reaches the speed of sound merely at point S to decrease just after it [18]).

According to Eq. (28), $dz = D dt$ and $d\sigma_i = N_i dt$. Therefore, at those points, finite changes Δz and $\Delta \sigma_i$ calculated by the numerical methods are equal to 0 regardless of the integration step size Δt. It means that, the numerical algorithms cannot neither "start from" nor "pass through" this kind of points (they simply "get stuck" in these points - in the theory of differential equations, such points are called equilibrium points). Therefore, contrary to remaining trajectories, the transonic trajectory cannot be determined by a conventional numerical forward-marching integration (even of the system 28).

In [18] it was shown that when $D = 0$ and an arbitrary $N_i = 0$ then all remaining Ns also vanish.

3.3. The topological analysis of the nonequilibrium mass transfer modelling

The review of the equations describing nonequilibrium interphase mass transfer presented earlier revealed a high diversity of these equations. The equations differ in the method of derivation (the phenomenological approaches or the approaches rooted in theories that translate the microscopic behaviour of the fluid into its macroscopic properties), the type of quantity whose difference is relaxed, and the relaxation rates. However, it turns out that from the topological point of view, all these differences are not important. Crucial is the physical nature of the equation in which the relaxation is used. Namely, equations having the form of a conservation equation do not pose topological problems. However, relations in the form of an advection equation (Eq. 10) may be problematic.

To prove the above statement, let us start by noting that the conservation equations, regardless of the choice of σ's components, always contain at least two gradients of different physical quantities. On the contrary, the advection equation for some choices of σ has just one gradient.

The above statement is true for every conservation equation, but in this work, we analyse mass transfer approaches, so we need to prove it only for the mass conservation equation, Eq. (1). To do so, let us extend the divergence term from its left-hand side:

$$\nabla(\alpha_k \rho_k u_k) = \rho_k u_k \nabla\alpha_k + \alpha_k u_k \nabla\rho_k + \alpha_k \rho_k \nabla u_k. \qquad (29)$$

We obtained two terms with different gradients ($\nabla\alpha_k$ and $\nabla\rho_k$) and the divergence term ($\alpha_k \rho_k \nabla u_k$).

Now, let us ponder on the advection equation, Eq. (10). It contains only one gradient $\nabla\beth_k$. The only possibility to get at least two gradients from it is to choose $\beth_k$ and σ in such a way that $\beth_k = \beth_k(\sigma_i, \sigma_j, \ldots)$. However, if this is not the case, Eq. 10 has only one gradient term that in general can be expressed as $a_c \nabla\sigma_j$, where a_c is a non-zero coefficient. Thus, the time-independent 1-D version of the advection equation (10) can be rearranged:

$$\frac{d\sigma_j}{dz} = \frac{K}{a_c}. \qquad (30)$$

The next thing to do is to show that the models that contain equations with only one gradient are topologically degenerated. Let us rearrange the equation system of the flow model in the non-autonomous form (Eq. 27) into the following form:

$$\frac{d\sigma_j}{dz} D(\sigma) = N_j(z, \sigma). \tag{31}$$

Substitution of Eq. (30) to Eq. (31) gives the equation that reads:

$$N_j(z, \sigma) = \frac{K}{a_c} D(\sigma). \tag{32}$$

It means that when the main determinant $D = 0$ then $N_j = 0$. However, $N_j = 0$ does not vanish the remaining Ns (the author proved it for the HRM and the DEM by recalling the momentum equation in [48]).

The consequence of the demonstrated fact is that any model applying such a simple form of the closure equation ("single gradient" equation) does not possess turning points (Fig. 1, the points F, G and H). Instead, other kinds of points appear when $D = 0$. Suppose that $D \to 0$, then according to Eq. (30), $d\sigma_j/dz \to Ka_c^{-1}$, while according to Eq. (27), the remaining derivatives $(i \neq j)$ approaches $\pm\infty$. However, there is no trajectory (a continuous multidimensional curve) that can satisfy such conditions (it is impossible for any curve to turn towards the opposite direction of the z-axis without being parallel to all other axes at the point of turning). In other words, the considered points refer to states that the analysed dynamical system [18] cannot archive.

In summary, the consequence of using "single gradient" closure equation is that the considered model is inconsistent with the previously described structure of the phase space (the model is degenerated). Therefore, there is a clear need for more complex closure equations. The obvious candidate to be tested is an equation containing two gradients.

To prove that the "two gradients" closure equation (thus, also any conservation equation with relaxation terms) does not introduce the topological flaw into the model, let us replace Eq. (30) with the following all-encompassing but simple relation:

$$a_{c,j}\frac{d\sigma_j}{dz} + a_{c,i}\frac{d\sigma_i}{dz} = K, \tag{33}$$

were $a_{c,i}$ and $a_{c,j}$ are non-zero coefficients. Application of this equation to Eq. (31) results with:

$$\left(\frac{K}{a_{c,j}} - \frac{a_{c,i}}{a_{c,j}}\frac{d\sigma_i}{dz}\right) D(\sigma) = N_j(z, \sigma). \tag{34}$$

From Eq. (27) we know that

$$d\sigma_i/dz = N_i(z, \sigma)/D(\sigma),$$

thus:

$$\frac{K}{a_{c,j}} D(\sigma) - \frac{a_{c,i}}{a_{c,j}} N_i = N_j(z, \sigma). \tag{35}$$

We can see that when $D = 0$ then not necessarily $N_j = 0$. Hoverer, having $D = 0$ and any of Ns equal to zero, vanishes the remaining N.

This proves that the presence of at least two different gradient terms in the relaxation equation results in a model with the correct structure of the phase space (at least in the context of considered topological aspects).

4. CONCLUSIONS

This paper presents a brief succinct of the models for phase transition flow, followed by a quite detailed review of the two-phase flow relaxation models just to create an appropriate background for an in-depth review of the nonequilibrium mass transport relaxation equations used in the mentioned models. The reviewed approaches are divided into five classes: simple thermodynamic relations, empirical phenomenological relations, more advanced thermodynamic approaches, relations based on the statistical phase change analysis, relations based on the nucleation theories and/or the kinetic theory of phase change. However, it is just one of many possible systematisations. A broader categorization can be established as follows: phenomenological relations and approaches based on theories that bridge the microscopic depiction of the fluid to properties characterizing its macroscopic behaviour. The considered equations can also be classified as those that have a form of an advection equation (Eq. 10) and those having a form of phasic mass conservation (Eq. 1).

The conducted topological analysis revealed that relaxation equations taking the form of an advection equation (or more precisely equation containing only one term with a gradient of velocity-state vector component), when integrated into the flow model, can lead to a violation of the phase space structure (making the model topologically degenerated).

While the aforementioned sentence describes a potential rather than an inevitability, it becomes evident that all models linked to the equations outlined in Tab. 1 (three B-N type models and eight HRMs) and linked to Eq. (15) and Eq. (17) are inherently topologically degenerated. This does not mean that they are therefore worthless. In fact, the majority of these models have been validated through comparison with experimental results, affirming their practical utility. Then, what practical implications arise from the described degeneration? Let us start with the most certain things.

The practical ramification of the identified flaw is that the determinant described by Eq. (32) cannot be employed as the second condition (alongside $D = 0$) for determining the singular point. Moreover, this determinant is unsuitable for discerning whether the flow is Possible or Impossible. Therefore, if this determinant is used, the conventional solution algorithms of the initial-value problem (the PIF and the NCP algorithms) will not converge to the solution. In general, not being aware of the flaw may lead to the erroneous recognition of any of the turning points as a singular point. The significance of this issues diminishes when modelling unsteady flows or when a steady flow description is achieved by asymptotical convergence of the time-dependent solutions. Since, in such cases, the determination of singular points is not a pivotal step in the solution process. However, mentioned time-dependent solution methods require a significantly longer computation time.

The author also suspects that topologically degenerated models are more difficult to set up to accurately predict experimental flows. In other words, replacing the advection equations with the equations of the phasic mass conservation equation will simplify the mathematical form of correlations for the relaxation time (or the rate of relaxation) or the evolution of the saturation index.

Among the equations reviewed, many are based on the relaxation of the difference in the chemical potential and the specific Gibbs free energy. The author considers these approaches to be the most justified since these quantities are the same for both phases in equilibrium but more importantly, they appear in the first

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law of thermodynamics written for an open multi-component system.

According to the author, relying on the relaxation of other physical quantities (such as pressure, temperature, entropy, etc.) is not deemed a mistake, as long as only two different quantities are utilized. After all, the chemical potential and the specific Gibbs free energy can be conceptualized as functions defined by precisely two distinct intensive properties. Therefore, paradoxically, some equations classified as "more advanced thermodynamic approaches", in the author's opinion, are not physically justified.

Despite awareness of the topological flaw being able to prevent potential problems, The author recommends the use of appropriately complex closure equations to maintain the physical and mathematical consistency of the models. It was proved that closure equations with at least two gradients of different physical quantities should be employed. It is worth recalling that conservation equations exhibit this feature.

Please recall that the theoretical expression for the relaxation time depends on the second-order derivative of specific Helmholtz free energy. However, using such an approach is tantamount to formulating a non-hyperbolic model. Perhaps the physical correctness of modelling will dictate the development of new techniques for solving the considered flow cases.

As a final conclusion, let us note that in the time when the "oldest" of the models considered here were formulated, the conditions of their hyperbolicity were mainly studied. Subsequently, the models of the considered class were examined for their compliance with the second law of thermodynamics. Therefore, the author expresses curiosity about whether the field has now entered an era where scrutiny extends to verifying whether the formulated model is topologically non-degenerate. Nevertheless, the author is confident that in the forthcoming phase of the research, he will focus on delving into unravelling the connection between topological aspects and the model's adherence to the second law, as well as the model's hyperbolicity. However, this is a long-term investigation, while proposing closure equations for the DEM that are topologically correct is now a simple matter for the author and will probably be crowned with an appropriate publication soon.

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Wojciech Angielczyk: iD https://orcid.org/0000-0001-6408-1354