SIMULATION OF TWO-PHASE FLOWS IN VERTICAL TUBES WITH THE CFD CODE *FLU*BOX

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Abstract

The Computational Fluid Dynamics (CFD) code *FLU*BOX is developed at GRS for the multidimensional simulation of two-phase flows. The single-pressure two-fluid model is used as basis of the simulation. A basic mathematical property of the two-fluid model of *FLU*BOX is the hyperbolic character of the convection. The numerical solution methods of *FLU*BOX make explicit use of the hyperbolic structure of the coefficient matrices. The simulation of two-phase flow phenomena needs, apart from the conservation equations for each phase, an additional transport equation for the interfacial area concentration. The concentration of the interfacial area is one of the key parameters for the modelling of interfacial friction forces and interfacial transfer terms. A new transport equation for the interfacial area concentration is in development. It describes the dynamic change of the interfacial area concentration due to mass exchange and a force balance at the phase boundary. Results from *FLU*BOX calculations for different experiments of two-phase flows in vertical tubes are presented as part of the validation.

Introduction

The EU project EUROFASTNET [1] identified industrial needs for the three-dimensional simulation of nuclear reactor thermal-hydraulics. As a consequence the OECD/NEA established Writing Groups concerning the extension of CFD codes to two-phase safety problems. The Writing Groups covered a wide range of two-phase NRS problems (e.g. DNB, dry-out, steam discharge, thermal stratification, etc) in nuclear reactors [2]. Such simulations of two-phase flow phenomena with a two-fluid model need, apart from the basic conservation equations for each phase, an additional transport equation for the interfacial area concentration. The concentration of the interfacial area is one of the key parameters that provide information on the flow pattern. It is also an important parameter for the modelling of interfacial friction forces and interfacial transfer terms. A transport equation for the interfacial area concentration based on the ideas of Papadimitriou [3] is in development. The transport equation describes the dynamic change of the interfacial area concentration due to mass exchange and a force balance at the phase boundary. The modelling of the force balance contains the solution of a momentum equation at the phase boundary. The computation of the dynamic change of the interfacial area concentration with only one transport equation is very attractive concerning the computational costs (in relation to the multi-group models). Validation calculations for vertical air/water flows with different pipe diameters were performed with this model. These include the experiments of Hibiki [4] in a 1 cm tube, the experiments of Kashyap [5] in a 5 cm tube and the experiments of Prasser [6] in a 20 cm tube.

The paper describes the two-phase model approach with a two-fluid model and a transport equation for the interfacial area concentration. The transport equation is solved simultaneously with the conservation equations, with which it is coupled via the interfacial friction. The three test cases mentioned above are described and comparisons of validation calculations with measurements are presented.

Two-Phase Model Equations

Two-fluid model

A general two-fluid model consists of six balance equations, but there remain seven dependent flow parameters: $\alpha_g, u_g, u_l, h_g, h_l, p_g, p_l$. There are two ways to obtain a complete set of equations. Either introduce further simplifications in order to reduce the number of dependent flow parameters or add a further differential equation on a heuristic basis. There have been various attempts in the literature to derive such an additional model equation [7]. However, none of them has reached a state of maturity for direct technical application. Therefore, in most of the present two-fluid models the assumption of equal local pressure $p = p_g = p_l$ is introduced, since the differences in local pressure between the phases are expected to be small and can be neglected for most technical applications. Assuming a single local pressure value the following conservation equations for mass, momentum and energy are derived:

Mass balance equations:

$$\frac{\partial}{\partial t}\alpha_k \rho_k + \nabla(\alpha_k \rho_k \mathbf{u}_k) = \Gamma_k \tag{1}$$

Momentum balance equations:

$$\frac{\partial}{\partial t}\alpha_k \rho_k \mathbf{u}_k + \nabla(\alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k) + \alpha_k \nabla p + (p - p_k^{\text{int}})\nabla \alpha_k = \alpha_k \rho_k \mathbf{g} + \mathbf{F}_k^{\text{int}} + \Gamma_k \mathbf{u}^{\text{int}} - \nabla \cdot (\alpha_k \mathbf{T}_k) \qquad (2)$$

Energy balance equations:

$$\frac{\partial}{\partial t}\alpha_k \rho_k h_k + \nabla(\alpha_k \rho_k h_k \mathbf{u}_k) - \alpha_k \frac{D_k p}{Dt} = \Gamma_k h_k^{\text{int}} + q_k^{ext} \qquad (3)$$

where k=g for gas or vapor and k=l for liquid or water. D_k / Dt is the material derivative $\frac{D_k}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}_k \cdot \nabla$ and $\mathbf{T}_k$ is the turbulent viscosity tensor. Between the volume fractions of the gas or vapor phase and the water phase exists the relation $\alpha_g + \alpha_l = 1$. The densities are calculated from the state equation $\rho_k = \rho(h_k, p)$ using pressure p and enthalpy h. The right hand sides of the two-fluid model equations (1), (2) and (3) describe the interfacial transfer terms of mass, momentum and energy between the phases. This mathematical formulation of the conservation equations means that both phases co-exist at any point in space. The volume fraction α alone is not sufficient to describe the spatial topological structure between the phases and consequently the flow regime cannot be determined from the conservation equations. For the determination of the flow regime one needs more information on the interfacial area. The interfacial area concentration a^{int} [1/m] is also important for the formulation of interfacial transfer terms. The interfacial transfer terms can be written as the product of the interfacial area concentration and a driving potential [8]. The interfacial friction, which is part of the momentum transfer term $\mathbf{F}_k^{\text{int}}$, is:

$$\mathbf{F}_l^D = -\mathbf{F}_g^D = -\frac{1}{8} C_D \, a^{\text{int}} \rho_m (\mathbf{u}_g - \mathbf{u}_l) \, | \mathbf{u}_g - \mathbf{u}_l | \qquad (4)$$

and the mass transfer term due to condensation or evaporation is

$$\Gamma_v = -\Gamma_l = \frac{a^{\text{int}} (h_l^c (T_l - T_{sat}) + h_v^c (T_v - T_{sat}))}{\Delta h^{sat}} \qquad (5)$$

Numerical solution

The balance equations of the two-fluid model (1) – (3) can be written in compact matrix form as

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{G}\,\nabla \mathbf{U} + \mathbf{H}\,\nabla^2 \mathbf{U} = \mathbf{R} \qquad (6)$$

with the vector **U** of appropriately chosen solution variables. The matrix **G** represents the convection and the matrix **H** the diffusion of the flow. The right hand side **R** is an algebraic source vector for interfacial transfer processes.

For the numerical integration of (6) an operator splitting is applied, where the diffusive part is mathematically less challenging. The hyperbolic convection part, however, is characterized by the propagation of waves with characteristic velocities in regions of dependence and influence. Hyperbolicity is a precondition for the well-posedness of the mathematical equations as an initial-boundary problem. Appropriate numerical schemes for hyperbolic systems are based on techniques which make explicit use of the eigenstructure of the flow equations. Representatives of hyperbolic methods are the Flux Vector Splitting, Approximate Riemann Solvers and others. In the *FLU*BOX

code we use the Split Coefficient Matrix (SCM) method of Chakravarthy [9], which was first applied by Romstedt [10] for transient two-phase flows. The numerical solution procedures are suitable to master typical two-phase flow phenomena. The calculations of the ASTAR Benchmark test cases [11], which address typical two-phase flow phenomena (e.g. void and pressure wave propagation, phase transitions, sharp interface movements, compressible and nearly incompressible conditions, thermal and mechanical non-equilibrium) showed the robustness, accuracy and efficiency of the numerical schemes of the code [12].

A remark on the benefits of hyperbolicity (real eigenvalues) might be appropriate. Care must be taken on the formulation of interfacial terms. An incomplete formulation of the interfacial momentum coupling $\mathbf{F}_k^{\text{int}}$ results in complex eigenvalues and such system does not represent a well-posed initial-boundary value problem. A consequence might be that certain physical phenomena, e.g. critical flow conditions, are not realistically described. Nevertheless numerical solvers that provide sufficient numerical diffusion in order to dampen short wave length instabilities (e.g. elliptic solvers) obtain stable results for many transient two-phase flow conditions.

Transport Equation for Interfacial Area Concentration

The interfacial area concentration plays a central role in the modelling of two-phase flows. Therefore, an additional model equation is added to the conservation equations:

$$\frac{\partial a^{\text{int}}}{\partial t} + \nabla \cdot (a^{\text{int}} \mathbf{u}^{\text{int}}) = \Phi \tag{7}$$

The right hand side Φ of the interfacial area transport equation describes the change of the interfacial area concentration due to phase interactions. The modelling of Φ is described in the following. The transportation velocity of the interfacial area concentration $\mathbf{u}^{\text{int}}$ must be determined from the conservation equations.

The modelling approach calculates the interfacial area concentration from the complete differential of the particle radius and from a momentum equation at the phase boundary (Rayleigh equation). Through this approach it is possible to avoid empirical constants completely. The model describes the dynamic change of the interfacial area concentration due to mass and energy transfer between the phases and due to forces, which act at the interface [3]. The procedure is independent of the description of observed phenomena. For example the phenomena such as bubble coalescence and bubble disintegration on the interfacial area concentration are not explicitly modeled, but their effect is included by the force interactions between the phases. The modelling approach is not restricted to bubbly flows, but here, the derivation is given exemplary for bubbly flows. The derivation of the interfacial area transport equation starts with the ratio of the volume fraction α_g to the interfacial area density a^{int} for spherical bubbles:

$$\frac{\alpha_g}{a^{\text{int}}} = \frac{R_g}{3} \tag{8}$$

with bubble radius R_g. The relation (8) has the advantage to be independent of the number of bubbles which is considered as an essential aspect. Differentiation of equation (8) yields

$$\frac{\alpha_g}{a^{\text{int}}}\left(\frac{\partial a^{\text{int}}}{\partial t}+\mathbf{u}^{\text{int}}\nabla a^{\text{int}}\right)=\frac{\partial \alpha_g}{\partial t}+\mathbf{u}^{\text{int}}\nabla \alpha_g-\frac{a^{\text{int}}}{3}(\dot{R}_{g,thermal}+\dot{R}_{g,inertial}) \tag{9}$$

With the help of the simplified mass balances $\frac{\partial \alpha_g}{\partial t}+\nabla(\alpha_g \mathbf{u}^{\text{int}})=\frac{\Gamma_g}{\rho_g}$ (please note that $\mathbf{u}^{\text{int}} \to \mathbf{u}_g$ for $\alpha_g \to 0$) and $a^{\text{int}}\dot{R}_{g,thermal}=\frac{\Gamma_g}{\rho_g}$ the following transport equation for the interfacial area concentration arises as a result of algebraic manipulations:

$$\frac{\partial a^{\text{int}}}{\partial t}+\nabla(a^{\text{int}}\mathbf{u}^{\text{int}})=\frac{2}{3}a^{\text{int}}\frac{\Gamma_g}{\alpha_g\rho_g}-\frac{(a^{\text{int}})^2}{3\alpha_g}\dot{R}_{g,inertial} \tag{10}$$

The change of the interfacial area due to evaporation or condensation is taken into consideration by the mass transfer term Γ_g. The change of the particle radius $\dot{R}_{g,inertial}$ is calculated by using the Rayleigh equation:

$$R_g\ddot{R}_g+\frac{3}{2}\dot{R}_g^2=\frac{p(R_g)-p_\infty}{\rho_l} \tag{11}$$

The Rayleigh equation is enlarged through the pressure equation at the interface which gives its dependence on surface tension, viscosity and turbulence:

$$p(R_g)=p_g^{\text{int}}-2\frac{\sigma}{R_g}-4\frac{\eta_l}{R_g}(\dot{R}_g+\frac{3\mathbf{u}_r}{2\pi})-\tau_{t,g} \tag{12}$$

with $p_g^{\text{int}}-p_\infty=\frac{1}{4}\rho_l\mathbf{u}_r^2$. The turbulent shear stress is derived from the impulsive motion of a particle (Rayleigh impulsive flow) [3]:

$$\tau_{t,g}=(12\pi\rho_l\dot{R}_g+6\rho_l\,|\mathbf{u}_r\,|)\left(\frac{\varepsilon_l\nu_l}{\mathrm{Re}_{t,l}}\right)^{1/4} \tag{13}$$

In analogy to the derivation of equation (10) in the bubbly flow regime, one can derive a transport equation for the interfacial area equation in the droplet flow regime:

$$\frac{\partial a^{\text{int}}}{\partial t}+\nabla(a^{\text{int}}\mathbf{u}^{\text{int}})=\frac{2}{3}a^{\text{int}}\frac{\Gamma_l}{\alpha_l\rho_l}-\frac{(a^{\text{int}})^2}{3\alpha_l}\dot{R}_{l,inertial} \tag{14}$$

For flow regimes between bubbly flow and droplet flow an interpolation of the two equations (10) and (14) will be used, e.q. $\alpha_l(10)+\alpha_g(14)$, which yields:

$$\frac{\partial a^{\text{int}}}{\partial t}+\nabla(a^{\text{int}}\mathbf{u}^{\text{int}})=\frac{2}{3}a^{\text{int}}\left(\frac{\alpha_l\Gamma_g}{\alpha_g\rho_g}+\frac{\alpha_g\Gamma_l}{\alpha_l\rho_l}\right)-\frac{(a^{\text{int}})^2}{3}\left(\frac{\alpha_l}{\alpha_g}\dot{R}_{g,inertial}+\frac{\alpha_g}{\alpha_l}\dot{R}_{l,inertial}\right) \tag{15}$$

This set of equations is implemented in *FLU*BOX and has been applied for several configurations. It follows three validation calculations in the area of upward vertical pipe flows with mixtures of air and water. The pipes vary in length and diameter.

Validation calculations with upward vertical pipe flows

Cocurrent air-water up-flow in a 5.08 cm pipe

For a first validation of the interfacial area transport equation (10), experimental data of a steady air-water cocurrent up-flow in a 5.08 cm diameter pipe are used [5]. In these experiments, interfacial area and void fraction were measured with a double-sensor conductivity probe at three different axial positions, L/D = 2, 32 and 62. The boundary conditions are summarized in Table 1 for three test cases.

	j_g [m/s]	j_l [m/s]	α_g [-]
Case 1	0.023	0.77	0.025
Case 2	0.117	0.77	0.100
Case 3	0.117	1.58	0.065

Table 1: Boundary conditions for the 5.08 cm diameter pipe

In case 1 with 2.5% void fraction and very low liquid flow rate, bubble breakup can be neglected and the change of interfacial area is only due to coalescence. In case 2 with the same liquid superficial velocity but a higher void fraction, the decrease of interfacial area due to coalescence is reduced by bubble breakup. In case 3, the coalescence rate is balanced by the breakup rate, resulting in a relative flat axial distribution of the interfacial area concentration.

In the paper of Q.Wu [13] these test cases were successfully post calculated with a modelling of coalescence and breakup. In our approach however, the model describes the forces acting on the interfacial area. The good agreement with the experimental data supports the chosen approach (Figure 1). The model equations are based on first principles and good agreement is achieved without empirical constants.

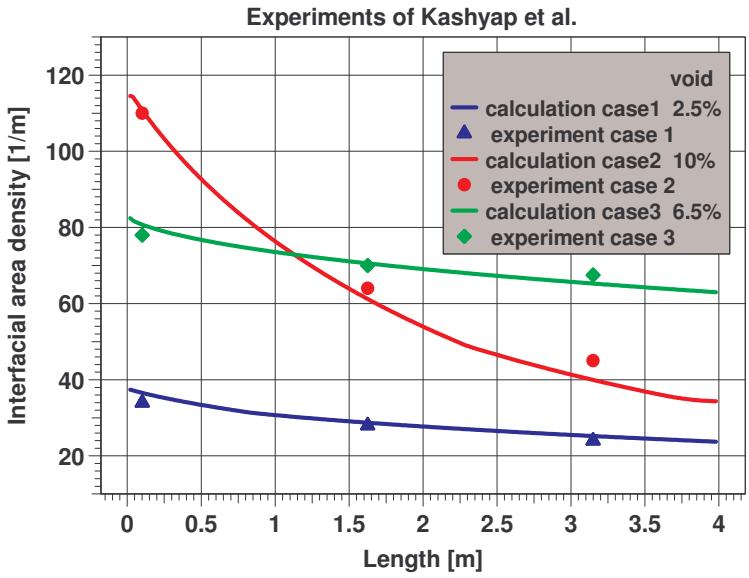

Figure 1: Vertical bubbly flow distribution of interfacial area concentration

Cocurrent air-water up-flow in small diameter pipe

The test section was a round tube with inner diameter of D = 9 mm and a length of L = 945 mm. The air and water were mixed in a mixing chamber and the mixture flowed upward through the test section. The water temperature was 20 °C at atmospheric pressure. Local measurements of flow parameters such as void fraction, interfacial area concentration and gas velocity were performed with the stereo image-processing method at six axial locations of z/D = 3, 6, 12, 24, 57 and 91 [4]. A comparison of the stereo-imaging method with the double sensor probe method showed a statistical accuracy in the order of 10 % [14]. From the measurements correlations were derived for the pressure, the void fraction and the gas velocity. In this experiment practically no disintegration of bubbles was observed, since the water flow was only weakly turbulent. The measured reductions of the interfacial area concentrations are thus due to bubble coalescence alone. The calculations show a reasonable agreement with the measured values, and/or the correlations derived from measured values, Figures 2-4. The boundary conditions of three test runs are specified in Table 2.

	j_g [m/s]	j_l [m/s]	α_g [-]
Run 1	0.013	0.58	0.021
Run 2	0.052	0.58	0.073
Run 3	0.052	1.00	0.044

Table 2: Boundary conditions for the small diameter pipe

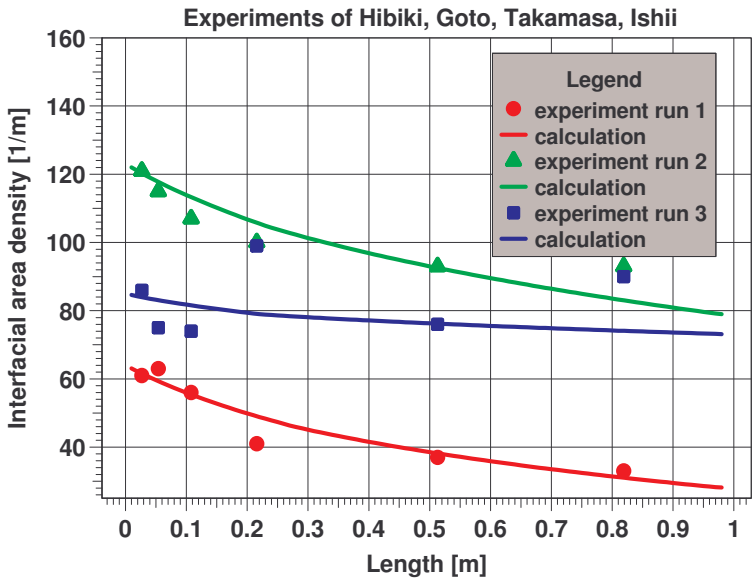

Figure 2: Axial distribution of interfacial area concentration

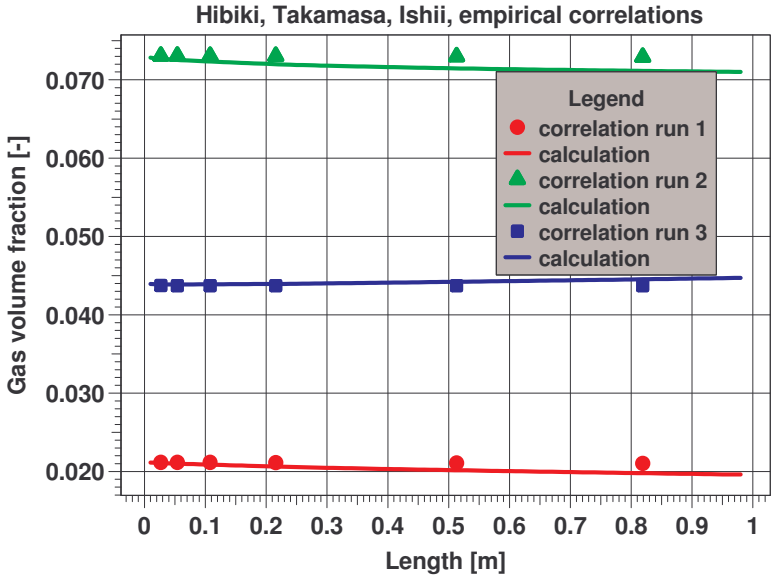

Figure 3: Axial distribution of gas volume fraction

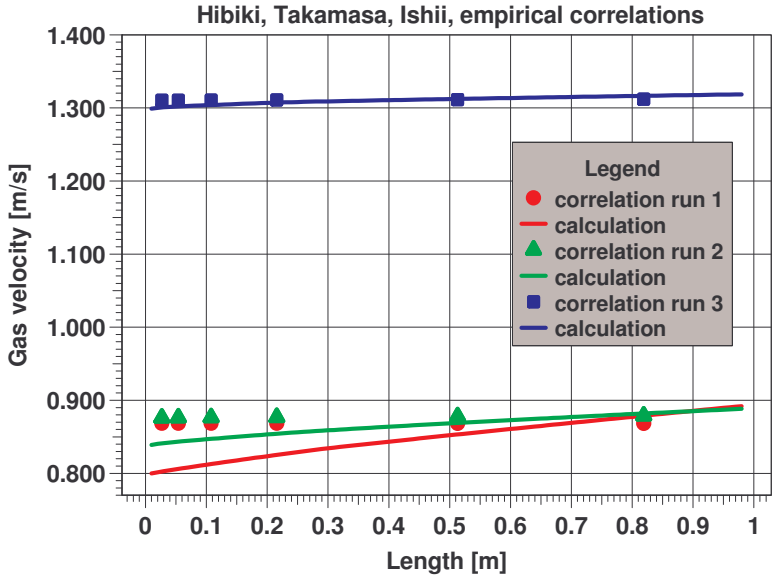

Figure 4: Axial distribution of gas velocity

Gas-liquid flow in a large vertical pipe

The test facility TOPFLOW of the Institute for Safety Research of the Research Center Rossendorf was established for the investigation of stationary and transient two-phase flows [6]. The test facility has, among others, a vertical test section with nominal diameter 200 mm. The vertical test section serves for the investigation of flow structure with stationary and transient two-phase air/water and/or steam/water flows. The test section is equipped with a variable injecting system that allows to inject gas or steam at 18 different positions upstream of the measuring position. Wire-mesh sensors are used to measure sequences of two-dimensional distributions of local instantaneous gas fraction within the complete pipe cross-section. The sensors reach a resolution of 3 mm at a measuring frequency of 2500 Hz.

In the test series (TS) air was fed from ring chambers through orifices in the pipe wall of 1 mm diameter. In all test series the superficial water velocity was $j_l = 1.016$ m/s at atmospheric pressure and 27 °C temperature. The superficial velocity of the gaseous phase j_g varied as indicated in Table 3.

TS	j_g [m/s]	α_g [-]
041	0.0094	0.010
074	0.0353	0.032
096	0.0862	0.057
118	0.2156	0.102
140	0.5331	0.176

Table 3: Boundary conditions of test series of the 200 mm pipe

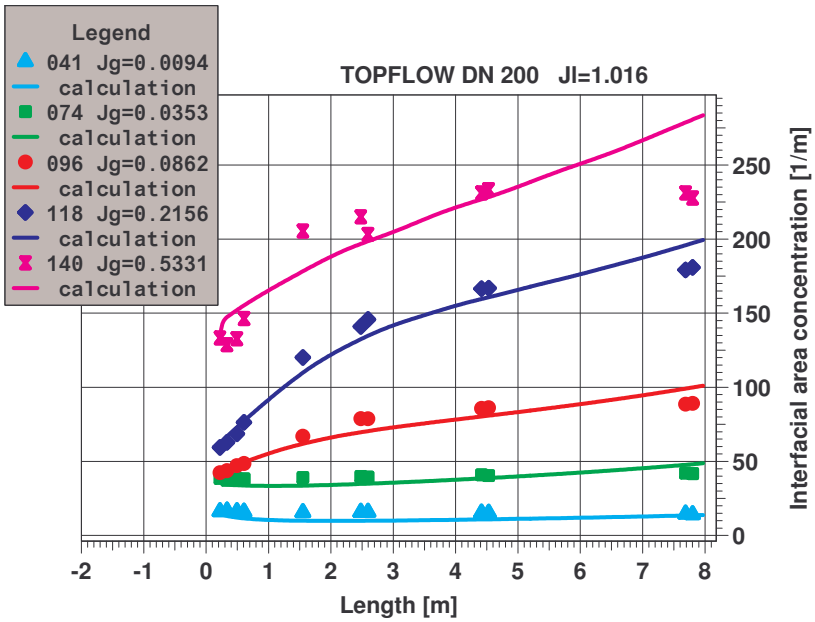

Figure 5: Axial distribution of interfacial area concentration

The axial distribution of the interfacial area concentration was post-calculated. The Figures 5 and 6 show the measured and computed axial distributions of the interfacial area concentration and the gas content. The rise of the interfacial area concentration along the pipe length at the superficial gas velocities of 0.086, 0.22 and 0.53 m/s points to bubble disintegration in the flow. The slight reduction of the interfacial area concentration at a superficial gas velocity of 0.0094 m/s points to bubble coalescence, however. These observed phenomena are represented correctly in tendency also in the calculation. Altogether, the post-calculations show a reasonable agreement with the measurement results.

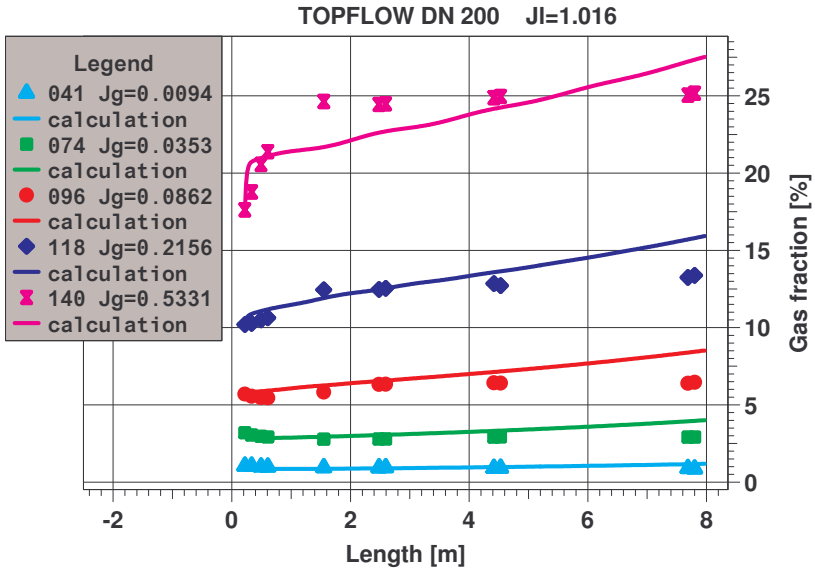

Figure 6: Axial distribution of gas volume fraction

Conclusions and Perspectives

The further development of multidimensional two-phase model equations is related to an extension of the basic two-fluid model with interfacial area transport processes and the inclusion of generic two-phase turbulence models. In a two-fluid model the interfacial area concentration is one of the key parameters in the constitutive relations in order to describe suitable the phase interactions. The proposed new model for the interfacial area transport equation is based on first principles (Rayleigh equation for momentum transport) and avoids empirical parameters. It differs from model suggestions in the literature which explicitly model bubble disintegration or bubble coalescence. The new modelling is based on a description of forces acting at the interface and observed phenomena are the result of the dynamic behavior at the interface. The computation of the dynamic change of the interfacial area concentration with only one transport equation is very attractive concerning the computational costs, in relation to the multi-group models. The presented validation calculations within the range of bubbly flows show a reasonable agreement with experimental data and confirm the new modelling concept. Further validation calculations in the range of drop flows are under way. Afterwards, the complex flow range between bubbly flow and drop flow will be addressed. The main idea behind the transport equation for the interfacial area concentration is to replace the flow pattern maps of the thermo-hydraulic codes. Flow regime maps have their uncertainty range and it is difficult to apply them suitably. There is also a lack on generally accepted criteria for intermediate flow transitions. The linear interpolation in equation (15) to cover intermediate flow regimes is a first attempt. Also nonlinear interpolations are thinkable, provided the weighting amounts to one.

Nomenclature

α volume fraction [-]
h enthalpy [J/kg]
p pressure [Pa]
ρ density [kg/m³]
Γ mass transfer term [kg/m³/s]
$\mathbf{u}$ velocity [m/s]
$\mathbf{u}_r = \mathbf{u}_g - \mathbf{u}_l$, relative velocity
$\mathbf{u}^{\mathrm{int}}$ interfacial velocity
j_k superficial velocity
a^{int} interfacial area concentration [1/m]
τ shear stress [Pa]
$\mathbf{x}$ space coordinates, $\mathbf{x}$=(x,y,z) [m]
ttime [s]

Indizes
k index for gas (g) or liquid (l)
m index for mixture
$t$index for turbulent

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