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The Three-Dimensional Transient Two-Phase Flow Computer Programme BACCHUS-3D/TP

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The three-dimensional single-phase flow version of the BACCHUS code, which describes the thermal behaviour of a coolant in hexagonal bundle geometry, developped earlier, provided the basis for the development of the two-phase flow version documented in this report.

A detailed description is given of the two-phase Slip Model (SM), and of the Homogeneous Equilibrium Model (HEM) as a subcase, which presents several improvements from both viewpoints of physical modelling and numerical treatment, with respect to usual models found in the literature. The most advanced Separated Phases Model (SPM) is then described in all analytical details necessary to fully understand its implementation in the code. Problems related to the link between the two above models into an integrated code version are then discussed. The code provides an additional option for modelling of active or passive, permeable or impermeable blockages. This option is documented separately. New numerical methods for solving the algebraic systems of equations derived from the linearization of the fundamental equations have completely superseded previous ones and are explained in detail.

Eventually a section is dedicated to an overview of the code verification, made over several years, which goes from steady state single-phase unheated bundle experiments up to fast transient two-phase flow experiments in electrically heated 37-pin bundles.

Das Computerprogramm BACCHUS-3D/TP für dreidimensionale transiente Zweiphasenströmungen

Die früher entwickelte dreidimensionale einphasige Version des Rechenprogrammes BACCHUS zur Beschreibung der Thermohydraulik eines Kühlmittels in hexagonaler Bündelgeometrie lieferte die Grundlage für die Entwicklung der zweiphasigen Version, die in diesem Bericht dokumentiert wird.

Das Zwei-Phasen-Schlupfmodell mit dem Spezialfall des homogenen Gleichgewichtsmodells wird detailliert beschrieben. Im Vergleich zu den üblichen Modellen, die in der Literatur beschrieben werden, enthält es mehrere Verbesserungen sowohl in der physikalischen Modellierung als auch in der numerischen Behandlung der Grundgleichungen. Das Modell der getrennten Phasen für höhere Dampfgehalte wird in allen analytischen Einzelheiten beschrieben, die zum vollen Verständnis seiner Implementierung im Rechenprogramm nötig sind. Probleme im Zusammenhang mit dem Übergang zwischen den beiden Modellen in einer integrierten Programmversion werden anschließend diskutiert.

Das Rechenprogramm enthält eine zusätzliche Option zur Modellierung von aktiven und passiven, durchlässigen und undurchlässigen Blockaden. Diese Option wird zusätzlich dokumentiert. Neue numerische Methoden zur Lösung des algebraischen Gleichungssystems, das durch die Linearisierung der Grundgleichungen entsteht, haben die Methoden, die früher für die einphasige Version des Rechenprogramms benutzt wurde, vollständig ersetzt und werden in diesem Bericht detailliert beschrieben.

Anschließend ist ein Abschnitt einem Überblick über die Verifikation des Programms gewidmet, die sich über mehrere Jahre erstreckt und von stationären einphasigen unbeheizten Bündelexperimenten bis zu schnellen transienten zweiphasigen Experimenten in elektrisch beheizten 37-Stabbündeln geht.

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Introduction

The three-dimensional two-phase flow version of the computer programme BACCHUS documented in this report has been developed from the single-phase flow version described in 1983 in reference [1]. Beside the new modelling of two-phase flow in bubbly and annular flow regimes and the provision of an option for blockage simulation, the basis version of 1983 has undergone a series of improvements concerning mainly: i) a replacement of the original explicit formulation of the code, where only friction terms were treated half-implicitly, by a completely implicit treatment of convective and diffusive terms in the transport equations; ii) the replacement of the numerical solution methods of the Poisson equations for pressure and enthalpy distributions, which were then available, with more advanced algorithms based on both direct and iterative methods; iii) the provision of plotting facilities and HISTORIAN packages for code bookkeeping; iv) the vectorization of the code.

The code version of 1983 has been therefore completely rewritten in the course of the implementation of the several topics involved. Beside the new physical modelling options, the code performances have been improved by a factor of 50 in computational speed with respect to the earlier version.

For these reasons only few of the topics documented in [1] still retain some actuality. These are:

i) The geometrical modelling of the bundle, as described in pages 3 - 13 of reference [1]. Because of the paramount importance of this information,and aiming at making the present report a self-contained one, we reproduced in the following "Preface on bundle modelling" this part of the earlier documentation, with only a few formal updating.

ii) The calculation of the temperature distribution in the fuel pins, as documented in pages 25 - 27, 45 - 54 and 137 - 147 of [1]. Although the basic algorithm for the numerical solution of the heat diffusion equation in the pins has remained unchanged, an improvement made in the present code version is worth mentioning. Since we model equivalent pins for every control volume and since a real pin is split in this way to belong to several contiguous control cells, we computed several and different pin temperatures at the axis. This inconsistency has been removed by imposing a further constraint on the calculation, namely that all computed central temperatures coincide. This in turn implies a more realistic azimuthal temperature distribution in the simulated pins. The better solution for this problem would, however, be a two-dimensional (radial and azimuthal) solution of the heat diffusion equation.

iii) The modelling of the turbulent exchanges of momentum and enthalpy, as described in pages 150 - 160 of [1]. This modelling is based on a sophisticated mixing-length concept which takes into account the anisotropy of the pin bundle and holds for single-phase flows. Its applicability to two-phase flow is object of current investigations.

The bulk of this report documents the to-date version of the code. In a few sections, mentioned in the following, we document an intermediate stage of the code evolution or give details about implementation of new modelling. The purpose of documenting some intermediate stages is twofold: first it allows one to understand how to proceed step by step in a code development from a preliminary stage (e.g. explicit) to an advanced stage (e.g. implicit); second, it allows comparisons of the theoretical background with other codes which have reached this degree of evolution. Since the to-date version of BACCHUS has reached an operational stage, but is still susceptible of improvements from both viewpoints of physical modelling and numerical treatment, we also explained the basis for future work in some sections.

The single-phase flow version of the code is not documented separately, because it is a subcase of the slip model to which Part I is reserved. Suppressing terms of the slip model containing the slip velocity one has the single-phase flow modelling. Sections 1 - 6, 9 and 11 - 12 of Part I refer to the to-date code version. Sections 7 and 10 document an intermediate evolution stage where diffusion terms in the momentum equation and in the enthalpy equation, respectively, were not yet treated fully implicitly. Section 8 explains how the Poisson equation for pressure can be solved for pressure increments $\delta p = p^{n+1} - p^n$ (over the time step) instead of solving for the pressure values p^{n+1}. The solution for pressure increments is more precise than the solution for pressure values because one has to deal with numbers in the range of magnitude of 10 - 10^2, instead of 10^5, and the relative algebraic equations are less stiff. The solution for δp was available in an earlier intermediate (now obsolete) code variant. It has not been taken over to the new code, but this could be done easily, if the need for increased precision were felt to be critical.

Part II is dedicated to the model of separated phases, where basically an annular flow regime is assumed. Sections 1to 7.2 refer to the present code version. Section 7.3 gives the rigorous theoretical treatment of the problem of calculating the mass of fluid vaporizing or condensing per unit time and volume, taking into account not only the power supplied to the coolant but also pressure variations. When power is suppressed the effect of pressure variations becomes dominant. This model has not yet been coded. Section 8 collects all partial derivatives of thermodynamical quantities for the liquid and for the vapour phase needed in the model of separated phases. As a preparation step for future modelling of superheated vapour and thermodynamic disequilibrium between the phases we complemented this set of derivatives with those of the vapour considered as a perfect gas (section 8.4). Section 9 sets the theoretical background for the modelling of a dispersed annular flow regime. This has not been coded so far. It is important for simulation of situations where large dry-out regions appear at the pin surfaces and the cooling effect of transported liquid droplet impinging onto this surface cannot be neglected.

Parts III to VI refer to the present code version.

Part VII gives an overview of the programme verifications made over the last ten years, including the earlier single-phase flow version of 1983. Numerical computations reported in section 1 refer to the calibration of this single-phase version against heated and unheated experiments in well-instrumented pin bundles. Section 2 refer to the verification of the Improved Slip Model (ISM) which has been performed over five years mainly on the basis of 7 and 37 electrically heated pin bundle experiments. The same experiments served for calibrating the Separated Phases Model (SPM) which has been eventually linked to the ISM in the combined code version. The verification of the integrated code version is not documented in this report, but has been explained in reference [39]. Likewise, the verification of the blockage option has been reported separately in references [18] and [19].

A quick information about the code is given in the following synopsis.

Synopsis of the BACCHUS-3D/TP code

Description of functions:

The programme describes single- and two-phase flow of coolant in hexagonal bundle geometry under normal or accident conditions like loss of flow, inlet blockages or reactivity transient. The programme is based on a three-dimensional representation of the bundle by means of the "porous-body" model. The thermal-hydraulic calculation for the coolant is coupled to a pin-model describing the temperature distribution in fuel and cladding. Heat losses out of the hexagonal duct and by-pass flows can be taken into account. An option is provided for the simulation of active or passive, central or displaced blockages of arbitrary thickness. The programme can be applied to reactor subassemblies as well as for the theoretical interpretation of in-pile or out-of-pile experiments. The single-phase flow version of the code has been extensively verified (see references [i] to [iv]).

The two-phase flow version is based on two physical models:

i) a slip model based on three conservation equations for the coolant mixture;

ii) a heterogeneous model of separated phases described by five conservation equations (two mass, two momentum conservation equations and one enthalpy equation for the mixture).

The two models have been coupled into an integrated code version which simulates a bubbly and annular flow regimes, with transition between them. An option is provided for using the slip model as stand alone code. Verification of the two-phase flow models has been reported in references [v] to [vii].

Numerical method:

The ICE (Implicit Continuous-fluid Eulerian) technique is used to derive a Poisson-like equation describing the pressure distribution in the coolant. The Poisson equation is solved numerically by means of an advanced variant of the ADI (Alternating Direction Implicit) method or with a fast L-U matrix decomposition technique or Gauss elimination. When the pressure field is known, the coolant mass flows are derived implicitly from the momentum equations. The coolant energy equation is also treated implicitly. It is also reduced to a Poisson-like equation solved numerically with the matrix decomposition technique or Gauss elimination. Alternatively, for single-phase flow calculations, a Runge-Kutta method of order four can be used (speed-up by a factor of two).

Vectorization:

The code is available in a version running both on scalar and VP vector computers. The vectorization degree is about 90% and implies a speed-up by a factor of 4 - 5 on the vector processor.

Running time:

It depends on the bundle size. For a 37 pin bundle with about 1000 meshes one hour of CPU time is required on the vector computer VP50 to calculate about 40 s problem time in single-phase flow or about 5 s in two-phase flow.

Programme size and core requirements:

The programme consists of about 30000 FORTRAN statements. Core requirements depend on the bundle size and on the axial discretization. For a 37-pin bundle with 40 axial meshes about 2000 K of core region are required including about 370 K for the matrix decomposition method or the Gauss elimination. When the ADI method is used about 170 K less are needed. Double precision calculation is compulsory.

Further facilities:

Dump restart files are written automatically with a given frequency and at the end of every run. A plot facility is available for i) axial, radial or azimuthal distributions of selected physical quantities at given time points; ii) time-dependent variations; iii) isotherms and velocity vectors for a given cut through the bundle.

Related programmes:

PLOTCP for the plotting facility. An independent library of material functions for fuel, cladding, coolant (sodium or water) and structural material is coupled to the programme.

A HISTORIAN package is available for code updating and management.

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Flow regime dependent modelling of two-phase flow in 3D-subassembly geometry and its experimental validation, Proc. ANS/ENS Int. Fast Reactor Safety Meeting, Snowbird, Utah, August 12 - 16, 1990.

Preface on bundle modelling

Some basic information about the geometrical model used for simulating the bundle, which is essential for understanding the conventions used in this report, is reproduced, with only slight updating, from reference [1].

i) Control volumes

We assume that the pins of the bundle are arranged on a hexagonal lattice, as shown in Fig. A.

The conservation equations describing the coolant flow are written first in a local form, then integrated over appropriate control volumes. A staggered mesh is used for defining the several dependent variables (components of coolant velocity, pressure, enthalpy etc.) and correspondingly different cells are used for the macroscopic balances. As shown in Figs. B1 and B2 the control cells are bounded in radial direction by planes parallel to the bundle z axis through the pin axes. Let Δr be the distance between the internal and external bounding planes, i.e. the width of the hexagonal ring. Planes perpendicular to the z axis define the following control cells of length Δz in the axial direction:

- Control volume V_I is bounded in axial direction by two planes perpendicular to the bundle z axis and a distance Δz apart, in radial direction by planes through the pin axes. This control cell is used for volume-averaging the coolant energy equation, and the continuity equation.

- Control volume V_{II} is obtained by displacing V_I by $\Delta r/2$ in radial direction. It is therefore bounded in the radial direction by planes parallel to the bundle axis passing midway between the pin axes. This control cell is used for volume - averaging the radial component of the coolant momentum equation.

- Control volume V_{III} is obtained by displacing V_I by $\Delta z/2$ in axial direction. It is used for volume - averaging the axial component of the coolant momentum equation.

- Control volume V_{IV} is obtained by taking the two adjacent halves of cells like V_I. V_{IV} is used for volume-averaging the azimuthal component of the coolant momentum equation.

- Control volume V_I to V_{IV} are bounded in the azimuthal direction by two planes passing through the bundle axis. Up to 48 azimuthal sectors can be considered.

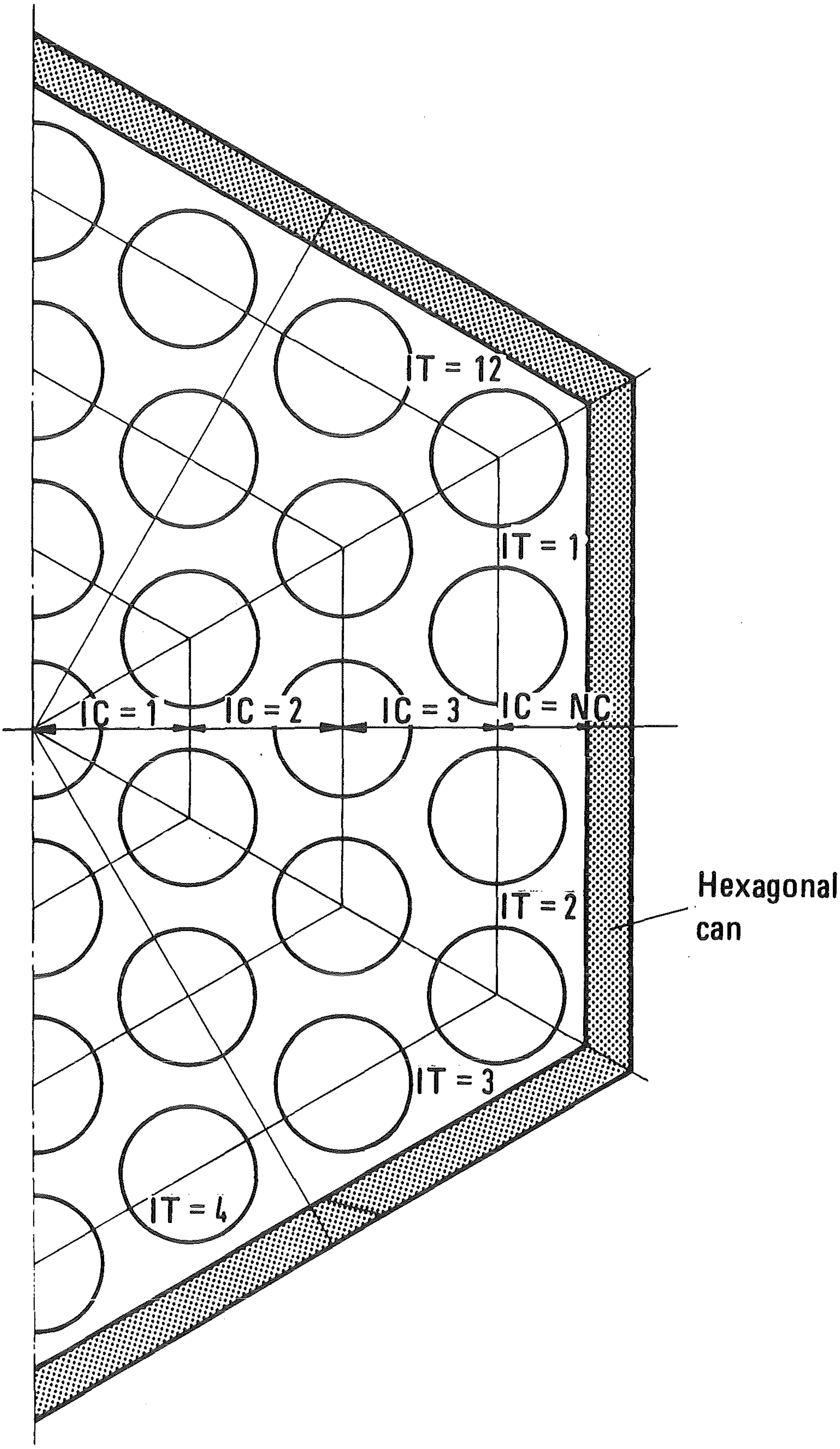

Fig. A: Radial and azimuthal discretization in BACCHUS.

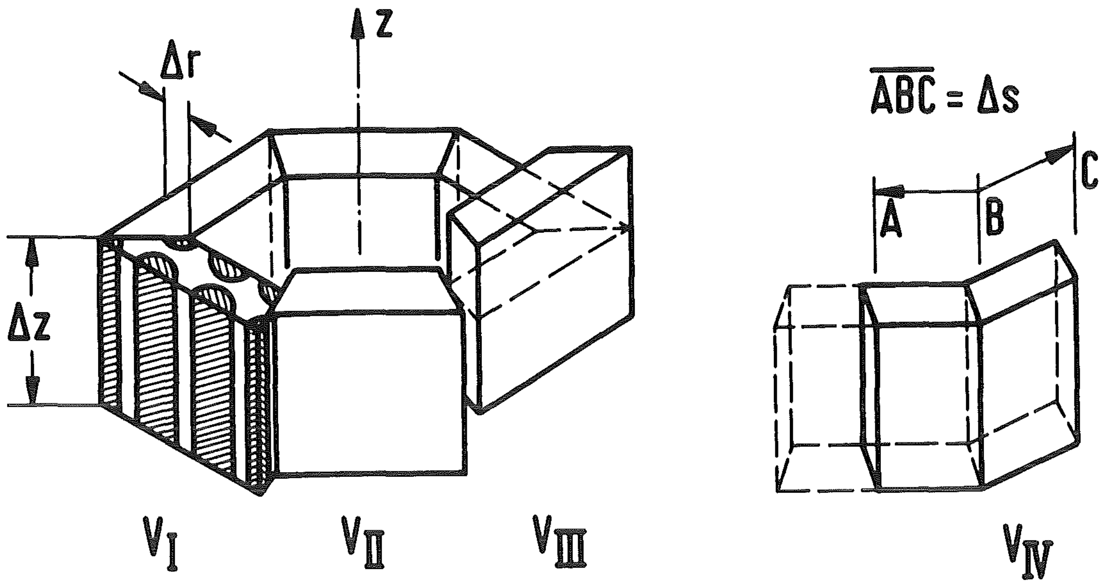

Fig. B1: Control volumes used for macroscopic balances.

ii) Indexing conventions

Following conventions are adopted for indexing the control cells:

- Axial direction. Index JC = 2, 3, ... MC denotes the control volumes V_I of length Δz. Control volumes V_{III} , displaced by + $\Delta z/2$ are indexed by JZ = 2, 3, ... MZ.

- Radial direction. Index IC = 1, 2, ... NC denotes the control volumes V_I. IC = 1 refers to the inner hexagonal control volume; IC = NC is the control volume bounded externally by the hexagonal can and internally by a plane through the axes of the outermost pins. Index IR = 1, 2, ... NR refers to the control volumes V_{II}.
  IR = NR is the control volume bounded externally by the hexagonal can and internally by a plane tangent to the outermost pins.

- Azimuthal direction. Index IT = 1, 2, ... NTH refers to the azimuthal sectors bounded by planes passing through the bundle axis. Index ITR = 1, 2, ... denotes these planes.

  Control cells and indexing conventions are shown in Fig. A for the case of a 37-pin bundle. (IC, JC, IT) is indexed as node (i, j, k). The cells faces are indexed as i ± 1/2, j ± 1/2, k ± 1/2, respectively.

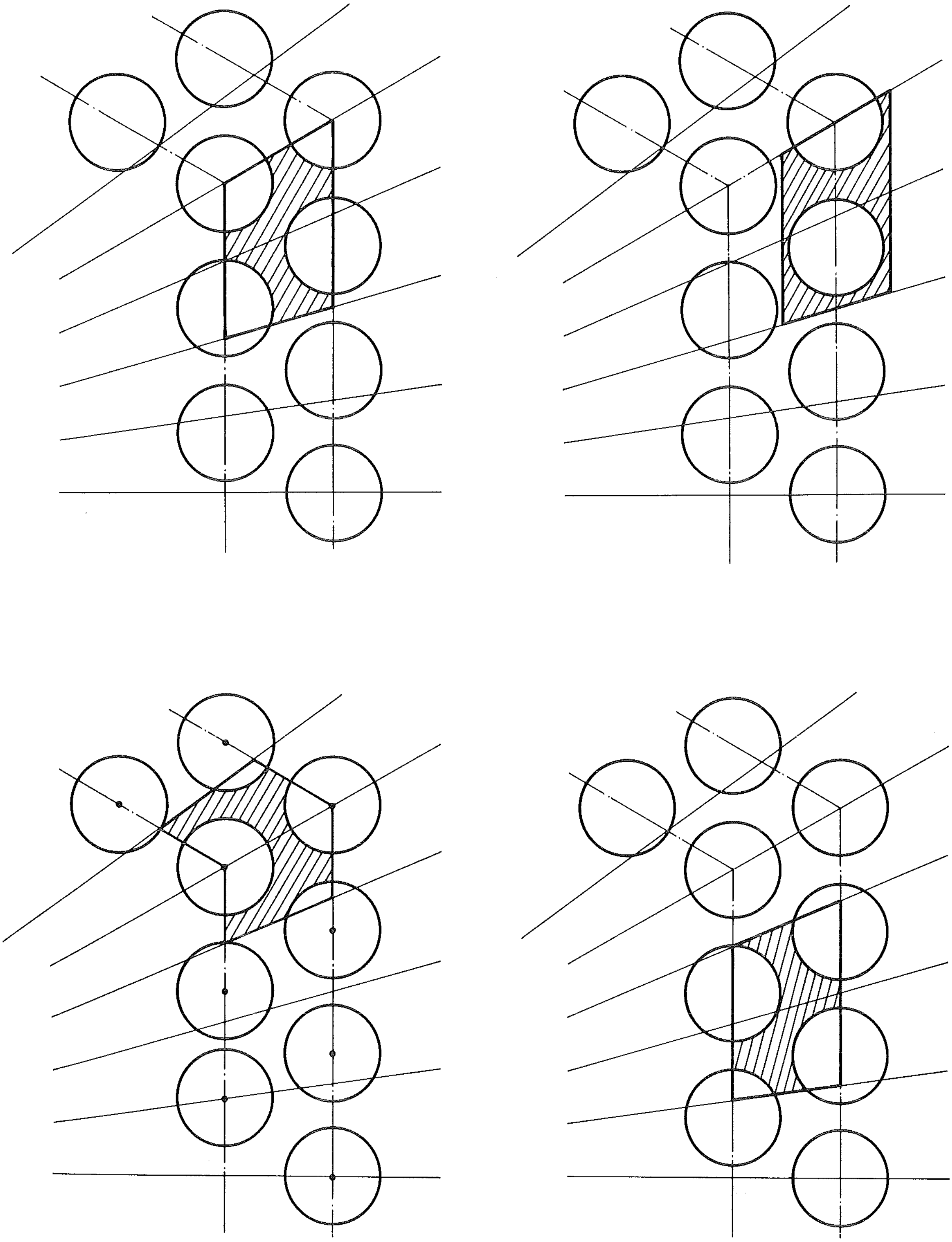

Fig. B2: Centred or axially displaced control volume V_I and V_{III} (top left),

radially displaced control volume V_{II} (top right),

azimuthal displaced control volume V_{IV} (negative direction) (bottom left),

azimuthal displaced control volume V_{IV} (positive direction) (bottom right),

iii) Definition of dependent variables

Space discretization of the conservation equations describing the fluid flow is done with reference to staggered meshes. Scalar quantities, like coolant pressure, enthalpy and other physical properties of the fluid, are defined at the centre point (i, j, k) of a control volume. Velocity components of the coolant (u, w, v for the r,z, s directions, respectively) are defined at the mid points of the boundary faces. These conventions are shown in Fig. C.

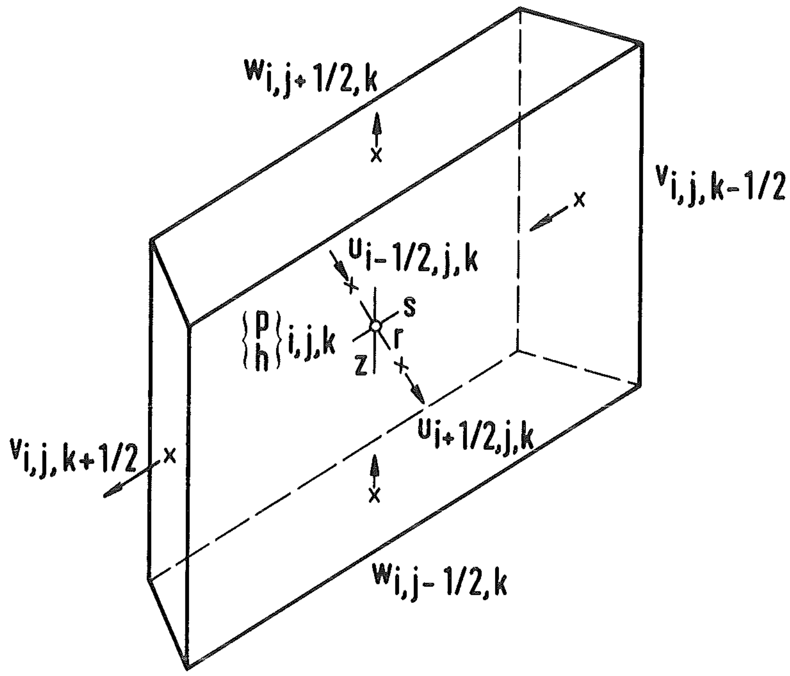

Fig. C: Definition of velocity components and scalar quantities on staggered meshes.

iv) Volume porosity and surface permeabilities

Conventions used for defining geometrical data are those customary in the so-called "porous body" approach. All cells are characterized by a total volume V, a volume occupied by the fluid V_f, an area A_w of the solid (wall)-fluid interfaces, by the areas of the lateral faces, S_t, S_b, (top, bottom, perpendicular to the z axis of the bundle), S_i, S_e (internal, external, perpendicular to the radial coordinate r),S_m, S_p (bounding the cell in the azimuthal direction, where the subscripts m (minus), p (plus) denote the sequence considered in the positive clockwise direction). These geometrical elements are used to define volumetric porosities and surface permeabilities for every cell.

Let S_{f_t}, S_{f_b}, S_{f_i}, S_{fe}, S_{f_m}, S_{f_p} be the cross flow areas of the bounding faces. For every cell we define surface permeabilities ζ, ψ, ξ for the axial, radial and azimuthal directions, respectively, as the ratio of the respective cross flow area to total area, for instance

$$\psi_i = S_{f_i} / S_i$$

$$\xi_b = S_{f_p} / S_p \; etc.$$

The volume porosity of a cell is defined as the ratio of the volume occupied by the fluid to the total cell volume, i.e.:

$$\varepsilon = V_f / V$$

In an undisturbed geometry the volume porosity is equal to the surface permeabilities in the axial direction. The definition of the surface permeabilities and of geometry coefficients for the radial direction is shown in detail in Fig. D with reference to the centred cells V_I and to the displaced cells V_{II}.

In the documentation following symbols are used according to Fig. D2:

$\psi_i = PSI(IC)$	$\psi_{i+1/2} = PSIR(IR)$
$S_i / S_{mi} = FACCM(IC)$	$S_e / S_{mi} = FACCP(IC)$
$S_{mi} / S_e = FACRM(IR)$	$S_{me} / S_e = FACRP(IR)$

Further details are given in Ref. [1].

v) Advantages offered by the porous medium approach

In the last two decades several computer programmes have been developed for the three-dimensional analysis of the coolant behaviour in fast reactor cores. Their degree of sophistication has grown together with the improvement of the computing facilities over the years. Their common feature consists in searching for an approximate solution of the conservation equations for mass, momentum and enthalpy by treating the numerical problem as an initial- value problem in time and a boundary value problem in space. However, some codes differ quite strongly from the viewpoint of the choice of the control volumes assumed for making the macroscopic balances of the dependent variables to be conserved.

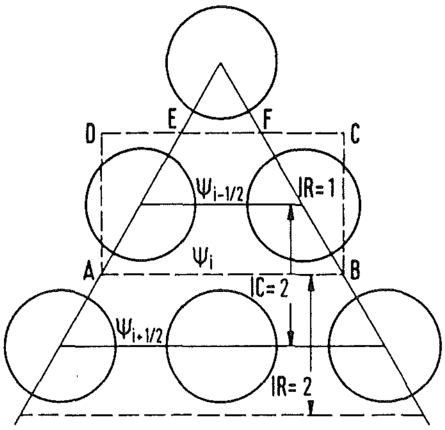

Fig. D1: Definition of surface permeabilities.

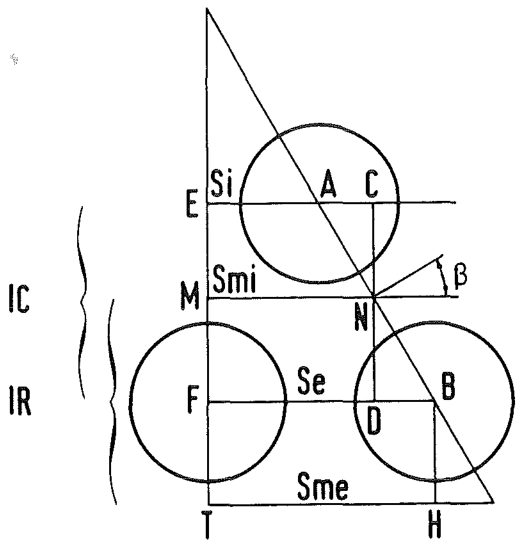

Fig. D2: Definition of geometry coefficients.

Most of the computer codes developed earlier than BACCHUS-3D were based on the "subchannel-analysis" concept which assumes as control volume the standard triangular subchannel between three rods. Computer programmes of this category present some basic limitations:

i) Scalar physical quantities (density, temperature etc.) are considered as constant in the control volume and velocity components are constant on the bounding surfaces (lumped parameter approach). Therefore the detailed distributions of temperature, pressure and velocity fields within a subchannel are ignored. The adoption of the lumped parameter approach arises from the mathematical treatment of the conservation equations as made in most codes. They are first "time-smoothed" to eliminate formally the fluctuations of the dependent variables due to turbulence (this process introduces however additional terms which are interpreted as the components of a turbulent stress tensor) then are integrated over the control cells to obtain volume - averaged physical quantities.

ii) The transversal components of the momentum equation are not treated with the same mathematical rigor as the axial component. This is a consequence of the non-orthogonality of the coordinate system used on a cross section of the bundle.

iii) The number of subchannels is very large in large bundles, thus implying long computer running times and high costs.

A successful attempt to cope with the drawbacks imposed by the subchannel analysis has been made by grouping some subchannels together to define a larger control volume for the macroscopic balance of the conservation equations. According to this, the real geometrical configurations of the subchannels grouped together to form a computational cell becomes irrelevant. We account for it, indirectly, by means of the new concepts of volume porosity, surface permeabilities, distributed frictional resistance and distributed heat source. Moreover, the new computational cells can be so defined that their bounding surfaces are orthogonal to a system of Cartesian coordinate axes. The basic limitation imposed by the non-orthogonality of the coordinate system employed by codes based on the subchannel-analysis concept is thus removed.

The porous-body concept allows one to calculate also real continuum regions like a reactor plenum or a mixing chamber in experimental assemblies. It is sufficient to define unity volume porosity and surface permeabilities in these regions. Thus both continuum and quasi-continuum subdomains can be handled in a single computer programme.

The performancies of a fuel assembly may be affected seriously by deformed geometry, as pin bowing due to power skew. Codes based on the subchannel concept have strong difficulties in taking into account a deformation properly because the definition of the control volumes is bounded to the real geometry. In the porous body approach, conversely, a deformed geometry can be simply accounted for by a modification of the coefficients representing the volume porosity and the surface permeabilities of the cells involved.

As in the case of codes based on the subchannel analysis, the lumped parameter approach is followed also in the porous body model. However, the following advantages are offered by the porous-medium formulation:

i) Reduction of the total number of cells considered, therefore of computer time. Obviously the control volumes should also be - on an average - larger than subchannels, but small enough compared with the scale of phenomena to be investigated.

ii) Use of an orthogonal coordinate system. This implies that the transverse momentum equations can be treated with the same rigor as the axial component.

iii) Suitability for simulating a continuum as well as an heterogeneous medium and geometrical deformations.

Part I

Slip Model - (Homogeneous Equilibrium Model) (SM-(HEM))

by M. Bottoni

1. Governing equations for the slip model

The governing equations for the conservation of mass, momentum, and energy of the coolant for the Slip Model have been derived in reference [2]. Neglecting some terms (like viscous dissipation in the fluid) which are small compared with the dominant ones (like power source) these equations can be written as follows:

Continuity Equation

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot \left(\rho_m \bar{v}_m \right) = 0 \, , \tag{1.1}$$

Momentum Equation

$$\frac{\partial}{\partial t} \left(\rho_m \bar{v}_m \right) + \nabla \cdot \left(\rho_m \bar{v}_m \bar{v}_m \right) + \nabla \cdot \left[x \left(1 - x \right) \rho_m \bar{V}_{Sl} \bar{V}_{Sl} \right] = \tag{1.2}$$

$$= - \nabla p + \nabla \cdot \left(\mu \nabla \bar{v}_m \right) + \rho_m \bar{g} - \bar{R} \, ,$$

Energy Equation

$$\frac{\partial}{\partial t} \left(\rho_m h_m \right) + \nabla \cdot \left(\rho_m \bar{v}_m h_m \right) + \nabla \cdot \left[x \left(1 - x \right) \rho_m \left(h_g - h_l \right) \bar{V}_{Sl} \right] = \tag{1.3}$$

$$= \frac{\partial p}{\partial t} + \bar{v}_m \cdot \nabla p + \left(\frac{1}{\rho_m} \alpha \left(1 - \alpha \right) \left(\rho_l - \rho_g \right) \bar{V}_{Sl} \right) \cdot \nabla p - \nabla \cdot \bar{q} + Q .$$

Indices g, l, m refer to vapour, liquid, and coolant mixture, respectively. The term $\vec{R}$ in the momentum equation represents the drag force per unit volume. The dynamic viscosity μ is the effective one, defined as sum of molecular and turbulent contributions (see Ref. [1] for details). ∇ is the Nabla operator.

The continuity equation, Eq. (1.1), is formally identical to the continuity equation for single-phase flow and reduces to it if the void fraction is zero. The energy and momentum equations, Eqs. (1.2) and (1.3), are similar to those for single-phase flow, but contain additional terms, which depend on the slip velocity V_{SL}. In case the slip velocity is zero (i.e. the phases have the same velocity) the equation obtained are those of the Homogeneous Equilibrium Model (HEM), as a subcase of the slip model.

2. Summary of basic relationships between two-phase flow parameters

With reference to the velocity components w_l and w_g of the coolant liquid and vapour phases in the z coordinate direction, we define the mass flow rate W, the volumetric flow rate Q, and the main flux G by:

$$W_p = \rho_p w_p A_p \qquad \left|Kg/s\right|, \tag{2.1}$$

$$Q_p = \frac{W_p}{\rho_p} \qquad \left|m^3/s\right|, \tag{2.2}$$

$$G_p = \frac{W_p}{A} \qquad \left|Kg/m^2/s\right|, \tag{2.3}$$

respectively. The index p (=l, g) refers to either phase; ρ and A are the coolant density and flow area, respectively. Similar definitions are used for the other coordinate directions. The contribution of each phase being additive, it holds

$$W = W_l + W_g, \tag{2.4}$$

$$Q = Q_l + Q_g,\ and \tag{2.5}$$

$$G = G_l + G_g. \tag{2.6}$$

The fraction of either phase is defined as the ratio of the cross-section occupied by the phase to the total cross section:

$$\alpha_p = \frac{A_p}{A} = \frac{A_p}{A_l + A_g}. \tag{2.7}$$

We define the phase weight fraction by

$$\omega_p = \frac{\alpha_p \rho_p}{\rho_m}, \tag{2.8}$$

where

$$\rho_m = \alpha_l \rho_l + \alpha_g \rho_g \tag{2.9}$$

is the mixture density. The flowing quality is defined for either phase by

$$x_{fp} = \frac{W_p}{W} = \frac{W_p}{W_l + W_g} = \frac{\alpha_p \rho_p w_p}{\alpha_l \rho_l w_l + \alpha_g \rho_g w_g}. \tag{2.10}$$

It holds

$$\alpha_l + \alpha_g = 1, \tag{2.11}$$

$$x_{fl} + x_{fg} = 1, \tag{2.12}$$

$$\omega_l + \omega_g = 1. \tag{2.13}$$

The total mass flux can be expressed as a function of the flowing qualities by

$$G = \frac{\alpha_g \rho_g w_g}{x_{fg}} = \frac{\alpha_l \rho_l w_l}{x_{fl}} . \tag{2.14}$$

The relationship between vapour void fraction and flowing quality is given by

$$a_g = \frac{1}{1 + \frac{1 - x_{fg}}{x_{fg}} \frac{\rho_g w_g}{\rho_l w_l}} . \tag{2.15}$$

The inverse relationship is:

$$x_{fg} = \frac{1}{1 + \frac{1 - a_g}{a_g} \frac{w_l \rho_l}{w_g \rho_g}} . \tag{2.16}$$

The relationship between vapour weight fraction ω_g and the vapour flowing quality x_{fg} is given by

$$x_{fg} = \omega_g \frac{w_g}{w_m} = \frac{\omega_g w_g}{\omega_g w_g + \omega_l w_l} , \tag{2.17}$$

where

$$w_m = \frac{1}{\rho_m} \Sigma_p \alpha_p \rho_p w_p \tag{2.18}$$

is the mixture velocity. If $w_m = w_g = w_l$ (slip ratio equal to 1), one derives $x_{fg} = \omega_g$.

The following relationships are also worth noting:

$$\frac{1 - x_{fg}}{x_{fg}} = \frac{1 - \alpha_g}{\alpha_g} \frac{w_l \rho_l}{w_g \rho_g} \tag{2.19}$$

$$= \frac{\omega_l w_l}{\omega_g w_l} = \frac{1 - \omega_g}{\omega_g} \frac{w_l}{w_g} \tag{2.10}$$

$$= \frac{1 - x}{x} \frac{w_l}{w_g} = \frac{1 - x}{x} \cdot \frac{1}{H} . \tag{2.21}$$

We define slip ratio as the ratio of the vapour velocity to the liquid phase velocity component in the respective coordinate direction:

$$H = \frac{w_g}{w_l} . \tag{2.22}$$

In the theoretical description of two-phase flow by means of a slip model ($H \neq 1$), the assumption is made that the slip ratio is constant. This assumption allows strong simplifications in programming. However, a more refined numerical treatment of two-phase flow, made by calculating the velocity components of both phases by means of separate systems of momentum equations in the Separated Phase Model, shows that the slip ratio is not constant.

From Eq. (2.19) one derives

$$H = \frac{w_g}{w_l} = \frac{x_{fg}}{1 - x_{fg}} \frac{1 - \alpha_g}{\alpha_g} \frac{\rho_l}{\rho_g} . \tag{2.23}$$

We define the thermodynamic quality of the mixture by

$$x = \frac{h_m - h_{ls}}{h_{gs} - h_{ls}} , \tag{2.24}$$

where h_{ls} and h_{gs} are the specific enthalpies of the liquid and vapour phases on the respective saturation lines and h_m is the specific enthalpy of the mixture defined by

$$h_m = \frac{1}{\rho_m} \left(\alpha_l \rho_l h_l + \alpha_g \rho_g h_g \right) . \tag{2.25}$$

From the definition of the vapour flowing quality (Eq. 2.10), one derives:

$$x_{fg} = \frac{1}{1 + \frac{1 - \alpha_g}{\alpha_g} \frac{\rho_l}{\rho_g} \frac{1}{H}} , \tag{2.26}$$

while solving Eq. (2.21) with respect to x_{fg} gives

$$x_{fg} = \frac{1}{1 + \frac{1}{H} \frac{1 - x}{x}} . \tag{2.27}$$

Combining Eqs. (2.26) and (2.27), one derives the important relationship between the thermodynamic quality and the vapour void fraction:

$$\frac{1 - x}{x} = \frac{1 - \alpha_g}{\alpha_g} \frac{\rho_l}{\rho_g} , \tag{2.28}$$

which can also be written

$$x = \frac{\alpha_g \rho_g}{\alpha_g \rho_g + \alpha_l \rho_l} = \frac{\alpha_g \rho_g}{\rho_m} = \frac{(1 - \alpha_l) \rho_g}{\rho_m} . \tag{2.29}$$

A useful expression for the mixture density ρ_m is obtained by combining Eqs. (2.9) and (2.15):

$$\rho_m = \frac{x_{fg} + (1 - x_{fg}) H}{\frac{x_{fg}}{\rho_g} + \frac{H}{\rho_l} (1 - x_{fg})} . \tag{2.30}$$

Introducing Eq. (2.27) into Eq. (2.30) one derives:

$$\rho_m = \frac{1}{\dfrac{x}{\rho_g} + \dfrac{1-x}{\rho_l}} = \frac{\rho_g \rho_l}{x\,\rho_l + (1-x)\,\rho_g} . \qquad (2.31)$$

Eq. (2.31) holds for every value of the slip ratio H.

3. Calculation of liquid and vapour velocity components from given slip velocity or slip ratio

For every coordinate direction, we define the slip velocity as the difference between the velocity of the vapour and liquid phase. With reference to the z coordinate direction, we have

$$W_{Sl} = w_g - w_l \ . \tag{3.1}$$

The normalized slip velocity is defined as the ratio of the slip velocity to the mixture velocity component in the same coordinate direction:

$$W_{Sl}^N = \frac{W_{Sl}}{w_m} = \frac{w_g - w_l}{w_m} \ . \tag{3.2}$$

Similar definitions apply for the r and s coordinate directions.

Relationships between the slip velocity, mixture velocity, and the velocity components of either phase can be obtained under the assumption of thermodynamic equilibrium between the phases ($T_g = T_l$). In this case one has $x = \omega_g = \alpha_g \rho_g / \rho_m$, $(1 - x) = \omega_l = \alpha_l \rho_l / \rho_m$, and given Eq. (2.18), one derives

$$(if \quad T_g = T_l) \qquad w_l = w_m - x\, W_{Sl} \ , \tag{3.3}$$

$$(if \quad T_g = T_l) \qquad w_g = w_m + (1 - x)\, W_{Sl} \ . \tag{3.4}$$

Combining the two previous equations yields the following relationship between the slip ratio H and the slip velocity W_{Sl}:

$$H = \frac{w_m + (1 - x)\, W_{Sl}}{w_m - x\, W_{Sl}} \tag{3.5}$$

or its inverse,

$$W_{Sl} = w_m \frac{H - 1}{1 + x\ (H - 1)} \ . \tag{3.6}$$

In the case of $H = 1$ (the Homogeneous Equilibrium Model), the slip velocity vanishes.

The slip velocity can be eliminated from Eqs. (3.3) and (3.4) using Eq. (3.1), thus obtaining the velocity components of either phase as a function of the mixture velocity w_m and of the slip ratio H:

$$w_l = \frac{w_m}{1 - x + x\, H} \tag{3.7}$$

$$w_g = H\, w_l \ . \tag{3.8}$$

Two options are commonly used for imposing either the slip ratio or the slip velocity:

- Option 1:

The slip ratios are prescribed for the three coordinate directions as

$$H_x = VSLIPR \;=\; u_g / u_l \;, \tag{3.9a}$$

$$H_y = VSLIPT \;=\; v_g / v_l \;, \; and \tag{3.9b}$$

$$H_z = VSLIPZ = w_g / w_l \;. \tag{3.9c}$$

In this case, Eqs. (3.7) and (3.8) and similar ones in the r and s coordinate directions give the velocity components of either phase (to be used for calculating the "momentum slip"and "energy slip", i.e. the terms containing the slip velocity, in the momentum and energy equations)

$$u_l = u_m / (1 - x + x \cdot \; H_s) \;, \tag{3.10a}$$

$$v_l = v_m / (1 - x + x \cdot \; H_r) \;, \tag{3.10b}$$

$$w_l = w_m / (1 - x + x \cdot \; H_z) \;, \tag{3.10c}$$

$$u_g = H_r \cdot \; u_l \;, \tag{3.11a}$$

$$v_g = H_s \cdot \; v_l \;, \tag{3.11b}$$

$$w_g = H_z \cdot \; w_l \;. \tag{3.11c}$$

The Homogeneous Equilibrium Model (HEM) is obtained as a subcase of the Slip Model (SM), setting $H_r = H_S = H_Z = 1$.

- Option 2:

In this case, the input parameters VSLIPR, VSLIPT, and VSLIPZ have the meaning of normalized slip velocities defined as

$$VSLRN \;(= VSLIPR) = U^N_{Sl} = (u_g \; - u_l)/u_m \;, \tag{3.12a}$$

$$VSLTN \;(= VSLIPT) = V^N_{Sl} = (v_g \; - v_l)/v_m \;, \tag{3.12b}$$

$$VSLZN \;(= VSLIPZ) = W^N_{Sl} = (w_g \; - w_l)/w_m \;. \tag{3.12c}$$

Using Eqs. 2, 3, and 4 (as well as the analogous equations for the r and s coordinate directions), one derives the following velocity components of the two phases:

$$u_l = u_m \left(1 - x\, U_{Sl}^N\right) \ , \tag{3.13a}$$

$$v_l = v_m \left(1 - x\, V_{Sl}^N\right) \ , \tag{3.13b}$$

$$w_l = w_m \left(1 - x\, W_{Sl}^N\right) \ , \tag{3.13c}$$

$$u_g = u_l \left(1 + \frac{U_{Sl}^N}{1 - x\, U_{Sl}^N}\right) = u_l + U_{Sl}^N \cdot \ u_m \ , \tag{3.14a}$$

$$v_g = v_l \left(1 + \frac{V_{Sl}^N}{1 - x\, V_{Sl}^N}\right) = v_l + V_{Sl}^N \cdot \ v_m \ , \tag{3.14b}$$

$$w_g = w_l \left(1 + \frac{W_{Sl}^N}{1 - x\, W_{Sl}^N}\right) = w_l + W_{Sl}^N \cdot \ w_m \ . \tag{3.14c}$$

The HEM is obtained again as a subcase in this second option setting

$$U_{Sl}^N = V_{Sl}^N = W_{Sl}^N = 0 \ .$$

In both options, one has

- For $x=0$: $u_l = u_m$,
  $v_l = v_m$,
  $w_l = w_m$,

  while the vapour velocity components are not defined (they are set to zero).

- In the limiting case $x=1$, the above equations for the phase velocity components are not applicable and we set

  $u_g = u_m$,
  $v_g = v_m$,
  $w_g = w_m$,

  while the liquid velocity components are set to zero.

4. Finite difference form of the continuity equation

We treat the convective terms in equations (1) fully implicitly. Integrating this equation over a centred cell, replacing the volume integral of the divergence term by means of surface fluxes one derives the following finite difference form:

$$\varepsilon_{ijk}\left(\frac{\partial\rho_m}{\partial t}\right)^{n+1}_{ijk} + \frac{1}{\Delta z_j}\left[\zeta_{j+1/2}\left(\rho_m w_m\right)^{n+1}_{i,j+1/2,k} - \zeta_{j-1/2}\left(\rho_m w_m\right)^{n+1}_{i,j-1/2,k}\right] +$$

$$+\frac{1}{\Delta r_i}\left[\left(\psi F_c\,\rho_m \upsilon_m\right)^{n+1}_{i+1/2,j,k} - \left(\psi F_c\,\rho_m \upsilon_m\right)^{n+1}_{i-1/2,j,k}\right] + \tag{4.1}$$

$$+\frac{1}{\Delta s_k}\left[\left(\frac{\xi\rho_m v_m}{\cos\beta}\right)^{n+1}_{i,j,k+1/2} - \left(\frac{\xi\rho_m v_m}{\cos\beta}\right)^{n+1}_{i,j,k-1/2}\right] = 0\,.$$

Equation (4.1) can be written in compact form as

$$\varepsilon_{ijk}\left(\frac{\partial\rho_m}{\partial t}\right)^{n+1}_{ijk} + \sum_1^3{}_i\ \frac{1}{\Delta l_i}\ \Delta\left(\gamma_i\, c_i < \rho_m u_{m\,i} >\right)^{n+1} = 0 \qquad (i = r, s, z) \tag{4.2}$$

with γ_i = surface permeability,
c_z = 1,
c_r = F_c = FACCM, FACCP
c_s = $1/\cos\beta$; β = angle between r-axis and azimuthal boundary surface of centred control volume (see Fig. D2).

Equation (4.1) is used to derive a Poisson-like equation for the pressure distribution, as explained in section 6. It is also used to derive the updated value of the void fraction. Discretizing the time derivative and solving with respect to ρ_m^{n+1} one has

$$\rho_m^{n+1} = \rho_m^n - \frac{\Delta t}{\varepsilon}\sum_1^3{}_i\ \frac{1}{\Delta l_i}\ \Delta\left(\gamma_i\, c_i < \rho_m u_{m\,i} >\right) \tag{4.3}$$

Hence, from the definition $\rho_m = \alpha\rho_g + (1-\alpha)\,\rho_l$,

$$\alpha^{n+1} = \frac{\rho_l^{n+1} - \rho_m^{n+1}}{\rho_l^{n+1} - \rho_g^{n+1}} = \tag{4.4}$$

$$= \frac{1}{\rho_l^{n+1} - \rho_g^{n+1}}\left[\rho_l^{n+1} - \rho_m^n - \frac{\Delta t}{\varepsilon}\sum_1^3{}_i\ \frac{1}{\Delta l_i}\ \Delta\left(\gamma_i\, c_i < \rho_m u_{m\,i} >\right)^{n+1}\right].$$

5. Fully implicit treatment of momentum conservation equation

The scalar component of the momentum conservation equation (1.2) in the z-coordinate direction can be written

$$\frac{\partial}{\partial t}\left(\rho_m w_m\right)+\frac{\partial}{\partial L_\alpha}\left[\left(\rho_m V_{m_\alpha}\right)w_m+x\left(1-x\right)\rho_m\left(V_g-V_l\right)_\alpha\left(w_g-w_l\right)\right]-$$

$$-\frac{\partial}{\partial L_\alpha}\left(\mu_m\frac{\partial w_m}{\partial L_\alpha}\right)=-\frac{\partial p}{\partial z}-\rho_m g_z-R_z\,. \qquad (L_\alpha=r,s,z) \tag{5.1}$$

L_α represent any of the coordinate directions (r, s, z in bundle geometry) and V_α is the respective velocity component.

Letting

$$G_{Sl}=x\,(1-x)\,\rho_m \qquad \textit{(momentum slip)} \tag{5.2}$$

$$S_z=-\frac{\partial p}{\partial z}-\rho_m g_z-R_z \qquad \textit{(source term)} \tag{5.3}$$

$$Jw_{m_\alpha}=\left(\rho_m V_{m_\alpha}\right)w_m+G_{Sl}\left(V_g-V_l\right)_\alpha\left(w_g-w_l\right)-\mu_m\frac{\partial w_m}{\partial L_\alpha}\,, \tag{5.4}$$

(convective plus diffusive flux of momentum)

equation (1) can be written

$$\frac{\partial}{\partial t}\left(\rho_m w_m\right)+\frac{\partial}{\partial L_\alpha}Jw_{m\alpha}=S_z\,. \tag{5.5}$$

Integration over the volume V_f of the fluid in a control cell yields

$$\int_{V_f}\frac{\partial}{\partial t}\left(\rho_m w_m\right)dV+\int_{V_f}\frac{\partial}{\partial L_\alpha}Jw_{m\alpha}\,dV=\int_{V_f}S_z\,dV\,. \tag{5.6}$$

The control volume for the z-component of the momentum equation is obtained displacing a centred control cell (i j k) by half-mesh in the z direction. Replacing the volume integral of the divergence term by means of the fluxes through the cell bounding surfaces one derives:

$$\int_{V_f}\frac{\partial}{\partial t}\left(\rho_m w_m\right)dV+\int_{A_{f\,i+1/2,j+1/2,k}}\left(Jw_m\right)_r dA-\int_{A_{f\,i-1/2,j+1/2,k}}\left(Jw_m\right)_r dA+$$

$$+\int_{A_{f\,i,j+1,k}}\left(Jw_m\right)_z dA-\int_{A_{f\,i,j,k}}\left(Jw_m\right)_z dA+\int_{A_{f\,i,j+1/2,k+1/2}}\left(Jw_m\right)_s dA- \tag{5.7}$$

$$-\int_{A_{f\,i,j+1/2,k-1/2}}\left(Jw_m\right)_s dA=\int_{V_f}S_z\,dV\,.$$

We discretize this equation with respect to time treating convective, diffusive, and the pressure gradient term fully implicitly and the friction term half-implicitly. Replacing the surface integrals by the mean values over the surfaces, denoted by the symbols $< >$, one obtains:

$$\frac{V_{f_{i,j+1/2,k}}}{\Delta t}\left[\left(\rho_m w_m\right)^{n+1}-\left(\rho_m w_m\right)^{n}\right]_{i,j+1/2,k}+$$

$$+<\left(Jw_m\right)_r A_f>^{n+1}_{i+1/2,j+1/2,k}-<\left(Jw_m\right)_r A_f>^{n+1}_{i-1/2,j+1/2,k}+$$

$$+<\left(Jw_m\right)_z A_f>^{n+1}_{i,j+1,k}-<\left(Jw_m\right)_z A_f>^{n+1}_{i\,j\,k}+ \tag{5.8}$$

$$+<\left(Jw_m\right)_s A_f>^{n+1}_{i,j+1/2,k+1/2}-<\left(Jw_m\right)_s A_f>^{n+1}_{i,j+1/2,k-1/2}=$$

$$=-\left(\frac{V_f}{\Delta z}\right)_{i,j+1/2,k}\left(p^{n+1}_{i,j+1,k}-p^{n+1}_{i\,j\,k}\right)-\left(V_f\,\rho_m\,g_z\right)^{n}_{i,j+1/2,k}-\left[\frac{V_f}{2D_h}f\,|w_m|^n\left(\rho_m w_m\right)^{n+1}\right]_{i,j+1/2,k}.$$

The averaged fluxes of the vector Jw_m are evaluated with the upwind discretization scheme given in eq. (5.13):

$$Jr+=\int_{A_{f\,i+1/2,j+1/2,k}}\left(Jw_m\right)_r dA=<Jw_m\cdot A_f>_{i+1/2,j+1/2,k}= \tag{5.9}$$

$$=\left\{A_f\,\rho_m\,u_m\,w_m+A_f\,G_{Sl}\left(u_g-u_l\right)\left(w_g-w_l\right)-\frac{A_f\,\mu_m}{\rho_m\,\Delta r}\,\Delta\left(\rho_m w_m\right)\right\}_{i+1/2,j+1/2,k}=$$

$$=\left\{F\cdot\rho_m\,w_m+G\left(w_g-w_l\right)-D\cdot\Delta\left(\rho_m w_m\right)\right\}_{i+1/2,j+1/2,k},$$

with the definitions:

$$F_{i+1/2,j+1/2,k}=\left(A_f\,u_m\right)_{i+1/2,j+1/2,k}, \tag{5.10}$$

$$G_{i+1/2,j+1/2,k}=\left[A_f\,G_{Sl}\left(u_g-u_l\right)\right]_{i+1/2,j+1/2,k}, \tag{5.11}$$

$$D_{i+1/2,j+1/2,k}=\left(A_f\frac{\mu_m}{\rho_m\,\Delta r}\right)_{i+1/2,j+1/2,k}, \tag{5.12}$$

$$\Delta\left(\rho_m w_m\right)_{i+1/2,j+1/2,k}=\left(\rho_m w_m\right)_{i+1,j+1/2,k}-\left(\rho_m w_m\right)_{i,j+1/2,k}.$$

For both $u_{i+1/2,j+1/2,k}$ positive and negative, formula (5.9) can be written

$$Jr+ = \left[0, F_{i+1/2,j+1/2,k}\right] \left(\rho_m \; w_m\right)_{i,j+1/2,k} - \left[0, -F_{i+1/2,j+1/2,k}\right] \left(\rho_m \; w_m\right)_{i+1,j+1/2,k} +$$

$$+ \left[0, G_{i+1/2,j+1/2,k}\right] \left(w_g - w_l\right)_{i,j+1/2,k} - \left[0, -G_{i+1/2,j+1/2,k}\right] \left(w_g - w_l\right)_{i+1,j+1/2,k} + \quad (5.13)$$

$$+ D_{i+1/2,j+1/2,k} \left\{ \left(\rho_m \; w_m\right)_{i,j+1/2,k} - \left(\rho_m \; w_m\right)_{i+1,j+1/2,k} \right\}.$$

The symbol [a, b] denotes the maximum of the two real numbers a, b.

Let us introduce the following subscripts to index the central node considered and the six neighbouring nodes in the three coordinate directions:

0	for	$i, j+1/2, k$
1	for	$i-1, j+1/2, k$
2	for	$i+1, j+1/2, k$
3	for	$i, j+1/2, k-1$
4	for	$i, j+1/2, k+1$
5	for	$i, j-1/2, k$
6	for	$i, j+3/2, k$.

The flux $Jr+$ and, similarly, the other ones in eq. (5.9) can be written:

$$Jr+ = \int_{A_{f\; i+1/2,j+1/2,k}} \left(Jw_m\right)_r \; dA = < \left(Jw_m\right)_r \cdot A_f >_{i+1/2,j+1/2,k} =$$

$$= \left[0, F_{i+1/2,j+1/2,k}\right] \left(\rho_m \; w_m\right)_0 - \left[0, -F_{i+1/2,j+1/2,k}\right] \left(\rho_m \; w_m\right)_2 +$$

$$+ \left[0, G_{i+1/2,j+1/2,k}\right] \left(w_g - w_l\right)_0 - \left[0, -G_{i+1/2,j+1/2,k}\right] \left(w_g - w_l\right)_2 + \quad (5.14a)$$

$$+ D_{i+1/2,j+1/2,k} \left\{ \left(\rho_m \; w_m\right)_0 - \left(\rho_m \; w_m\right)_2 \right\},$$

$$Jr- = \int_{A_{f\; i-1/2,j+1/2,k}} \left(Jw_m\right)_r \; dA = < \left(Jw_m\right)_r \cdot A_f >_{i-1/2,j+1/2,k} =$$

$$= \left[0, F_{i-1/2,j+1/2,k}\right] \left(\rho_m \; w_m\right)_1 - \left[0, -F_{i-1/2,j+1/2,k}\right] \left(\rho_m \; w_m\right)_0 +$$

$$+ \left[0, G_{i-1/2,j+1/2,k}\right] \left(w_g - w_l\right)_1 - \left[0, -G_{i-1/2,j+1/2,k}\right] \left(w_g - w_l\right)_0 + \quad (5.14b)$$

$$+ D_{i-1/2,j+1/2,k} \left\{ \left(\rho_m \; w_m\right)_1 - \left(\rho_m \; w_m\right)_0 \right\},$$

$$Jz+ = \int_{A_{f\ i,j+1,k}} \left(Jw_m\right)_z \ dA = < \left(Jw_m\right)_z \cdot A_f >_{i,j+1,k} =$$

$$= \left[0, F_{i,j+1,k}\right] \left(\rho_m \ w_m\right)_0 - \left[0, -F_{i,j+1,k}\right] \left(\rho_m \ w_m\right)_6 +$$

$$+ \left[0, G_{i,j+1,k}\right] \left(w_g - w_l\right)_0 - \left[0, -G_{i,j+1,k}\right] \left(w_g - w_l\right)_6 + \qquad (5.14c)$$

$$+ D_{i,j+1,k} \left\{ \left(\rho_m \ w_m\right)_0 - \left(\rho_m \ w_m\right)_6 \right\} ,$$

$$Jz- = \int_{A_{f\ i,j\,k}} \left(Jw_m\right)_z \ dA = < \left(Jw_m\right)_z \cdot A_f >_{i,j\,k} =$$

$$= \left[0, F_{i\,j\,k}\right] \left(\rho_m \ w_m\right)_5 - \left[0, -F_{i\,j\,k}\right] \left(\rho_m \ w_m\right)_0 +$$

$$+ \left[0, G_{i\,j\,k}\right] \left(w_g - w_l\right)_5 - \left[0, -G_{i\,j\,k}\right] \left(w_g - w_l\right)_0 + \qquad (5.14d)$$

$$+ D_{i\,j\,k} \left\{ \left(\rho_m \ w_m\right)_5 - \left(\rho_m \ w_m\right)_0 \right\} ,$$

$$Js+ = \int_{A_{f\ i,j+1/2,\,k+1/2}} \left(Jw_m\right)_s \ dA = < \left(Jw_m\right)_s \cdot A_f >_{i,j+1/2,k+1/2} =$$

$$= \left[0, F_{i,j+1/2,\,k+1/2}\right] \left(\rho_m \ w_m\right)_0 - \left[0, -F_{i,j+1/2,\,k+1/2}\right] \left(\rho_m \ w_m\right)_4 +$$

$$+ \left[0, G_{i,j+1/2,\,k+1/2}\right] \left(w_g - w_l\right)_0 - \left[0, -G_{i,j+1/2,\,k+1/2}\right] \left(w_g - w_l\right)_4 + \qquad (5.14e)$$

$$+ D_{i,j+1/2,\,k+1/2} \left\{ \left(\rho_m \ w_m\right)_0 - \left(\rho_m \ w_m\right)_4 \right\} ,$$

$$Js- = \int_{A_{f\ i,j+1/2,\,k-1/2}} \left(Jw_m\right)_s \ dA = < \left(Jw_m\right)_s \cdot A_f >_{i,j+1/2,k-1/2} = \qquad (5.14f)$$

$$= \left[0, F_{i,j+1/2,\,k-1/2}\right] \left(\rho_m \ w_m\right)_3 - \left[0, -F_{i,j+1/2,\,k+1/2}\right] \left(\rho_m \ w_m\right)_0 +$$

$$+\left[0, G_{i,j+1/2,k-1/2}\right]\left(w_g - w_l\right)_3 - \left[0, -G_{i,j+1/2,k+1/2}\right]\left(w_g - w_l\right)_0 +$$

$$+ D_{i,j+1/2,k-1/2}\left\{\left(\rho_m w_m\right)_3 - \left(\rho_m w_m\right)_0\right\} .$$

Let

$$H_r = u_g / u_l , \tag{5.15a}$$

$$H_s = v_g / v_l , \tag{5.15b}$$

$$H_z = w_g / w_l \tag{5.15c}$$

be the slip ratios for the three velocity components in the radial, azimuthal and axial directions, respectively.

The slip velocities can be written in terms of the mixture velocity and of the thermodynamic quality (see (3.6)) as

$$U_{Sl} = u_g - u_l = u_m \frac{H_r - 1}{1+x\ (H_r - 1)} = \rho_m\ u_m \cdot \frac{\widetilde{H}_r}{\rho_m}, \tag{5.16a}$$

$$V_{Sl} = v_g - v_l = v_m \frac{H_s - 1}{1+x\ (H_s - 1)} = \rho_m\ v_m \cdot \frac{\widetilde{H}_s}{\rho_m}, \tag{5.16b}$$

$$W_{Sl} = w_g - w_l = w_m \frac{H_z - 1}{1+x\ (H_z - 1)} = \rho_m\ w_m \cdot \frac{\widetilde{H}_z}{\rho_m}, \tag{5.16c}$$

with the definitions:

$$\widetilde{H}_i = \frac{H_i - 1}{1+x\ (H_i - 1)} \qquad (i = r, s, z) . \tag{5.17}$$

With this artifice we can calculate the sum of convective terms one and three in formula (5.14a) as

$$\begin{aligned} &\left[0, F_{i+1/2,j+1/2,k}\right]\left(\rho_m\ w_m\right)_0 + \left[0, +\ G_{i+1/2,j+1/2,k}\right]\left(w_g - w_l\right)_0 = \\ &= \left[0, F_{i+1/2,j+1/2,k} + G_{i+1/2,j+1/2,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right]\left(\rho_m\ w_m\right)_0 \end{aligned} \tag{5.18}$$

and similarly for the other convective fluxes.

Thus formulas (5.14a) to (5.14f) can be written in more compact form:

$$Jr+ \;=\; D_{i+1/2}\;\left[\left(\rho_m\; w_m\right)_0 - \left(\rho_m\; w_m\right)_2\right] \;+ \tag{5.19a}$$

$$+\left[0, F_{i+1/2} + G_{i+1/2}\cdot\;\left(\frac{\widetilde{H}_{z\,0}}{\rho_{m\,0}}\right)\right]\left(\rho_m\; w_m\right)_0 - \left[0, -\left(F_{i+1/2} + G_{i+1/2}\cdot\;\frac{\widetilde{H}_{z\,2}}{\rho_{m\,2}}\right)\right]\left(\rho_m\; w_m\right)_2 ,$$

$$Jr- \;=\; D_{i-1/2}\;\left[\left(\rho_m\; w_m\right)_1 - \left(\rho_m\; w_m\right)_0\right] \;+ \tag{5.19b}$$

$$+\left[0, F_{i-1/2} + G_{i-1/2}\cdot\;\left(\frac{\widetilde{H}_{z\,1}}{\rho_{m\,1}}\right)\right]\left(\rho_m\; w_m\right)_1 - \left[0, -\left(F_{i-1/2} + G_{i-1/2}\cdot\;\frac{\widetilde{H}_{z\,0}}{\rho_{m\,0}}\right)\right]\left(\rho_m\; w_m\right)_0 ,$$

$$Jz+ \;=\; D_{j+1}\;\left[\left(\rho_m\; w_m\right)_0 - \left(\rho_m\; w_m\right)_6\right] \;+ \tag{5.19c}$$

$$+\left[0, F_{j+1} + G_{j+1}\cdot\;\left(\frac{\widetilde{H}_{z\,0}}{\rho_{m\,0}}\right)\right]\left(\rho_m\; w_m\right)_0 - \left[0, -\left(F_{j+1} + G_{j+1}\cdot\;\frac{\widetilde{H}_{z\,6}}{\rho_{m\,6}}\right)\right]\left(\rho_m\; w_m\right)_6 ,$$

$$Jz- \;=\; D_{j}\;\left[\left(\rho_m\; w_m\right)_5 - \left(\rho_m\; w_m\right)_0\right] \;+ \tag{5.19d}$$

$$+\left[0, F_{j} + G_{j}\cdot\;\left(\frac{\widetilde{H}_{z\,5}}{\rho_{m\,5}}\right)\right]\left(\rho_m\; w_m\right)_5 - \left[0, -\left(F_{j} + G_{j}\cdot\;\frac{\widetilde{H}_{z\,0}}{\rho_{m\,0}}\right)\right]\left(\rho_m\; w_m\right)_0 ,$$

$$Js+ \;=\; D_{k+1/2}\;\left[\left(\rho_m\; w_m\right)_0 - \left(\rho_m\; w_m\right)_4\right] \;+ \tag{5.19e}$$

$$+\left[0, F_{k+1/2} + G_{k+1/2}\cdot\;\left(\frac{\widetilde{H}_{z\,0}}{\rho_{m\,0}}\right)\right]\left(\rho_m\; w_m\right)_0 - \left[0, -\left(F_{k+1/2} + G_{k+1/2}\cdot\;\frac{\widetilde{H}_{z\,4}}{\rho_{m\,4}}\right)\right]\left(\rho_m\; w_m\right)_4 ,$$

$$Js- \;=\; D_{k-1/2}\;\left[\left(\rho_m\; w_m\right)_3 - \left(\rho_m\; w_m\right)_0\right] \;+ \tag{5.19f}$$

$$+\left[0, F_{k-1/2} + G_{k-1/2}\cdot\;\left(\frac{\widetilde{H}_{z\,3}}{\rho_{m\,3}}\right)\right]\left(\rho_m\; w_m\right)_3 - \left[0, -\left(F_{k-1/2} + G_{k-1/2}\cdot\;\frac{\widetilde{H}_{z\,0}}{\rho_{m\,0}}\right)\right]\left(\rho_m\; w_m\right)_0 .$$

Here and in the following equations indices i, j, and k are partly suppressed. Recalling the definitions of G (5.11), of momentum slip G_{Sl} (5.2), and using (5.16a), the terms in brackets can be calculated as follows:

$$F_{i-1/2,j+1/2,k} + G_{i-1/2,j+1/2,k} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_1 =$$

(5.20a)

$$= \left(A_f \, u_m \right)_{i-1/2,j+1/2,k} \left\{ 1 + \left(x \left(1-x \right) \rho_m \; \widetilde{H}_r \right)_{i-1/2,j+1/2,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m} \right)_1 \right\} ,$$

$$F_{i+1/2,j+1/2,k} + G_{i+1/2,j+1/2,k} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_2 =$$

(5.20b)

$$= \left(A_f \, u_m \right)_{i+1/2,j+1/2,k} \left\{ 1 + \left(x \left(1-x \right) \rho_m \; \widetilde{H}_r \right)_{i+1/2,j+1/2,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m} \right)_2 \right\} ,$$

$$F_{i,j,k} + G_{i,j,k} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_5 =$$

(5.20c)

$$= \left(A_f \, w_m \right)_{ijk} \left\{ 1 + \left(x \left(1-x \right) \rho_m \; \widetilde{H}_z \right)_{ijk} \cdot \left(\frac{\widetilde{H}_z}{\rho_m} \right)_5 \right\} ,$$

$$F_{i,j+1,k} + G_{i,j+1,k} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_6 =$$

(5.20d)

$$= \left(A_f \, w_m \right)_{i,j+1,k} \left\{ 1 + \left(x \left(1-x \right) \rho_m \; \widetilde{H}_z \right)_{i,j+1,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m} \right)_6 \right\} ,$$

$$F_{i,j+1/2,k-1/2} + G_{i,j+1/2,k-1/2} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_3 =$$

(5.20e)

$$= \left(A_f \, v_m \right)_{i,j+1/2,k-1/2} \left\{ 1 + \left(x \left(1-x \right) \rho_m \; \widetilde{H}_s \right)_{i,j+1/2,k-1/2} \cdot \left(\frac{\widetilde{H}_z}{\rho_m} \right)_3 \right\} ,$$

$$F_{i,j+1/2,k+1/2} + G_{i,j+1/2,k+1/2} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_4 =$$

(5.20f)

$$= \left(A_f \, v_m \right)_{i,j+1/2,k+1/2} \left\{ 1 + \left(x \left(1-x \right) \rho_m \; \widetilde{H}_s \right)_{i,j+1/2,k+1/2} \cdot \left(\frac{\widetilde{H}_z}{\rho_m} \right)_4 \right\} ,$$

$$F_{i+1/2,j+1/2,k} + G_{i+1/2,j+1/2,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 =$$

$$= \left(A_f\, u_m\right)_{i+1/2,j+1/2,k}\left\{1+\left(x\left(1-x\right)\rho_m\ \widetilde{H}_r\right)_{i+1/2,j+1/2,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right\}, \tag{5.20g}$$

$$F_{i-1/2,j+1/2,k} + G_{i-1/2,j+1/2,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 =$$

$$= \left(A_f\, u_m\right)_{i-1/2,j+1/2,k}\left\{1+\left(x\left(1-x\right)\rho_m\ \widetilde{H}_r\right)_{i-1/2,j+1/2,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right\}, \tag{5.20h}$$

$$F_{i,\,j+1,\,k} + G_{i,\,j+1,\,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 =$$

$$= \left(A_f\, w_m\right)_{i,j+1,k}\left\{1+\left(x\left(1-x\right)\rho_m\ \widetilde{H}_z\right)_{i,j+1,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right\}, \tag{5.20i}$$

$$F_{i,\,j,\,k} + G_{i,\,j,\,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 =$$

$$= \left(A_f\, w_m\right)_{i,j,k}\left\{1+\left(x\left(1-x\right)\rho_m\ \widetilde{H}_z\right)_{i,j,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right\}, \tag{5.20j}$$

$$F_{i,\,j+1/2,\,k+1/2} + G_{i,\,j+1/2,\,k+1/2}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 =$$

$$= \left(A_f\, v_m\right)_{i,j+1/2,k+1/2}\left\{1+\left(x\left(1-x\right)\rho_m\ \widetilde{H}_s\right)_{i,j+1/2,k+1/2}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right\}, \tag{5.20k}$$

$$F_{i,\,j+1/2,\,k-1/2} + G_{i,\,j+1/2,\,k-1/2}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 =$$

$$= \left(A_f\, v_m\right)_{i,j+1/2,k-1/2}\left\{1+\left(x\left(1-x\right)\rho_m\ \widetilde{H}_s\right)_{i,j+1/2,k-1/2}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right\}. \tag{5.20l}$$

The diffusion coefficients in formulas (5.19a) to (5.19f) are given by

$$D_{i \pm 1/2,\, j+1/2,\, k} = \left(\frac{A_f\, \mu_m}{\rho_m\, \Delta r} \right)_{i \pm 1/2, j+1/2,\, k} , \tag{5.21a}$$

$$\underset{(j)}{D_{i,j+1,\,k}} = \left(\frac{A_f\, \mu_m}{\rho_m\, \Delta z} \right)_{\underset{(j)}{i,j+1,\,k}} , \tag{5.21b}$$

$$D_{i,\, j+1/2,\ k \pm 1/2} = \left(\frac{A_f\, \mu_m}{\rho_m\, \Delta s} \right)_{i,j+1/2,\ k \pm 1/2} . \tag{5.21c}$$

Using $V_f = \varepsilon V$, introducing the convective and diffusive fluxes (5.19) evaluated at time level $n+1$ into (5.8) and rearranging, one derives

$$\begin{aligned}
&\left(\rho_m\, w_m\right)_0^{n+1} \left\{ \frac{(\varepsilon V)_0}{\Delta t} + \left(\frac{\varepsilon V}{2D_h}\, f\, |w_m|^n \right)_0 + \right. \\
&+ \left[0, F^{n+1}_{i+1/2,j+1/2,\,k} + G^{n+1}_{i+1/2,j+1/2,\,k} \cdot \left(\frac{\tilde{H}_z}{\rho_m} \right)_0 \right] + \left[0, -\left(F^{n+1}_{i-1/2,j+1/2,\,k} + G^{n+1}_{i-1/2,j+1/2,\,k} \cdot \left(\frac{\tilde{H}_z}{\rho_m} \right)_0 \right) \right] + \\
&+ \left[0, F^{n+1}_{i,j+1,\,k} + G^{n+1}_{i,j+1,\,k} \cdot \left(\frac{\tilde{H}_z}{\rho_m} \right)_0 \right] + \left[0, -\left(F^{n+1}_{i\,j\,k} + G^{n+1}_{i\,j\,k} \cdot \left(\frac{\tilde{H}_z}{\rho_m} \right)_0 \right) \right] + \\
&+ \left[0, F^{n+1}_{i,j+1/2,\,k+1/2} + G^{n+1}_{i,j+1/2,\,k+1/2} \cdot \left(\frac{\tilde{H}_z}{\rho_m} \right)_0 \right] + \left[0, -\left(F^{n+1}_{i,j+1/2,\,k-1/2} + G^{n+1}_{i,j+1/2,\,k-1/2} \cdot \left(\frac{\tilde{H}_z}{\rho_m} \right)_0 \right) \right] + \\
&\left. + D^{n+1}_{i+1/2,j+1/2,\,k} + D^{n+1}_{i-1/2j+1/2,\,k} + D^{n+1}_{ij+1,\,k} + D^{n+1}_{i\,j\,k} + D^{n+1}_{ij+1/2,\,k+1/2} + D^{n+1}_{ij+1/2,\,k-1/2} \right\} + \\
&- \left(\rho_m\, w_m\right)_1^{n+1} \left\{ \left[0, F^{n+1}_{i-1/2,j+1/2,\,k} + G^{n+1}_{i-1/2,j+1/2,\,k} \left(\frac{\tilde{H}_z}{\rho_m} \right)_1 \right] + D^{n+1}_{i-1/2,j+1/2,\,k} \right\} + \\
&- \left(\rho_m\, w_m\right)_2^{n+1} \left\{ \left[0, -\left(F^{n+1}_{i+1/2,j+1/2,\,k} + G^{n+1}_{i+1/2,j+1/2,\,k} \left(\frac{\tilde{H}_z}{\rho_m} \right)_2 \right) \right] + D^{n+1}_{i+1/2,j+1/2,\,k} \right\} + \\
&- \left(\rho_m\, w_m\right)_5^{n+1} \left\{ \left[0, F^{n+1}_{i\,j\,k} + G^{n+1}_{i\,j\,k} \left(\frac{\tilde{H}_z}{\rho_m} \right)_5 \right] + D^{n+1}_{ij\,k} \right\} + \\
&- \left(\rho_m\, w_m\right)_6^{n+1} \left\{ \left[0, -\left(F^{n+1}_{i,j+1,\,k} + G^{n+1}_{i,j+1,\,k} \left(\frac{\tilde{H}_z}{\rho_m} \right)_6 \right) \right] + D^{n+1}_{i,j+1,\,k} \right\} +
\end{aligned} \tag{5.22}$$

$$-\left(\rho_m\, w_m\right)_3^{n+1} \left\{ \left[0, F^{n+1}_{i,j+1/2,\,k-1/2} + G^{n+1}_{i,j+1/2,\,k-1/2} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_3 \right] + D^{n+1}_{i,j+1/2,\,k-1/2} \right\} +$$

$$-\left(\rho_m\, w_m\right)_4^{n+1} \left\{ \left[0, -\left(F^{n+1}_{i,j+1/2,\,k+1/2} + G^{n+1}_{i,j+1/2,\,k+1/2} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_4\right) \right] + D^{n+1}_{i,j+1/2,\,k+1/2} \right\} =$$

$$= \frac{(\varepsilon\, V)_0}{\Delta t} \left(\rho_m\, w_m\right)_0^n - \left(\varepsilon\, V\, \rho_m\, g_z\right)_0^n - \left(\frac{\varepsilon\, V}{\Delta z}\right)_0 \left(p^{n+1}_{i,j+1,\,k} - p^{n+1}_{i\;j\;k}\right).$$

This equation can be written in the compact form

$$a_0^w \left(\rho_m\, w_m\right)_0^{n+1} - \sum_1^6{}_\beta\; a_\beta^w \left(\rho_m\, w_m\right)_\beta^{n+1} = b_0^w - d_0^w \left(p^{n+1}_{i,j+1,\,k} - p^{n+1}_{i\;j\;k}\right) \tag{5.23}$$

with the following definitions of the coefficients :

$$a_0^w = \frac{(\varepsilon\, V)_0}{\Delta t} + \left(\frac{\varepsilon\, V}{2D_h}\, f\,|\,w_m|^n\right)_0 + \tag{5.24a}$$

$$+ \left[0, F^{n+1}_{i+1/2,\,j+1/2,\,k} + G^{n+1}_{i+1/2,\,j+1/2,\,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right] + \left[0, -\left(F^{n+1}_{i-1/2,\,j+1/2,\,k} + G^{n+1}_{i-1/2,\,j+1/2,\,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right)\right] +$$

$$+ \left[0, F^{n+1}_{i,j+1,\,k} + G^{n+1}_{i,j+1,\,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right] + \left[0, -\left(F^{n+1}_{i\;j\;k} + G^{n+1}_{i\;j\;k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right)\right] +$$

$$+ \left[0, F^{n+1}_{i,j+1/2,\,k+1/2} + G^{n+1}_{i,j+1/2,\,k+1/2} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right] + \left[0, -\left(F^{n+1}_{i,j+1/2,\,k-1/2} + G^{n+1}_{i,j+1/2,\,k-1/2} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right)\right] +$$

$$+ D^{n+1}_{i+1/2,\,j+1/2,\,k} + D^{n+1}_{i-1/2 j+1/2,\,k} + D^{n+1}_{i,j+1,\,k} + D^{n+1}_{i j\;k} + D^{n+1}_{i,j+1/2,\,k+1/2} + D^{n+1}_{i,j+1/2,\,k-1/2} \Big\} \,,$$

$$a_1^w = \left\{ \left[0, F^{n+1}_{i-1/2,\,j+1/2,\,k} + G^{n+1}_{i-1/2,\,j+1/2,\,k} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_1\right] + D^{n+1}_{i-1/2,\,j+1/2,\,k} \right\} \,, \tag{5.24b}$$

$$a_2^w = \left\{ \left[0, -\left(F^{n+1}_{i+1/2,\,j+1/2,\,k} + G^{n+1}_{i+1/2,\,j+1/2,\,k} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_2\right)\right] + D^{n+1}_{i+1/2,\,j+1/2,\,k} \right\} \,, \tag{5.24c}$$

$$a_3^w = \left\{ \left[0, F^{n+1}_{i,j+1/2,\,k-1/2} + G^{n+1}_{i,j+1/2,\,k-1/2} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_3 \right] + D^{n+1}_{i,j+1/2,\,k-1/2} \right\} \,, \tag{5.24d}$$

$$a_4^w = \left\{ \left[0, -\left(F^{n+1}_{i,j+1/2,\,k+1/2} + G^{n+1}_{i,j+1/2,\,k+1/2} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_4\right) \right] + D^{n+1}_{i,j+1/2,\,k+1/2} \right\} \,, \tag{5.24e}$$

$$a_5^w = \left\{ \left[0,\, F_{i\,j\,k}^{n+1} + G_{i\,j\,k}^{n+1} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_5 \right] + D_{i\,j\,k}^{n+1} \right\} , \tag{5.24f}$$

$$a_6^w = \left\{ \left[0,\, - \left(F_{i,j+1,k}^{n+1} + G_{i,j+1,k}^{n+1} \left(\frac{\widetilde{H}_z}{\rho_m} \right)_6 \right) \right] + D_{i,j+1,k}^{n+1} \right\} , \tag{5.24g}$$

$$b_0^w = \frac{(\varepsilon V)_0}{\Delta t} \left(\rho_m \, w_m \right)_0^n - \left(\varepsilon V \rho_m \, g_z \right)_0^n , \tag{5.24h}$$

$$d_0^w = \left(\frac{\varepsilon V}{\Delta z} \right)_0 . \tag{5.25}$$

Defining

$$\hat{w}_6 = \frac{1}{a_0^w} \left\{ \sum_1^6 {}_\beta \; a_\beta^w \left(\rho_m \, w_m \right)_\beta^{n+1} + b_0^w \right\} , \tag{5.26}$$

$$d_6^w = \frac{d_0^w}{a_0^w} = \frac{1}{a_0^w} \left(\frac{\varepsilon V}{\Delta z} \right)_0 , \tag{5.27}$$

equation (5.23) can be written

$$\left(\rho_m \, w_m \right)_{i,j+1/2,k}^{n+1} = \hat{w}_6 - d_6^w \left(p_{i,j+1,k}^{n+1} - p_{i\,j\,k}^{n+1} \right) . \tag{5.28a}$$

Similarly one derives for the radial and azimuthal components of the momentum equation

$$\left(\rho_m \, u_m \right)_{i+1/2,j,k}^{n+1} = \hat{u}_2 - d_2^u \left(p_{i+1,j,k}^{n+1} - p_{i,\,j\,k}^{n+1} \right) , \tag{5.28b}$$

$$\left(\rho_m \, v_m \right)_{i,j,k+1/2}^{n+1} = \hat{v}_4 - d_4^v \left(p_{i,\,j,\,k+1}^{n+1} - p_{i\,j\,k}^{n+1} \right) , \tag{5.28c}$$

with

$$\hat{u}_2 = \frac{1}{a_0^u} \left\{ \sum_1^6 {}_\beta \; a_\beta^u \left(\rho_m \, u_m \right)_\beta^{n+1} + b_0^u \right\} , \tag{5.29}$$

$$\hat{v}_4 = \frac{1}{a_0^v} \left\{ \sum_1^6 {}_\beta \; a_\beta^v \left(\rho_m \, v_m \right)_\beta^{n+1} + b_0^v \right\} , \tag{5.30}$$

$$d_2^u = \frac{1}{a^u_{i+1/2,j,k}} \left(\frac{\varepsilon V}{\Delta r} \right)_{i+1/2,j,k} , \tag{5.31}$$

$$d_4^v = \frac{1}{a^v_{i,j,k+1/2}} \left(\frac{\varepsilon V}{\Delta s} \right)_{i,j,k+1/2} . \tag{5.32}$$

For the three components of the momentum equations, written for control volumes displaced by half-cell in the respective backward direction, one has (with similar definitions of symbols):

$$\left(\rho_m \, u_m \right)^{n+1}_{i-1/2,j,k} = \hat{u}_1 - d_1^u \left(p^{n+1}_{ijk} - p^{n+1}_{i-1,j\,k} \right) , \tag{5.33a}$$

$$\left(\rho_m \, v_m \right)^{n+1}_{i,j,k-1/2} = \hat{v}_3 - d_3^v \left(p^{n+1}_{ijk} - p^{n+1}_{i,j,k-1} \right) , \tag{5.33b}$$

$$\left(\rho_m \, w_m \right)^{n+1}_{i,j-1/2,k} = \hat{w}_5 - d_5^w \left(p^{n+1}_{ijk} - p^{n+1}_{i,j-1,k} \right) . \tag{5.33c}$$

6. Poisson equation describing the pressure distribution

The Poisson equation describing the coolant pressure distribution is obtained by combining the continuity and momentum equations. By introducing eqs. (5.28) and (5.33) into (4.1) one derives:

$$
\begin{aligned}
&\varepsilon_{ijk}\left(\frac{\partial\rho_m}{\partial t}\right)^{n+1}_{ijk} + \frac{1}{\Delta z_j}\left\{ \zeta_{i+1/2}\left[\hat{w}_6 - d^w_6\left(p^{n+1}_{i,j+1,k} - p^{n+1}_{ijk}\right)\right] - \right.\\
&\left. -\zeta_{j-1/2}\left[\hat{w}_5 - d^w_5\left(p^{n+1}_{ijk} - p^{n+1}_{i,j-1,k}\right)\right]\right\} +\\
&+\frac{1}{\Delta r_i}\left\{\left(\Psi F_c\right)_{i+1/2}\left[\hat{u}_2 - d^u_2\left(p^{n+1}_{i+1,j,k} - p^{n+1}_{ijk}\right)\right] - \right.\\
&\left. -\left(\Psi F_c\right)_{i-1/2}\left[\hat{u}_1 - d^u_1\left(p^{n+1}_{ijk} - p^{n+1}_{i-1,jk}\right)\right]\right\} +\\
&+\frac{1}{\Delta s_k}\left\{\left(\frac{\xi}{\cos\beta}\right)_{k+1/2}\left[\hat{v}_4 - d^v_4\left(p^{n+1}_{i,j,k+1} - p^{n+1}_{ijk}\right)\right] - \right.\\
&\left. -\left(\frac{\xi}{\cos\beta}\right)_{k-1/2}\left[\hat{v}_3 - d^v_3\left(p^{n+1}_{ijk} - p^{n+1}_{i,j,k-1}\right)\right]\right\} = 0\,.
\end{aligned}
\tag{6.1}
$$

The time derivative of the coolant mixture density is calculated by using the equation of state

$$\rho_m = \rho_m\left(p,\, h_m\right) \tag{6.2}$$

as

$$\left(\frac{\partial\rho_m}{\partial t}\right)^{n+1} = \left(\frac{\partial\rho_m}{\partial p}\right)^n_{h_m}\frac{p^{n+1}_{ijk} - p^n_{ijk}}{\Delta t} + \left(\frac{\partial\rho_m}{\partial h_m}\right)^n_p\frac{\left(h^{n+1}_m - h^n_m\right)_{ijk}}{\Delta t}\,. \tag{6.3}$$

Therefore the first term in eq. (6.1) is approximated by

$$
\begin{aligned}
&\varepsilon_{ijk}\left(\frac{\partial\rho_m}{\partial t}\right)^{n+1}_{ijk} = p^{n+1}_{ijk}\left[\frac{\varepsilon_{ijk}}{\Delta t}\left(\frac{\partial\rho_m}{\partial p}\right)^n_{h_m}\right] -\\
&-\frac{\varepsilon_{ijk}}{\Delta t}\left[\left(\frac{\partial\rho_m}{\partial p}\right)^n_{h_m}p^n_{ijk} - \left(\frac{\partial\rho_m}{\partial h_m}\right)^n_p\left(h^{n+1}_m - h^n_m\right)_{ijk}\right]
\end{aligned}
\tag{6.4}
$$

The derivatives of the coolant mixture density with respect to specific enthalpy and pressure are given [3] by

$$\left(\frac{\partial\rho_m}{\partial h_m}\right)_p = -\frac{\rho^2_m}{T_s\,\dfrac{dp}{dT_s}}\,, \tag{6.5}$$

$$\left(\frac{\partial \rho_m}{\partial p}\right)_{h_m} = \frac{x\left[h'_{gs} + T_s \frac{dp}{dT_s} \frac{\rho'_{gs}}{\rho_g^2}\right] + \left(1-x\right)\left[h'_{ls} + T_s \frac{dp}{dT_s} \frac{\rho'_{ls}}{\rho_l^2}\right]}{\frac{T_s}{\rho_m^2} \frac{dp}{dT_s}} . \tag{6.6}$$

T_S ist the saturation temperature and the derivative dp/dT_S is given by the Clapeyron's equation

$$\frac{1}{T'_s} = \frac{dp}{dT_s} = \frac{h_g - h_l}{T_s\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right)} . \tag{6.7}$$

The derivatives h'_{is} and ρ'_{is} ($i = l, g$) are obtained from the functional expressions of density and specific enthalpy of the phases on the respective saturation lines

$$h_{is} = h_{is}\left(p, T_s\right) , \qquad (i = l, g) \tag{6.8}$$

$$\rho_{is} = \rho_{is}\left(p, h_{is}\right) . \tag{6.9}$$

Formal differentiation yields

$$d\,h_{is} = \left(\frac{\partial h_{is}}{\partial p}\right)_{T_s} dp + \left(\frac{\partial h_{is}}{\partial T_s}\right)_p d\,T_s , \tag{6.10}$$

$$d\,\rho_{is} = \left(\frac{\partial \rho_{is}}{\partial p}\right)_{h_{is}} dp + \left(\frac{\partial \rho_{is}}{\partial h_{is}}\right)_p d\,h_{is} . \tag{6.11}$$

Using $d\,T_S = T'_S \cdot dp$, $dh_{is} = h'_{is} \cdot dp$ and $d\rho_{is} = \rho'_{is} \cdot dp$ one has:

$$h'_{is} = \frac{dh_{is}}{dp} = \left(\frac{\partial h_{is}}{\partial p}\right)_{T_s} + \left(\frac{\partial h_{is}}{\partial T_s}\right)_p T'_s = \left(\frac{\partial h_{is}}{\partial p}\right)_{T_s} + c_{p_{is}} \cdot T'_s , \tag{6.12}$$

$$\rho'_{is} = \frac{d\rho_{is}}{dp} = \left(\frac{\partial \rho_{is}}{\partial p}\right)_{h_{is}} + \left(\frac{\partial \rho_{is}}{\partial h_{is}}\right)_p h'_{is} . \tag{6.13}$$

The subscript s denotes saturation conditions. The derivatives in eqs (6.7), (6.12) and (6.13) are calculated as explained in section 9.

Introducing eq. (6.4) into eq. (6.1) and rearranging one derives the following Poisson-like equation:

$$p_{ijk}^{n+1} \left\{ \frac{\varepsilon_{ijk}}{\Delta t} \left(\frac{\partial \rho_m}{\partial p}\right)_{h_m}^n + \frac{1}{\Delta z_j} \left(\zeta_{j+1/2}\, d_6^w + \zeta_{j-1/2}\, d_5^w \right) + \right.$$

$$+ \frac{1}{\Delta r_i} \left[\left(\Psi F_c\right)_{i+1/2} \cdot d_2^u + \left(\Psi F_c\right)_{i-1/2} \; d_1^u \right] +$$

$$+ \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos\beta}\right)_{k+1/2} d_4^v + \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} d_3^v \right] \Bigg\} -$$

$$- p_{i,j+1,k}^{n+1} \left[\frac{\zeta_{j+1/2}}{\Delta z_j} d_6^w \right] - p_{i,j-1,k}^{n+1} \left[\frac{\zeta_{j-1/2}}{\Delta z_j} d_5^w \right] -$$

$$- p_{i+1,j,k}^{n+1} \left[\frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} d_2^u \right] - p_{i-1,j,k}^{n+1} \left[\frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} d_1^u \right] -$$

$$- p_{i,j,k+1}^{n+1} \left[\frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k+1/2} d_4^v \right] - p_{i,j,k-1}^{n+1} \left[\frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} d_3^v \right] = \tag{6.14}$$

$$= \frac{\varepsilon_{ijk}}{\Delta t} \left[\left(\frac{\partial \rho_m}{\partial p}\right)_{h_m}^n p_{ijk}^n - \left(\frac{\partial \rho_m}{\partial h}\right)_p^n \left(h_m^{n+1} - h_m^n\right)_{ijk} \right] -$$

$$- \frac{\zeta_{j+1/2}}{\Delta z_j} \hat{w}_6 + \frac{\zeta_{j-1/2}}{\Delta z_j} \hat{w}_5 - \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} \hat{u}_2 + \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \hat{u}_1 -$$

$$- \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k+1/2} \hat{v}_4 + \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} \hat{v}_3 \,.$$

This equation can be written in the compact form

$$A^{n+1} p_{ijk}^{n+1} - B^{n+1} p_{i,j-1,k}^{n+1} - C^{n+1} p_{i,j+1,k}^{n+1} - D^{n+1} p_{i-1,j,k}^{n+1} - E^{n+1} p_{i+1,j\,k}^{n+1} -$$

$$- J^{n+1} p_{ij,k-1}^{n+1} - K^{n+1} p_{i,j,k+1}^{n+1} = R^{n+1} \,, \tag{6.15}$$

with the following definitions of the coefficients:

$$B^{n+1} = \frac{\zeta_{j-1/2}}{\Delta z_j} d_5^w = \left(\frac{\zeta_{j-1/2}}{\Delta z_j} \frac{\left(\varepsilon V\right)_{j-1/2}}{\Delta z_{j-1/2}} \right) \frac{1}{a_{j-1/2}^w} = CKS \cdot FWZ_{j-1/2}^{n+1} \,, \tag{6.16a}$$

$$C^{n+1} = \frac{\zeta_{j+1/2}}{\Delta z_j} d_6^w = \frac{\zeta_{j+1/2} \left(\varepsilon V\right)_{j+1/2}}{\Delta z_j \; \Delta z_{j+1/2}} \frac{1}{a_{j+1/2}^w} = CKN \cdot FWZ_{j+1/2}^{n+1} \,, \tag{6.16b}$$

$$D^{n+1} = \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \; d_1^u = \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \; \frac{\left(\varepsilon V\right)_{i-1/2}}{\Delta r_{i-1/2}} \; \frac{1}{a^u_{i-1/2}} = CKW \cdot \; FWR^{n+1}_{i-1/2}, \tag{6.16c}$$

$$E^{n+1} = \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} \; d_2^u = \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} \; \frac{\left(\varepsilon V\right)_{i+1/2}}{\Delta r_{i+1/2}} \; \frac{1}{a^u_{i+1/2}} = CKE \cdot \; FWR^{n+1}_{i+1/2} \quad , \tag{6.16d}$$

$$J^{n+1} = \frac{1}{\Delta s_k} \; \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} \; d_3^v = \frac{\left(\frac{\xi}{\cos\beta}\right)_{k-1/2}}{\Delta s_k} \; \frac{\left(\varepsilon V\right)_{k-1/2}}{\Delta s_{k-1/2}} \; \frac{1}{a^v_{k-1/2}} = CKTM \cdot \; FWT^{n+1}_{k-1/2}, \tag{6.16e}$$

$$K^{n+1} = \frac{1}{\Delta s_k} \; \left(\frac{\xi}{\cos\beta}\right)_{k+1/2} \; d_4^v = \frac{\left(\frac{\xi}{\cos\beta}\right)_{k+1/2}}{\Delta s_k} \; \frac{\left(\varepsilon V\right)_{k+1/2}}{\Delta s_{k+1/2}} \; \frac{1}{a^v_{k+1/2}} = CKTP \cdot \; FWT^{n+1}_{k+1/2}, \tag{6.16f}$$

and:

$$CKS = \frac{\zeta_{j-1/2}}{\Delta z_j} \; \frac{\left(\varepsilon V\right)_{j-1/2}}{\Delta z_{j-1/2}} \quad , \tag{6.17a}$$

$$CKN = \frac{\zeta_{j+1/2}}{\Delta z_j} \; \frac{\left(\varepsilon V\right)_{j+1/2}}{\Delta z_{j+1/2}} \quad , \tag{6.17b}$$

$$CKW = \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \; \frac{\left(\varepsilon V\right)_{i-1/2}}{\Delta r_{i-1/2}} \quad , \tag{6.17c}$$

$$CKE = \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} \; \frac{\left(\varepsilon V\right)_{i+1/2}}{\Delta r_{i+1/2}} \quad , \tag{6.17d}$$

$$CKTM = \frac{\left(\frac{\xi}{\cos\beta}\right)_{k-1/2}}{\Delta s_k} \; \frac{\left(\varepsilon V\right)_{k-1/2}}{\Delta s_{k-1/2}} \quad , \tag{6.17e}$$

$$CKTP = \frac{\left(\frac{\xi}{\cos\beta}\right)_{k+1/2}}{\Delta s_k} \; \frac{\left(\varepsilon V\right)_{k+1/2}}{\Delta s_{k+1/2}} \quad , \tag{6.17f}$$

$$FWZ_{j\pm 1/2} = \frac{1}{a^{w}_{j\pm 1/2}} , \tag{6.18a}$$

$$FWR_{i\pm 1/2} = \frac{1}{a^{u}_{i\pm 1/2}} , \tag{6.18b}$$

$$FWT_{k\pm 1/2} = \frac{1}{a^{v}_{k\pm 1/2}} , \tag{6.18c}$$

$$A^{n+1} = \frac{\varepsilon_{ijk}}{\Delta t} \left(\frac{\partial \rho_m}{\partial p}\right)^n_{h_m} + B^{n+1} + C^{n+1} + D^{n+1} + E^{n+1} + J^{n+1} + K^{n+1} , \tag{6.19}$$

$$R^{n+1} = \frac{\varepsilon_{ijk}}{\Delta t} \left[\left(\frac{\partial \rho_m}{\partial p}\right)^n_{h_m} p^n_{ijk} - \left(\frac{\partial \rho_m}{\partial h_m}\right)^n_p \left(h^{n+1}_m - h^n_m\right)_{ijk} \right] -$$

$$- \frac{\zeta_{j+1/2}}{\Delta z_j} \hat{w}_6 + \frac{\zeta_{j-1/2}}{\Delta z_j} \hat{w}_5 - \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} \hat{u}_2 + \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \hat{u}_1 - \tag{6.20}$$

$$- \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k+1/2} \hat{v}_4 + \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} \hat{v}_3 .$$

The complete analytical expressions of the coefficients of the Poisson equation (6.15) are given, for the three coordinate directions, in Appendix I.A.

7. Alternative half-implicit treatment of diffusion terms in the momentum equation

When convective tems in the momentum equation are treated explicitly the time step constraint ($\Delta t < \Delta l/v$) is very restrictive for small mesh lengths Δl and large fluid velocity V. The time step contraint imposed by diffusive terms ($\Delta t < \Delta l^2/v$) is, on the contrary, not very restrictive. It is therefore very important to remove the first constraint by treating the convective terms implicitly while diffusive terms can still be treated explicitly or half-implicitly.

In section 5 we have shown a fully implicit treatment of both convective and diffusive terms, the latter ones without the turbulent contributions. We now present a half-implicit treatment of the diffusive terms taking into account the turbulent contributions $\nabla\cdot\tau^t$ on the basis of the generalized mixing length model explained in reference [1].

In this case the numerical treatment of the momentum equations follows the path explained in section 5, but without including the diffusive terms in the definition of the vector J. The scalar component of the momentum equation for the z coordinate direction is written

$$\frac{\partial}{\partial t}\left(\rho_m\, w_m\right) + \frac{\partial}{\partial L_\alpha} Jw_{m\alpha} - \frac{\partial}{\partial L_\alpha}\left[\left(\mu^l_m + \mu^t_m\right)\frac{\partial w_m}{\partial L_\alpha}\right] = S_z \qquad \left(L_\alpha = r, s, z\right), \tag{7.1}$$

with

$$Jw_{m_\alpha} = \left(\rho_m\, V_{m_\alpha}\right) w_m + G_{Sl}\left(V_g - V_l\right)_\alpha \left(w_g - w_l\right). \tag{7.2}$$

The same procedure as in section 5 yields the following equation (corresponding to (5.22)):

$$\left(\rho_m\, w_m\right)^{n+1}_0 \left\{\left(\frac{\varepsilon V}{\Delta t}\right)_0 + \left(\frac{\varepsilon V}{2D_h} f\,|w|^n\right)_0 + \right. \tag{7.3}$$

$$+\left[0, F^{n+1}_{i+1/2,j+1/2,k} + G^{n+1}_{i+1/2,j+1/2,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right] + \left[0, -\left(F^{n+1}_{i-1/2,j+1/2,k} + G^{n+1}_{i-1/2,j+1/2,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right)\right] +$$

$$+\left[0, F^{n+1}_{i,j+1,k} + G^{n+1}_{i,j+1,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right] + \left[0, -\left(F^{n+1}_{i\,j\,k} + G^{n+1}_{i\,j\,k}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right)\right] +$$

$$\left. +\left[0, F^{n+1}_{i,j+1/2,k+1/2} + G^{n+1}_{i,j+1/2,k+1/2}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right] + \left[0, -\left(F^{n+1}_{i,j+1/2,k-1/2} + G^{n+1}_{i,j+1/2,k-1/2}\cdot\left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right)\right]\right\} -$$

$$-\left(\rho_m\, w_m\right)^{n+1}_1 \left\{\left[0, F^{n+1}_{i-1/2,j+1/2,k} + G^{n+1}_{i-1/2,j+1/2,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_1\right]\right\} -$$

$$- \left(\rho_m\, w_m\right)_2^{n+1} \left\{ \left[0, -\left(F^{n+1}_{i+1/2,j+1/2,k} + G^{n+1}_{i+1/2,j+1/2,k} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_2 \right) \right] \right\} -$$

$$- \left(\rho_m\, w_m\right)_5^{n+1} \left\{ \left[0,\ F^{n+1}_{i\,j\,k} + G^{n+1}_{i\,j\,k} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_5 \right] \right\} -$$

$$- \left(\rho_m\, w_m\right)_6^{n+1} \left\{ \left[0,\ -\left(F^{n+1}_{i,j+1,k} + G^{n+1}_{i,j+1,k} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_6 \right) \right] \right\} -$$

$$- \left(\rho_m\, w_m\right)_3^{n+1} \left\{ \left[0, F^{n+1}_{i,j+1/2,k-1/2} + G^{n+1}_{i,j+1/2,k-1/2} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_3 \right] \right\} -$$

$$- \left(\rho_m\, w_m\right)_4^{n+1} \left\{ \left[0, -\left(F^{n+1}_{i,j+1/2,k+1/2} + G^{n+1}_{i,j+1/2,k+1/2} \left(\frac{\widetilde{H}_z}{\rho_m}\right)_4 \right) \right] \right\} =$$

$$= \frac{(\varepsilon V)_0}{\Delta t} \left(\rho_m\, w_m\right)_0^n - \left(\varepsilon V \rho_m\, g_z\right)_0^n - \left(\frac{\varepsilon V}{\Delta z}\right)_0 \left(p^{n+1}_{i,j+1,k} - p^{n+1}_{i\,j\,k} \right) +$$

$$+ \left(\zeta A\right)_{i,j+1,k} < \left(\mu^l_m + \mu^t_m\right) \frac{\partial w_m}{\partial z} >_{i,j+1,k} - \left(\zeta A\right)_{i,j,k} < \left(\mu^l_m + \mu^t_m\right) \frac{\partial w}{\partial z} >_{i,j,k} +$$

$$+ \left(\Psi A\right) < \left(\mu^l_m + \mu^t_m\right) \frac{\partial w}{\partial r} >_{i+1/2,\,j+1/2,\,k} - \left(\Psi A\right) < \left(\mu^l_m + \mu^t_m\right) \frac{\partial w}{\partial r} >_{i-1/2,\,j+1/2,\,k} +$$

$$+ \left(\xi A\right) < \left(\mu^l_m + \mu^t_m\right) \frac{\partial w}{\partial s} >_{i,j+1/2,\,k+1/2} - \left(\xi A\right) < \left(\mu^l_m + \mu^t_m\right) \frac{\partial w}{\partial s} >_{i,j+1/2,\,k-1/2} .$$

This equation can be written in the compact form

$$a^w_0 \left(\rho_m\, w_m\right)_0^{n+1} - \sum_1^6{}_\beta\ a^w_\beta \left(\rho_m\, w_m\right)_\beta^{n+1} = b^w_0 - d^w_0 \left(p^{n+1}_{i,j+1,k} - p^{n+1}_{i\,j\,k} \right) \tag{7.4}$$

with the following definitions :

$$a^w_0 = \frac{(\varepsilon V)_0}{\Delta t} + \left(\frac{\varepsilon V}{2D_h} f\,|\,w\,|^n \right)_0 + \tag{7.5a}$$

$$+ \left[0, F^{n+1}_{i+1/2,j+1/2,k} + G^{n+1}_{i+1/2,j+1/2,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 \right] + \left[0, -\left(F^{n+1}_{i-1/2,j+1/2,k} + G^{n+1}_{i-1/2,j+1/2,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 \right) \right] +$$

$$+ \left[0, F^{n+1}_{i,j+1,k} + G^{n+1}_{i,j+1,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 \right] + \left[0, -\left(F^{n+1}_{i\,j\,k} + G^{n+1}_{i\,j\,k} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0 \right) \right] +$$

$$+\left[0, F^{n+1}_{i,j+1/2,k+1/2} + G^{n+1}_{i,j+1/2,k+1/2} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right] + \left[0, -\left(F^{n+1}_{i,j+1/2,k-1/2} + G^{n+1}_{i,j+1/2,k-1/2} \cdot \left(\frac{\widetilde{H}_z}{\rho_m}\right)_0\right)\right],$$

$$a^w_1 = \left\{\left[0, F^{n+1}_{i-1/2,j+1/2,k} + G^{n+1}_{i-1/2,j+1/2,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_1\right]\right\}, \tag{7.5b}$$

$$a^w_2 = \left\{\left[0, -\left(F^{n+1}_{i+1/2,j+1/2,k} + G^{n+1}_{i+1/2,j+1/2,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_2\right)\right]\right\}, \tag{7.5c}$$

$$a^w_5 = \left\{\left[0, F^{n+1}_{i\,j\,k} + G^{n+1}_{i\,j\,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_5\right]\right\}, \tag{7.5d}$$

$$a^w_6 = \left\{\left[0, -\left(F^{n+1}_{i,j+1,k} + G^{n+1}_{i,j+1,k}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_6\right)\right]\right\}, \tag{7.5e}$$

$$a^w_3 = \left\{\left[0, F^{n+1}_{i,j+1/2,k-1/2} + G^{n+1}_{i,j+1/2,k-1/2}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_3\right]\right\}, \tag{7.5f}$$

$$a^w_4 = \left\{\left[0, -\left(F^{n+1}_{i,j+1/2,k+1/2} + G^{n+1}_{i,j+1/2,k-1/2}\left(\frac{\widetilde{H}_z}{\rho_m}\right)_4\right)\right]\right\}, \tag{7.5g}$$

$$b^w_0 = \frac{(\varepsilon V)_0}{\Delta t}\left(\rho_m w_m\right)^n - \left(\varepsilon V \rho_m g_z\right)^n_0 + \tag{7.5h}$$

$$+\left(\zeta A\right)_{i,j+1,k} < \left(\mu^l_m + \mu^t_m\right)\frac{\partial w_m}{\partial z} >_{i,j+1,k} - \left(\zeta A\right)_{i,j,k} < \left(\mu^l_m + \mu^t_m\right)\frac{\partial w}{\partial z} >_{i,j,k} +$$

$$+\left(\Psi A\right) < \left(\mu^l_m + \mu^t_m\right)\frac{\partial w}{\partial r} >_{i+1/2,\,j+1/2,\,k} - \left(\Psi A\right) < \left(\mu^l_m + \mu^t_m\right)\frac{\partial w}{\partial r} >_{i-1/2,\,j+1/2,\,k} +$$

$$+\left(\xi A\right) < \left(\mu^l_m + \mu^t_m\right)\frac{\partial w}{\partial s} >_{i,j+1/2,k+1/2} - \left(\xi A\right) < \left(\mu^l_m + \mu^t_m\right)\frac{\partial w}{\partial s} >_{i,j+1/2,k-1/2},$$

$$d^w_0 = \left(\frac{\varepsilon V}{\Delta z}\right)_0 . \tag{7.6}$$

The subsequent treatment is formally identical with that of the section 5 starting from formula (5.26) on.

8. Solution for pressure increments

In terms of pressure increments over a time step

$$\delta_p^{n+1} = p^{n+1} - p^n \tag{8.1}$$

equation (5.28) can be written

$$\left(\rho_m u_m\right)_{i+1/2,j,k}^{n+1} = \hat{\hat{u}}_2 - d_2^u \left(\delta p_{i+1,j,k}^{n+1} - \delta p_{i,j\,k}^{n+1}\right), \tag{8.2a}$$

$$\left(\rho_m v_m\right)_{i,j,k+1}^{n+1} = \hat{\hat{v}}_4 - d_4^v \left(\delta p_{i,j,k+1}^{n+1} - \delta p_{i,j,k}^{n+1}\right), \tag{8.2b}$$

$$\left(\rho_m w_m\right)_{i,j+1/2,k}^{n+1} = \hat{\hat{w}}_6 - d_6^w \left(\delta p_{i,j+1,k}^{n+1} - \delta p_{i\,j\,k}^{n+1}\right), \tag{8.2c}$$

with:

$$\hat{\hat{u}}_2 = \hat{u}_2 - d_2^u \left(p_{i+1,j,k}^n - p_{i,j\,k}^n\right), \tag{8.3a}$$

$$\hat{\hat{v}}_4 = \hat{v}_4 - d_4^v \left(p_{i,j,k+1}^n - p_{i,j,k}^n\right), \tag{8.3b}$$

$$\hat{\hat{w}}_6 = \hat{w}_6 - d_6^w \left(p_{i,j+1,k}^n - p_{i\,j\,k}^n\right). \tag{8.3c}$$

With similar definitions of symbols it holds

$$\left(\rho_m u_m\right)_{i-1/2,j,k}^{n+1} = \hat{\hat{u}}_1 - d_1^u \left(\delta p_{i,j,k}^{n+1} - \delta p_{i-1,j\,k}^{n+1}\right), \tag{8.4a}$$

$$\left(\rho_m v_m\right)_{i,j,k-1/2}^{n+1} = \hat{\hat{v}}_3 - d_3^v \left(\delta p_{i,j,k}^{n+1} - \delta p_{i,j,k-1}^{n+1}\right), \tag{8.4b}$$

$$\left(\rho_m w_m\right)_{i,j-1/2,k}^{n+1} = \hat{\hat{w}}_5 - d_5^w \left(\delta p_{i,j,k}^{n+1} - \delta p_{i,j-1,k}^{n+1}\right), \tag{8.4c}$$

with

$$\hat{\hat{u}}_1 = \hat{u}_1 - d_1^u \left(p_{i,j\,k}^n - p_{i-1,j,k}^n\right), \tag{8.5a}$$

$$\hat{\hat{v}}_3 = \hat{v}_3 - d_3^v \left(p_{i\,j\,k}^n - p_{i,j,k-1}^n\right), \tag{8.5b}$$

$$\hat{\hat{w}}_5 = \hat{w}_5 - d_5^w \left(p_{i\,j\,k}^n - p_{i,j-1,k}^n\right). \tag{8.5c}$$

The new form of the Poisson equation for pressure is obtained by inserting equations (8.2) and (8.4) into eq. (4.1):

$$
\begin{aligned}
&\varepsilon_{ijk}\left(\frac{\partial \rho_m}{\partial t}\right)^{n+1}_{ijk} + \frac{1}{\Delta z_j}\left\{ \zeta_{i+1/2}\left[\hat{\hat{w}}_6 - d^w_6\left(\delta p^{n+1}_{i,j+1,k} - \delta p^{n+1}_{ijk}\right)\right] - \right.\\
&\qquad \left. -\zeta_{j-1/2}\left[\hat{\hat{w}}_5 - d^w_5\left(\delta p^{n+1}_{ijk} - \delta p^{n+1}_{i,j-1,k}\right)\right]\right\} + \\
&+ \frac{1}{\Delta z_j}\left\{\left(\Psi F_c\right)_{i+1/2\,k}\left[\hat{\hat{u}}_2 - d^u_2\left(\delta p^{n+1}_{i+1,j,k} - \delta p^{n+1}_{ijk}\right)\right] - \right.\\
&\qquad \left. - \left(\Psi F_c\right)_{i-1/2}\left[\hat{\hat{u}}_1 - d^u_1\left(\delta p^{n+1}_{ijk} - \delta p^{n+1}_{i-1,jk}\right)\right]\right\} + \qquad (8.6)\\
&+ \frac{1}{\Delta s_k}\left\{\left(\frac{\xi}{\cos\beta}\right)_{k+1/2}\left[\hat{\hat{v}}_4 - d^v_4\left(\delta p^{n+1}_{i,j,k+1} - \delta p^{n+1}_{ijk}\right)\right] - \right.\\
&\qquad \left. - \left(\frac{\xi}{\cos\beta}\right)_{k-1/2}\left[\hat{\hat{v}}_3 - d^v_3\left(\delta p^{n+1}_{ijk} - \delta p^{n+1}_{i,j,k-1}\right)\right]\right\} = 0\,.
\end{aligned}
$$

The time derivative of the coolant mixture density is calculated by using the equation of state yielding

$$
\begin{aligned}
\left(\frac{\partial \rho_m}{\partial t}\right)^{n+1} &= \left(\frac{\partial \rho_m}{\partial p}\right)^n_{h_m}\frac{p^{n+1}_{ijk} - p^n_{ijk}}{\Delta t} + \left(\frac{\partial \rho_m}{\partial h_m}\right)_p \frac{\left(h^{n+1}_m - h^n_m\right)_{ijk}}{\Delta t} = \qquad (8.7)\\
&= \left(\frac{\partial \rho_m}{\partial p}\right)^n_{h_m}\frac{\delta p^{n+1}_{ijk}}{\Delta t} + \left(\frac{\partial \rho_m}{\partial h_m}\right)_p \frac{\left(h^{n+1}_m - h^n_m\right)_{ijk}}{\Delta t}\,.
\end{aligned}
$$

Introducing (8.7) into (8.6) and rearranging one derives the following Poisson-like equation:

$$
\begin{aligned}
&\delta p^{n+1}_{ijk}\left\{\frac{\varepsilon_{ijk}}{\Delta t}\left(\frac{\partial \rho_m}{\partial p}\right)^n_{h_m} + \frac{1}{\Delta z_j}\left(\zeta_{j+1/2}\, d^w_6 + \zeta_{j-1/2}\, d^w_5\right) + \right. \qquad (8.8)\\
&\qquad + \frac{1}{\Delta r_i}\left[\left(\Psi F_c\right)_{i+1/2} d^u_2 + \left(\Psi F_c\right)_{i-1/2} d^u_1\right] + \\
&\qquad \left. + \frac{1}{\Delta s_k}\left[\left(\frac{\xi}{\cos\beta}\right)_{k+1/2} d^v_4 + \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} d^v_3\right]\right\} - \\
&\qquad - \delta p^{n+1}_{i,j+1,k}\left[\frac{\zeta_{j+1/2}}{\Delta z_j}\, d^w_6\right] - \delta p^{n+1}_{i,j-1,k}\left[\frac{\zeta_{j-1/2}}{\Delta z_j}\, d^w_5\right] -
\end{aligned}
$$

$$- \delta p^{n+1}_{i+1,j,k} \left[\frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} d^u_2 \right] - \delta p^{n+1}_{i-1,j,k} \left[\frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} d^u_1 \right] -$$

$$- \delta p^{n+1}_{i,j,k+1} \left[\frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta} \right)_{k+1/2} d^v_4 \right] - \delta p^{n+1}_{i,j,k-1} \left[\frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta} \right)_{k-1/2} d^v_3 \right] =$$

$$= - \frac{\varepsilon_{ijk}}{\Delta t} \left(\frac{\partial \rho_m}{\partial h_m} \right)_p \left(h^{n+1}_m - h^n_m \right)_{ijk} -$$

$$- \frac{\zeta_{j+1/2}}{\Delta z_j} \hat{\hat{w}}_6 + \frac{\zeta_{j-1/2}}{\Delta z_j} \hat{\hat{w}}_5 - \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} \hat{\hat{u}}_2 + \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \hat{\hat{u}}_1 -$$

$$- \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta} \right)_{k+1/2} \hat{\hat{v}}_4 + \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta} \right)_{k-1/2} \hat{\hat{v}}_3 .$$

This equation can be written in the compact form

$$A^{n+1}\, \delta p^{n+1}_{ijk} - B^{n+1}\, \delta p^{n+1}_{i,j-1,k} - C^{n+1}\, \delta p^{n+1}_{i,j+1,k} - D^{n+1}\, \delta p^{n+1}_{i-1,j,k} - E^{n+1}\, \delta p^{n+1}_{i+1,j\;k} -$$

$$- J^{n+1}\, \delta p^{n+1}_{ij,k-1} - K^{n+1}\, \delta p^{n+1}_{i,j,k+1} = R^{n+1} , \tag{8.9}$$

with the following definitions of the coefficients:

$$B^{n+1} = \frac{\zeta_{j-1/2}}{\Delta z_j} d^w_5 = \left(\frac{\zeta_{j-1/2}}{\Delta z_j} \frac{\left(\varepsilon V\right)_{j-1/2}}{\Delta z_{j-1/2}} \right) \frac{1}{a^w_{j-1/2}} = CKS \cdot\ FWZ^{n+1}_{j-1/2} , \tag{8.10a}$$

$$C^{n+1} = \frac{\zeta_{j+1/2}}{\Delta z_j} d^w_6 = \frac{\zeta_{j+1/2} \left(\varepsilon V\right)_{j+1/2}}{\Delta z_j \quad \Delta z_{j+1/2}} \frac{1}{a^w_{j+1/2}} = CKN \cdot\ FWZ^{n+1}_{j+1/2} , \tag{8.10b}$$

$$D^{n+1} = \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} d^u_1 = \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \frac{\left(\varepsilon V\right)_{i-1/2}}{\Delta r_{i-1/2}} \frac{1}{a^u_{i-1/2}} = CKW \cdot\ FWR^{n+1}_{j-1/2} , \tag{8.10c}$$

$$E^{n+1} = \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} d^u_2 = \frac{\left(\Psi F_c\right)_{i+1/2} \left(\varepsilon V\right)_{i+1/2}}{\Delta r_i \qquad \Delta r_{i+1/2}} \frac{1}{a^u_{i+1/2}} = CKE \cdot\ FWR^{n+1}_{j+1/2} , \tag{8.10d}$$

$$J^{n+1} = \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} d_3^v = \frac{\left(\frac{\xi}{\cos\beta}\right)_{k-1/2}}{\Delta s_k} \frac{\left(\varepsilon V\right)_{k-1/2}}{\Delta s_{k-1/2}} \frac{1}{a^v_{k-1/2}} = CKTM \cdot FWT^{n+1}_{k-1/2}, \tag{8.10e}$$

$$K^{n+1} = \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k+1/2} d_4^v = \frac{\left(\frac{\xi}{\cos\beta}\right)_{k+1/2}}{\Delta s_k} \frac{\left(\varepsilon V\right)_{k+1/2}}{\Delta s_{k+1/2}} \frac{1}{a^v_{k+1/2}} = CKTP \cdot FWT^{n+1}_{k+1/2}, \tag{8.10f}$$

and:

$$FWZ_{j\pm 1/2} = \frac{1}{a^w_{j\pm 1/2}} , \tag{8.11a}$$

$$FWR_{i\pm 1/2} = \frac{1}{a^u_{j\pm 1/2}} , \tag{8.11b}$$

$$FWT_{k\pm 1/2} = \frac{1}{a^v_{k\pm 1/2}} , \tag{8.11c}$$

$$A^{n+1} = \frac{\varepsilon_{ijk}}{\Delta t} \left(\frac{\partial \rho_m}{\partial p}\right)^n_{h_m} + B^{n+1} + C^{n+1} + D^{n+1} + E^{n+1} + J^{n+1} + K^{n+1} , \tag{8.12}$$

$$R^{n+1} = - \frac{\varepsilon_{ijk}}{\Delta t} \left(\frac{\partial \rho_m}{\partial h_m}\right)^n_p \left(h^{n+1}_m - h^n_m\right)_{ijk} -$$

$$- \frac{\zeta_{j+1/2}}{\Delta z_j} \hat{\hat{w}}_6 + \frac{\zeta_{j-1/2}}{\Delta z_j} \hat{\hat{w}}_5 - \frac{\left(\Psi F_c\right)_{i+1/2}}{\Delta r_i} \hat{\hat{u}}_2 + \frac{\left(\Psi F_c\right)_{i-1/2}}{\Delta r_i} \hat{\hat{u}}_1 - \tag{8.13}$$

$$- \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k+1/2} \hat{\hat{v}}_4 + \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} \hat{\hat{v}}_3 .$$

A formally identical derivation holds for the half-implicit treatment of the diffusive terms.

9. Program functions for calculating the partial derivatives of the coolant mixture density

The partial derivatives of the coolant mixture density with respect to mixture enthalpy and pressure are calculated using the analytical expressions (6.5) and (6.6), respectively. The following auxiliary program functions are used for this purpose:

DRODHL Derivative of subcooled and saturated liquid density with respect to enthalpy at constant pressure $(\partial\rho_\ell/\partial h_\ell)_p$ (see Eq. 9.2);

DRODHV Derivative of saturated and superheated vapour density with respect to enthalpy at constant pressure $(\partial\rho_g/\partial h_g)_p$ (see Eq. 9.5);

DRODPL Derivative of subcooled and saturated liquid density with respect to pressure at constant enthalpy $(\partial\rho_\ell/\partial p)_{h_\ell}$ (see Eq. 9.18);

DRODPV Derivative of saturated and superheated vapour density with respect to pressure at constant enthalpy $(\partial\rho_g/\partial p)_{h_g}$ (see Eq. 9.19);

DPSADT Derivative of saturation pressure with respect to temperature $[dp\,(T_S)\,/\,dT_S]$ (see Eq. 9.20);

DHDPL Derivative of subcooled or saturated liquid coolant enthalpy with respect to pressure at constant temperature $(\partial h_\ell/\partial p)_T$ (see Eq. 9.21);

DHDPV Derivative of saturated or superheated vapour enthalpy with respect to pressure at constant temperature $(\partial h_g/\partial p)_T$ (see Eq. 9.22).

Details about these program functions are as follows:

Function DRODHL:

Derivative of subcooled and saturated liquid density with respect to enthalpy at constant pressure $(\partial\rho_\ell/\partial h_\ell)_p$.

From the functional dependence

$$\rho_l = \rho_l\left(h_l, p\right) \tag{9.1}$$

one derives

$$\left(\frac{\partial\rho_l}{\partial h_l}\right)_p = \left(\frac{\partial\rho_l}{\partial T_l}\right)_p \cdot \left(\frac{\partial T_l}{\partial h_l}\right)_p = \left(\frac{\partial\rho_l}{\partial T_l}\right)_p \cdot \frac{1}{c_{pl}}, \tag{9.2}$$

with

$$c_{pl} = \left(\frac{\partial h_l}{\partial T_l}\right)_p. \tag{9.3}$$

Function DRODHV:

Derivative of saturated and superheated vapour density with respect to enthalpy at constant pressure $(\partial \rho_g / \partial h_g)_p$.

From the functional dependence

$$\rho_g = \rho_g \left(h_g , p \right), \tag{9.4}$$

one derives

$$\left(\frac{\partial \rho_g}{\partial h_g} \right)_p = \left(\frac{\partial \rho_g}{\partial T_g} \right)_p \left(\frac{\partial T_g}{\partial h_g} \right)_p = \frac{\partial \rho_g}{\partial T_g} \cdot \frac{1}{c_{pg}} , \tag{9.5}$$

with

$$c_{pg} = \left(\frac{\partial h_g}{\partial T_g} \right)_p . \tag{9.6}$$

For a perfect gas one has

$$\left(\frac{\partial \rho_g}{\partial h_g} \right)_p = - \frac{\rho_g}{T \, c_p} . \tag{9.7}$$

Function DRODPL:

Derivative of subcooled and saturated liquid density with respect to pressure at constant enthalpy $(\partial \rho_\ell / \partial p)_{h_\ell}$.

Letting $v_l = 1/\rho_l$ be the liquid coolant specific volume, we have

$$\left(\frac{\partial \rho_l}{\partial p} \right)_{h_l} = - \rho_l^2 \left(\frac{\partial v_l}{\partial p} \right)_{h_l} . \tag{9.8}$$

From the thermodynamic formulas of Ref. [3] we obtain:

$$\left(\frac{\partial \rho_l}{\partial p} \right)_{h_l} = - \frac{\rho_l^2}{c_{pl}} \left[c_{pl} \left(\frac{\partial v_l}{\partial p} \right)_{T_l} + T_l \left(\frac{\partial v_l}{\partial T_l} \right)_p^2 - v_l \left(\frac{\partial v_l}{\partial T_l} \right)_p \right] . \tag{9.9}$$

For practical applications, Eq. (9.9) can be simplified as follows. We define for either phase

$$\beta_i = \frac{1}{v_i} \left(\frac{\partial v_i}{\partial T_i} \right)_p = - \frac{1}{\rho_i} \left(\frac{\partial \rho_i}{\partial T_i} \right)_p \qquad \left(i = l, g \right) \tag{9.10}$$

and

$$K_i = - \frac{1}{v_i} \left(\frac{\partial v_i}{\partial p} \right)_{T_i} = \frac{1}{\rho_i} \left(\frac{\partial \rho_i}{\partial p} \right)_{T_i} \qquad \left(i = l, g \right) . \tag{9.11}$$

The liquid specific heat at constant volume is, by definition,

$$c_{vl} = \left(\frac{\partial u_l}{\partial T_l}\right)_v , \tag{9.12}$$

where $u_l = h_l - pv_l$ is the specific internal energy.

From the tables of Ref. [3]

$$c_{vl} = \frac{c_{pl}\left(\frac{\partial v_l}{\partial p}\right)_{T_l} + T_l \left(\frac{\partial v_l}{\partial T_l}\right)_p^2}{\left(\frac{\partial v_l}{\partial p}\right)_{T_l}} ; \tag{9.13}$$

hence, using Eq. (9.11)

$$- K_l v_l \cdot c_{vl} = c_{pl} \left(\frac{\partial v_l}{\partial p}\right)_{T_l} + T_l \left(\frac{\partial v_l}{\partial T_l}\right)_p^2 . \tag{9.14}$$

Eventually, one derives the following relationship between the specific heats at constant pressure and at constant volume:

$$c_{pl} = c_{vl} + \frac{T_l \beta_l^2 v_l}{K_l} . \tag{9.15}$$

The ratio between the specific heats is given by:

$$\gamma_l = \frac{c_{pl}}{c_{vl}} = \frac{1}{1 - \frac{T_l \beta_l^2 v_l}{K_l c_{pl}}} . \tag{9.16}$$

Using Eq. (9.14) and the definitions (9.10) and (9.11), Eq. (9.9) simplifies to

$$\left(\frac{\partial \rho_l}{\partial p}\right)_{h_l} = \frac{\rho_l}{c_{pl}} \left(K_l c_{vl} + \beta_l v_l\right) . \tag{9.17}$$

Using Eq. (9.16), one derives:

$$\left(\frac{\partial \rho_l}{\partial p}\right)_{h_l} = \rho_l K_l + \frac{\beta_l}{c_{pl}} \left(1 - T_l \beta_l\right) . \tag{9.18}$$

Assuming that, for the liquid phase, the density is a function of the temperature only [$\rho_l = \rho_l(T_l)$], the approximation $K_l = 0$ in Eq. (9.18) is justifiable.

Function DRODPV:

Derivative of saturated and superheated vapour density with respect to pressure at constant enthalpy $(\partial\rho_g/\partial p)_{h_g}$.

The same analytical treatment as before yields:

$$\left(\frac{\partial \rho_g}{\partial p}\right)_{h_g} = \rho_g K_g + \frac{\beta_g}{c_{pg}} \left(1 - T_g \beta_g\right) . \tag{9.19}$$

Function DPSADT:

Derivative of saturation pressure with respect to temperature $[dp\,(T_S)/dT_S]$.

This derivative is calculated from the Clapeyron equation

$$\frac{dp\left(T_s\right)}{dT_s} = \frac{h_{gs} - h_{ls}}{T_s\left(\dfrac{1}{\rho_{gs}} - \dfrac{1}{\rho_{ls}}\right)} . \tag{9.20}$$

Function DHDPL:

Derivative of subcooled or saturated liquid coolant enthalpy with respect to pressure at constant temperature $(\partial h_\ell/\partial p)_T$.

From the thermodynamic formulas of Ref. [3], we have

$$\left(\frac{\partial h_l}{\partial p}\right)_T = \frac{1}{\rho_l} - T_l \left[\frac{\partial\left(1/\rho_l\right)}{\partial T_l}\right]_p = \frac{1}{\rho_l} - \frac{T_l}{\rho_l^2}\left(\frac{\partial \rho_l}{\partial T}\right)_p = \frac{1}{\rho_l}\left(1 - T_l\,\beta_l\right) . \tag{9.21}$$

Function DHDPV:

Derivative of saturated or superheated vapour enthalpy with respect to pressure at constant temperature $(\partial h_g/\partial p)_T$.

As in the previous case,

$$\left(\frac{\partial h_g}{\partial p}\right)_T = \frac{1}{\rho_g} - T_g \left[\frac{\partial\left(1/\rho_g\right)}{\partial T_g}\right]_p = \frac{1}{\rho_g}\left(1 - T_g\,\beta_g\right) . \tag{9.22}$$

10. Treatment of energy equation with implicit convective terms and explicit diffusion terms

Using the identities

$$\nabla \cdot \left(p\, \bar{v}_m\right) = p \left(\nabla\, \bar{v}_m\right) + \bar{v}_m \cdot \nabla p \,, \tag{10.1}$$

$$\nabla \cdot \left(\frac{p}{\rho_m}\, \alpha \left(1-\alpha\right) \left(\rho_l - \rho_g\right) \bar{V}_{Sl} \right) = \tag{10.2}$$

$$= p \left[\nabla \cdot \left(\frac{\alpha}{\rho_m} \left(1-\alpha\right) \left(\rho_l - \rho_g\right) \bar{V}_{Sl} \right) \right] + \frac{\alpha}{\rho_m} \left(1-\alpha\right) \left(\rho_l - \rho_g\right) \bar{V}_{Sl} \cdot \nabla p$$

and the following definitions of "enthalpy-slip" and "density-Slip"

$$H_{Sl} = x \left(1-x\right) \rho_m \left(h_g - h_l\right) , \tag{10.3}$$

$$R_{oSl} = \frac{\alpha}{\rho_m} \left(1-\alpha\right) \left(\rho_l - \rho_g\right) , \tag{10.4}$$

the energy conservation equation (1.3) can be written

$$\frac{\partial \left(\rho_m\, h_m\right)}{\partial t} + \nabla \cdot \left(\rho_m\, h_m\, \bar{v}_m\right) = \frac{\partial p}{\partial t} + \nabla \cdot \left(p\, \bar{v}_m\right) - p \left(\nabla \cdot\, \bar{v}_m\right) + \tag{10.5}$$

$$+ \nabla \cdot \left(p\, R_{oSl}\, \bar{V}_{Sl}\right) - p \cdot \left(\nabla \cdot\, R_{oSl}\, \bar{V}_{Sl}\right) - \nabla \cdot \bar{q} + Q - \nabla \cdot H_{Sl}\, \bar{V}_{Sl} \,.$$

Expressing the heat flux in terms of temperature gradient ($\bar{q} = -\lambda_m \nabla T$) and introducing the definition of the energy flux vector

$$\bar{J}^E_m = \rho_m\, h_m\, \bar{v}_m + H_{Sl}\, \bar{V}_{Sl} \,, \tag{10.6}$$

equation (10.5) becomes

$$\frac{\partial \left(\rho_m\, h_m\right)}{\partial t} + \nabla \cdot \bar{J}^E_m = \frac{\partial p}{\partial t} + \nabla \cdot \left(p\, \bar{v}_m\right) - p \left(\nabla \cdot\, \bar{v}_m\right) + \tag{10.7}$$

$$+ \nabla \cdot \left(p\, R_{oSl}\, \bar{V}_{Sl}\right) - p \cdot \left(\nabla \cdot\, R_{oSl}\, \bar{V}_{Sl}\right) + \nabla \cdot \lambda_m\, \nabla T + Q \,.$$

Integrating over the control cell occupied by the fluid volume $V_f = \varepsilon\, V$ and denoting $\bar{n}$ an outward directed vector normal to the cell bounding surfaces one derives, with the application of the Gauss theorem:

$$\int_{V_f} \frac{\partial}{\partial t} \left(\rho_m\, h_m\right) dV + \int_{V_f} \frac{\partial}{\partial L_\alpha}\, \bar{J}^E_{m_\alpha}\, dV = \int_{V_f} \frac{\partial p}{\partial t}\, dV + \int_{A_f} p\, \bar{v}_m \cdot \bar{n}\; dA \; -$$

$$- < p > \int_{A_f} \bar{v}_m \cdot \bar{n} \; dA + \int_{A_f} p \, R_{o\,Sl} \; \bar{V}_{Sl} \cdot \bar{n} \; dA - < p > \int_{A_f} R_{o\,Sl} \; \bar{V}_{Sl} \cdot \bar{n} \; dA +$$

$$+ \int_{V_f} Q \, dV + \int_{V_f} \frac{\partial}{\partial L_a} \left(\lambda_m \frac{\partial T}{\partial L_a} \right) dV . \qquad (10.8)$$

L_a represents the general coordinate direction and the symbol < > denotes mean value over a bounding surface.

Equation (10.8) is discretized as follows:

$$\left(\frac{\varepsilon V}{\Delta t} \right)_{ijk} \left[\left(\rho_m \, h_m \right)^{n+1}_{ijk} - \left(\rho_m \, h_m \right)^{n}_{ijk} \right] + \qquad (10.9)$$

$$+ < J^E_r \, A_f >^{n+1}_{i+1/2,j,k} - < J^E_r \, A_f >^{n+1}_{i-1/2,j,k} + < J^E_z \, A_f >^{n+1}_{i,j+1/2,k} - < J^E_z \, A_f >^{n+1}_{i,j-1/2,k}$$

$$+ < J^E_s \, A_f >^{n+1}_{i,j,k+1/2} - < J^E_s \, A_f >^{n+1}_{i,j,k-1/2} = \left(\varepsilon V \right)_{ijk} \cdot < Q >^{n+1}_{3} +$$

$$+ \left(A \, \zeta \right)_{j+1/2} < \lambda_m \frac{\partial T}{\partial z} >^{n}_{i,j+1/2,k} - \left(A \, \zeta \right)_{j-1/2} < \lambda_m \frac{\partial T}{\partial z} >^{n}_{i,j-1/2,k} +$$

$$+ \left(A \, \Psi \right)_{i+1/2} < \lambda_m \frac{\partial T}{\partial r} >^{n}_{i+1/2,j,k} - \left(A \, \Psi \right)_{i-1/2} < \lambda_m \frac{\partial T}{\partial r} >^{n}_{i-1/2,j,k} +$$

$$+ \left(A \, \xi \right)_{k+1/2} < \lambda_m \frac{\partial T}{\partial s} >^{n}_{i,j,k+1/2} - \left(A \, \xi \right)_{k-1/2} < \lambda_m \frac{\partial T}{\partial s} >^{n}_{i,j,k-1/2} +$$

$$+ \frac{\left(\varepsilon V \right)_{ijk}}{\Delta t} \left(p^{n+1}_{ijk} - p^{n}_{ijk} \right) +$$

$$+ < A_f \, p \, w_m >_{i,j+1/2,k} - < A_f \, p \, w_m >_{i,j-1/2,k} + < A_f \, p \, u_m >_{i+1/2,j,k} - < A_f \, p \, u_m >_{i-1/2,j,k} +$$

$$+ < A_f \, p \, v_m >_{i,j,k+1/2} - < A_f \, p \, v_m >_{i,j,k-1/2} -$$

$$- p^{n+1}_{ijk} \Big[A_f < w_m + R_{o\,Sl} \left(w_g - w_l \right) >_{i,j+1/2,k} - A_f < w_m + R_{o\,Sl} \left(w_g - w_l \right) >_{i,j-1/2,k} +$$

$$+ A_f < u_m + R_{o\,Sl} \left(u_g - u_l \right) >_{i+1/2,j,k} - A_f < u_m + R_{o\,Sl} \left(u_g - u_l \right) >_{i-1/2,j,k} +$$

$$+ A_f < v_m + R_{o\,Sl} \left(v_g - v_l \right) >_{i,j,k+1/2} - A_f < v_m + R_{o\,Sl} \left(v_g - v_l \right) >_{i,j,k-1/2} \Big] +$$

$$+ <A_f\ p\ R_{oSl}\left(w_g - w_l\right)>_{i,j+1/2,k} - <A_f\ p\ R_{oSl}\left(w_g - w_l\right)>_{i,j-1/2,k} +$$

$$+ <A_f\ p\ R_{oSl}\left(u_g - u_l\right)>_{i+1/2,j,k} - <A_f\ p\ R_{oSl}\left(u_g - u_l\right)>_{i-1/2,j,k} +$$

$$+ <A_f\ p\ R_{oSl}\left(v_g - v_l\right)>_{i,j,k+1/2} - <A_f\ p\ R_{oSl}\left(v_g - v_l\right)>_{i,j,k-1/2} .$$

With an upwind differencing scheme and using equations (5.16) the convective enthalpy fluxes are calculated as follows

$$< J_r^E A_f >^{n+1}_{i+1/2,j,k} = \left[0, \left(F^E_{i+1/2,j,k} + G^E_{i+1/2,j,k} \cdot \frac{1}{h_{m,ijk}}\right)\right] h_{m,ijk} - \tag{10.10}$$

$$- \left[0, -\left(F^E_{i+1/2,j,k} + G^E_{i+1/2,j,k} \cdot \frac{1}{h_{m,i+1jk}}\right)\right] h_{m,i+1,jk} ,$$

$$< J_r^E A_f >^{n+1}_{i-1/2,j,k} = \left[0,\ F^E_{i-1/2,j,k} + G^E_{i-1/2,j,k} \cdot \frac{1}{h_{m,i-1,jk}}\right] h_{m,i-1,jk} - \tag{10.11}$$

$$- \left[0, -\left(F^E_{i-1/2,j,k} + G^E_{i-1/2,j,k} \cdot \frac{1}{h_{m,ijk}}\right)\right] h_{m,ijk} ,$$

with the definitions:

$$F^E_{i\pm 1/2,j,k} = \left(A_f\ \rho_m\ u_m\right)_{i\pm 1/2,j,k} , \tag{10.12}$$

$$G^E_{i\pm 1/2,j,k} = \left(A_f\ x\left(1-x\right)\ \rho_m\ \left(h_g - h_l\right)\ u_m\ \widetilde{H}_r\right)_{i\pm 1/2,j,k} , \tag{10.13}$$

and similarly for the other coordinate directions.

Introducing these convective fluxes into equation (10.9) one derives

$$\left(\frac{\varepsilon V}{\Delta t}\right)_{ijk} \left[\left(\rho_m\ h_m\right)^{n+1}_{ijk} - \left(\rho_m\ h_m\right)^{n}_{ijk}\right] + \tag{10.14}$$

$$+ \left[0,\ F^E_{i+1/2} + \frac{G^E_{i+1/2}}{h_{m,ijk}}\right] \cdot h^{n+1}_{m,ijk} - \left[0, -\left(F^E_{i+1/2,j,k} + \frac{G^E_{i+1/2}}{h_{m,i+1,jk}}\right)\right] h^{n+1}_{m,i+1,jk} -$$

$$- \left\{ \left[0, F^E_{i-1/2,j,k} + \frac{G^E_{i-1/2}}{h_{m,i-1,j,k}}\right] h^{n+1}_{m,i-1,jk} - \left[0, -\left(F^E_{i-1/2,j,k} + \frac{G^E_{i-1/2}}{h_{m,ij,k}}\right)\right] h^{n+1}_{m,ijk} \right\} +$$

$$+ \left[0,\ F^E_{i,j+1/2,k} + \frac{G^E_{j+1/2}}{h_{m,ijk}}\right] h^{n+1}_{m,ijk} - \left[0, -\left(F^E_{i,j+1/2,k} + \frac{G^E_{j+1/2}}{h_{m,i,j+1,k}}\right)\right] h^{n+1}_{m,i,j+1k} -$$

$$- \left\{ \left[0, F^{E}_{i,j-1/2,k} + \frac{G^{E}_{j-1/2}}{h_{m,i,j-1,k}} \right] h^{n+1}_{m,i,j-1,k} - \left[0, -\left(F^{E}_{i,j-1/2,k} + \frac{G^{E}_{i-1/2}}{h_{m,ij,k}} \right) \right] h^{n+1}_{m,ijk} \right\} +$$

$$+ \left[0, F^{E}_{i,j,k+1/2} + \frac{G^{E}_{k+1/2}}{h_{m,ijk}} \right] h^{n+1}_{m,ijk} - \left[0, -\left(F^{E}_{i,j,k+1/2} + \frac{G^{E}_{k+1/2}}{h_{m,i,j,k+1}} \right) \right] h^{n+1}_{m,i,j\,k+1} -$$

$$- \left\{ \left[0, F^{E}_{i,j,k-1/2} + \frac{G^{E}_{k-1/2}}{h_{m,i,j,k-1}} \right] h^{n+1}_{m,i,j,k-1} - \left[0, -\left(F^{E}_{i,j,k-1/2} + \frac{G^{E}_{k-1/2}}{h_{m,ij,k}} \right) \right] h^{n+1}_{m,ijk} \right\} =$$

cont. (10.14)

$$= \left(\varepsilon V \right)_{ijk} \cdot \; < Q >^{n+1}_{3} +$$

$$+ \left(A\,\zeta \right)_{j+1/2} < \lambda_m \frac{\partial T}{\partial z} >^{n}_{i,j+1/2,k} - \left(A\,\zeta \right)_{j-1/2} < \lambda_m \frac{\partial T}{\partial z} >^{n}_{i,j-1/2,k} +$$

$$+ \left(A\,\Psi \right)_{i+1/2} < \lambda_m \frac{\partial T}{\partial r} >^{n}_{i+1/2,j,k} - \left(A\,\Psi \right)_{i-1/2} < \lambda_m \frac{\partial T}{\partial r} >^{n}_{i-1/2,j,k} +$$

$$+ \left(A\,\xi \right)_{k+1/2} < \lambda_m \frac{\partial T}{\partial s} >^{n}_{i,j,k+1/2} - \left(A\,\xi \right)_{k-1/2} < \lambda_m \frac{\partial T}{\partial s} >^{n}_{i,j,k-1/2} +$$

$$+ \frac{\left(\varepsilon V \right)_{ijk}}{\Delta t} \left(p^{n+1}_{ijk} - p^{n}_{ijk} \right) +$$

$$+ < A_f \; p\,w_m >_{i,j+1/2,k} - < A_f \; p\,w_m >_{i,j-1/2,k} + < A_f \; p\,u_m >_{i+1/2,j,k} - < A_f \; p\,u_m >_{i-1/2,j,k} +$$

$$+ < A_f \; p\,u_m >_{i,j,k+1/2} - < A_f \; p\,u_m >_{i,j,k-1/2} -$$

$$- p^{n+1}_{ijk} \Big[A_f < w_m + R_{oSl} \left(w_g - w_l \right) >_{i,j+1/2,k} - A_f < w_m + R_{oSl} \left(w_g - w_l \right) >_{i,j-1/2,k} +$$

$$+ A_f < u_m + R_{oSl} \left(u_g - u_l \right) >_{i+1/2,j,k} - A_f < u_m + R_{oSl} \left(u_g - u_l \right) >_{i-1/2,j,k} +$$

$$+ A_f < v_m + R_{oSl} \left(v_g - v_l \right) >_{i,j,k+1/2} - A_f < v_m + R_{oSl} \left(v_g - v_l \right) >_{i,j,k-1/2} \Big] +$$

$$+ < A_f \; p\,R_{oSl} \left(w_g - w_l \right) >_{i,j+1/2,k} - < A_f \; p\,R_{oSl} \left(w_g - w_l \right) >_{i,j-1/2,k} +$$

$$+ < A_f \; p\,R_{oSl} \left(u_g - u_l \right) >_{i+1/2,j,k} - < A_f \; p\,R_{oSl} \left(u_g - u_l \right) >_{i-1/2,j,k} +$$

$$+ < A_f \; p \; R_{o\,Sl} \left(v_g - v_l \right) >_{i,j,k+1/2} - < A_f \; p \; R_{o\,Sl} \left(v_g - v_l \right) >_{i,j,k-1/2} .$$

Rearranging one obtains

$$h^{n+1}_{m_{ijk}} \left\{ \left(\frac{\varepsilon V}{\Delta t} \rho^{n+1}_m \right)_{ijk} + \left[0, F_{i+1/2,jk} + \frac{G^E_{i+1/2,jk}}{h^{n+1}_{m,ijk}} \right] + \left[0, -\left(F_{i-1/2,j,k} + \frac{G^E_{i-1/2,j,k}}{h_{m,ijk}} \right) \right] + \right.$$

$$+ \left[0, F_{i,j+1/2,k} + \frac{G^E_{i,j+1/2,k}}{h_{m,ijk}} \right] + \left[0, -\left(F_{i,j-1/2,k} + \frac{G^E_{i,j-1/2,k}}{h_{m,ij,k}} \right) \right] +$$

$$\left. + \left[0, F^E_{i,j,k+1/2} + \frac{G^E_{i,j,k+1/2}}{h_{m,ijk}} \right] + \left[0, -\left(F_{i,j,k-1/2} + \frac{G^E_{i,j,k-1/2}}{h_{m,ij,k}} \right) \right] \right\} - \tag{10.15}$$

$$- h^{n+1}_{m_{j+1}} \left[0, -\left(F_{i,j+1/2,k} + \frac{G^E_{i,j+1/2,k}}{h_{m,i,j+1,k}} \right) \right] - h^{n+1}_{m_{i,j-1,k}} \left[0, F_{i,j-1/2,k} + \frac{G^E_{i,j-1/2,k}}{h_{m,ij-1,k}} \right] -$$

$$- h^{n+1}_{m_{i+1}} \left[0, -\left(F_{i+1/2,j,k} + \frac{G^E_{i+1/2,j,k}}{h_{m,i+1,jk}} \right) \right] - h^{n+1}_{m_{i-1,jk}} \left[0, F_{i-1/2,jk} + \frac{G^E_{i-1/2,j,k}}{h_{m,i-1,jk}} \right] -$$

$$- h^{n+1}_{m_{k+1}} \left[0, -\left(F_{i,j,k+1/2} + \frac{G^E_{i,j,k+1/2}}{h_{m,i,j,k+1}} \right) \right] - h^{n+1}_{m_{i,j,k-1}} \left[0, F_{i,j,k-1/2} + \frac{G^E_{i,j,k-1/2}}{h_{m,ij,k-1}} \right] =$$

$$= \left(\varepsilon V \right)_{ijk} \cdot < Q >^{n+1}_3 + \left[\frac{\varepsilon V}{\Delta t} \left(\rho_m h_m \right)^n \right]_{ijk} +$$

$$+ \left(A \zeta \right)_{j+1/2} < \lambda_m \frac{\partial T}{\partial z} >^n_{i,j+1/2,k} - \left(A \zeta \right)_{j-1/2} < \lambda_m \frac{\partial T}{\partial z} >^n_{i,j-1/2,k} +$$

$$+ \left(A \Psi \right)_{i+1/2} < \lambda_m \frac{\partial T}{\partial r} >^n_{i+1/2,j,k} - \left(A \Psi \right)_{i-1/2} < \lambda_m \frac{\partial T}{\partial r} >^n_{i-1/2,j,k} +$$

$$+ \left(A \xi \right)_{k+1/2} < \lambda_m \frac{\partial T}{\partial s} >^n_{i,j,k+1/2} - \left(A \xi \right)_{k-1/2} < \lambda_m \frac{\partial T}{\partial s} >^n_{i,j,k-1/2} +$$

$$+ \frac{\left(\varepsilon V \right)_{ijk}}{\Delta t} \left(p^{n+1}_{ijk} - p^n_{ijk} \right) +$$

$$+ < A_f \; p \, w_m >_{i,j+1/2,k} - < A_f \; p \, w_m >_{i,j-1/2,k} + < A_f \; p \, u_m >_{i+1/2,j,k} - < A_f \; p \, u_m >_{i-1/2,j,k} +$$

$$+ < A_f \; p \, u_m >_{i,j,k+1/2} - < A_f \; p \, u_m >_{i,j,k-1/2} -$$

$$- p^{n+1}_{ijk} \Big[A_f < w_m + R_{oSl} \left(w_g - w_l \right) >_{i,j+1/2,k} - A_f < w_m + R_{oSl} \left(w_g - w_l \right) >_{i,j-1/2,k} +$$

$$+ A_f < u_m + R_{oSl} \left(u_g - u_l \right) >_{i+1/2,j,k} - A_f < u_m + R_{oSl} \left(u_g - u_l \right) >_{i-1/2,j,k} +$$

$$+ A_f < v_m + R_{oSl} \left(v_g - v_l \right) >_{i,j,k+1/2} - A_f < v_m + R_{oSl} \left(v_g - v_l \right) >_{i,j,k-1/2} \Big] + \qquad \text{(10.15)cont.}$$

$$+ < A_f \; p \, R_{oSl} \left(w_g - w_l \right) >_{i,j+1/2,k} - < A_f \; p \, R_{oSl} \left(w_g - w_l \right) >_{i,j-1/2,k} +$$

$$+ < A_f \; p \, R_{oSl} \left(u_g - u_l \right) >_{i+1/2,j,k} - < A_f \; p \, R_{oSl} \left(u_g - u_l \right) >_{i-1/2,j,k} +$$

$$+ < A_f \; p \, R_{oSl} \left(v_g - v_l \right) >_{i,j,k+1/2} - < A_f \; p \, R_{oSl} \left(v_g - v_l \right) >_{i,j,k-1/2} .$$

Equation (10.15) can be written in the compact form

$$A^{E,n+1} \; h^{n+1}_{m,i,jk} + B^{E,n+1} \; h^{n+1}_{m,i,j-1,k} + C^{E,n+1} \; h_{m,i,j+1,k} + D^{E,n+1} \; h_{m,i-1,j,k} + \qquad \text{(10.16)}$$

$$+ E^{E,n+1} \; h^{n+1}_{m,i+1,jk} + J^{E,n+1} \; h^{n+1}_{m,i,j,k-1} + K^{E,n+1} \; h_{m,i,j,k+1} = R^{E,n+1} .$$

The coefficients and right-hand side are given by

$$A^{E,n+1} = \left(\frac{\varepsilon V}{\Delta t} \; \rho^{n+1}_m \right)_{ijk} + \left[0, F^E_{i+1/2,jk} + \frac{G^E_{i+1/2,jk}}{h^{n+1}_{m,ijk}} \right] + \left[0, - \left(F^E_{i-1/2,j,k} + \frac{G^E_{i-1/2j,k}}{h_{m,ijk}} \right) \right] +$$

$$+ \left[0, F_{i,j+1/2,k} + \frac{G^E_{i,j+1/2,k}}{h_{m,ijk}} \right] + \left[0, - \left(F^E_{i,j-1/2,k} + \frac{G^E_{i,j-1/2,k}}{h_{m,ijk}} \right) \right] + \qquad \text{(10.17a)}$$

$$+ \left[0, F^E_{i,j,k+1/2} + \frac{G^E_{i,j,k+1/2}}{h_{m,ijk}} \right] + \left[0, - \left(F^E_{i,j,,k-1/2} + \frac{G^E_{i,j,k-1/2}}{h_{m,ijk}} \right) \right],$$

$$D^{E,n+1} = \left[0, F^{E,n+1}_{i-1/2,jk} + \frac{G^{E,n+1}_{i-1/2,jk}}{h^{n+1}_{m,i-1,jk}} \right], \qquad \text{(10.17b)}$$

$$E^{E,n+1} = \left[0, - F^{E,n+1}_{i+1/2,jk} + \frac{G^{E,n+1}_{i,j+1/2,k}}{h_{m,i+1,jk}} \right], \qquad \text{(10.17c)}$$

$$J^{E,n+1} = \left[0,\ F^{E,n+1}_{i,j\,k-1/2} + \frac{G^{E,n+1}_{i,j,k-1/2}}{h_{m,i,j,k-1}} \right], \tag{10.17d}$$

$$K^{E,n+1} = \left[0,\ -\left(F^{E,n+1}_{i,j\,k+1/2} + \frac{G^{E,n+1}_{i,j,k+1/2}}{h_{m,i,j,k+1}} \right) \right], \tag{10.17e}$$

$$B^{E,n+1} = \left[0,\ F^{E,n+1}_{i,j-1/2,k} + \frac{G^{E,n+1}_{i,j-1/2,k}}{h_{m,i,j-1,k}} \right], \tag{10.17f}$$

$$C^{E,n+1} = \left[0,\ -\left(F^{E,n+1}_{i,j+1/2,k} + \frac{G^{E,n+1}_{i,j+1/2,k}}{h_{m,i,j+1,k}} \right) \right], \tag{10.17g}$$

$$R^{E,n+1} = \left(\varepsilon V\right)_{i\,j\,k} \cdot < Q >^{n+1}_{3} + \left[\frac{\varepsilon V}{\Delta t} \left(\rho_m\, h_m\right)^n \right]_{ijk} + \tag{10.17h}$$

$$+ \left(A\,\zeta\right)_{j+1/2} < \lambda_m \frac{\partial T}{\partial z} >^{n}_{i,j+1/2,k} - \left(A\,\zeta\right)_{j-1/2} < \lambda_m \frac{\partial T}{\partial z} >^{n}_{i,j-1/2,k} +$$

$$+ \left(A\,\Psi\right)_{i+1/2} < \lambda_m \frac{\partial T}{\partial r} >^{n}_{i+1/2,j,k} - \left(A\,\Psi\right)_{i-1/2} < \lambda_m \frac{\partial T}{\partial r} >^{n}_{i-1/2,j,k} +$$

$$+ \left(A\,\xi\right)_{k+1/2} < \lambda_m \frac{\partial T}{\partial s} >^{n}_{i,j,k+1/2} - \left(A\,\xi\right)_{k-1/2} < \lambda_m \frac{\partial T}{\partial s} >^{n}_{i,j,k-1/2} +$$

$$+ \frac{\left(\varepsilon V\right)_{i\,j\,k}}{\Delta t} \left(p^{n+1}_{i\,j\,k} - p^{n}_{i\,j\,k} \right) +$$

$$+ < A_f\ p\, w_m >_{i,j+1/2,k} - < A_f\ p\, w_m >_{i,j-1/2,k} + < A_f\ p\, u_m >_{i+1/2,j,k} - < A_f\ p\, u_m >_{i-1/2,j,k} +$$

$$+ < A_f\ p\, u_m >_{i,j,k+1/2} - < A_f\ p\, u_m >_{i,j,k-1/2} -$$

$$- p^{n+1}_{i\,j\,k} \Big[A_f < w_m + R_{o\,Sl}\left(w_g - w_l\right) >_{i,j+1/2,k} - A_f < w_m + R_{o\,Sl}\left(w_g - w_l\right) >_{i,j-1/2,k} +$$

$$+ A_f < u_m + R_{o\,Sl}\left(u_g - u_l\right) >_{i+1/2,j,k} - A_f < u_m + R_{o\,Sl}\left(u_g - u_l\right) >_{i-1/2,j,k} +$$

$$+ A_f < v_m + R_{o\,Sl}\left(v_g - v_l\right) >_{i,j,k+1/2} - A_f < v_m + R_{o\,Sl}\left(v_g - v_l\right) >_{i,j,k-1/2} \Big] +$$

$$+ < A_f\ p\ R_{o\,Sl}\left(w_g - w_l\right) >_{i,j+1/2,k} - < A_f\ p\ R_{o\,Sl}\left(w_g - w_l\right) >_{i,j-1/2,k} + \tag{10.15)ct.$$

$$+ < A_f \, p \, R_{oSl} \left(u_g - u_l \right) >_{i+1/2,j,k} - < A_f \, p \, R_{oSl} \left(u_g - u_l \right) >_{i-1/2,j,k} +$$

$$+ < A_f \, p \, R_{oSl} \left(v_g - v_l \right) >_{i,j,k+1/2} - < A_f \, p \, R_{oSl} \left(v_g - v_l \right) >_{i,j,k-1/2} .$$

The solution of the energy conservation equation is therefore reduced to the numerical solution of a system of algebraic equations (10.16) formally identical to the Poisson equation (6.15) describing the pressure distribution and can therefore be carried out with the same numerical algorithm.

Programming note

For the application in the code, equation (10.9) is devided by the cell volume.
Using the relationships (F_c is the coefficient c_r defined in the Appendix I.A)

$$\frac{A_{f_{i\pm 1/2}}}{V_{ijk}} = \frac{\left(\Psi F_c \right)_{i\pm 1/2}}{\Delta r_i} , \qquad (10.18)$$

$$\frac{A_{f_{j\pm 1/2}}}{V_{ijk}} = \frac{\zeta_{j\pm 1/2}}{\Delta z_j} , \qquad (10.19)$$

$$\frac{A_{f_{k\pm 1/2}}}{V_{ijk}} = \frac{1}{\Delta s_k} \left(\frac{\xi}{\cos \beta} \right)_{k\pm 1/2} , \qquad (10.20)$$

one derives

$$\left(\frac{\varepsilon}{\Delta t} \right)_{ijk} \left[\left(\rho_m \, h_m \right)^{n+1} - \left(\rho_m \, h_m \right)^{n} \right] + \qquad (10.21)$$

$$+ \frac{1}{\Delta r_i} \left[< J_r^E \, \Psi F_c >^{n+1}_{i+1/2,j,k} - < J_r^E \, \Psi F_c >^{n+1}_{i-1/2,j,k} \right] + \frac{1}{\Delta z_j} \left[< J_z^E \, \zeta >^{n+1}_{i,j+1/2,k} - < J_z^E \, \zeta >^{n+1}_{i,j-1/2,k} \right] +$$

$$+ \frac{1}{\Delta s_k} \left[< J_s^E \, \frac{\xi}{\cos \beta} >^{n+1}_{i,j,k+1/2} - < J_s^E \, \frac{\xi}{\cos \beta} >^{n+1}_{i,j,k-1/2} \right] = \varepsilon_{ijk} \cdot < Q >^{n+1}_3 +$$

$$+ \frac{1}{\Delta z_j} \left[\left(\zeta \right)_{j+1/2} < \lambda_m \, \frac{\partial T}{\partial z} >^{n}_{i,j+1/2,k} - \left(\zeta \right)_{j-1/2} < \lambda_m \, \frac{\partial T}{\partial z} >^{n}_{i,j-1/2,k} \right] +$$

$$+ \frac{1}{\Delta r_i} \left[\left(F\Psi\right) < \lambda_m \frac{\partial T}{\partial r} >^n_{i+1/2,j,k} - \left(F\Psi\right) < \lambda_m \frac{\partial T}{\partial r} >^n_{i-1/2,j,k} \right] +$$

$$+ \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos\beta}\right) < \lambda_m \frac{\partial T}{\partial s} >^n_{i,j,k+1/2} - \left(\frac{\xi}{\cos\beta}\right) < \lambda_m \frac{\partial T}{\partial s} >^n_{i,j.k-1/2} \right] +$$

$$+ \left(\frac{\varepsilon}{\Delta t}\right)_{ijk} \left(p^{n+1}_{ijk} - p^n_{ijk}\right) +$$

$$+ \frac{1}{\Delta z_j} \left[< \zeta p w_m >_{j+1/2} - < \zeta p w_m >_{j-1/2} \right] +$$

$$+ \frac{1}{\Delta r_i} \left[< F \Psi p u_m >_{i+1/2} - < F \Psi p u_m >_{i-1/2} \right] +$$

$$+ \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos\beta}\right)_{k+1/2} < p v_m >_{k+1/2} - \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} < p v_m >_{k-1/2} \right] -$$

$$- p^{n+1}_{ijk} \left\{ \frac{1}{\Delta z_j} \left[\zeta < w_m + R_{oSl}\left(w_g - w_l\right) >_{j+1/2} - \zeta < w_m + R_{oSl}\left(w_g - w_l\right) >_{j-1/2} \right] + \right.$$

$$+ \frac{1}{\Delta r_i} \left[\Psi F < u_m + R_{oSl}\left(u_g - u_l\right) >_{i+1/2} - \Psi F < u_m + R_{oSl}\left(u_g - u_l\right) >_{i-1/2} \right] +$$

$$\left. + \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos\beta}\right)_{k+1/2} < v_m + R_{oSl}\left(v_g - v_l\right) >_{k+1/2} - \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} < v_m + R_{oSl}\left(v_g - v_l\right) >_{k-1/2} \right] \right\} +$$

$$+ \frac{1}{\Delta z_j} \left[< \zeta\, p\, R_{oSl}\left(w_g - w_l\right) >_{j+1/2} - < \zeta\, p\, R_{oSl}\left(w_g - w_l\right) >_{j-1/2} \right] +$$

$$+ \frac{1}{\Delta r_i} \left[F\Psi < p\, R_{oSl}\left(u_g - u_l\right) >_{i+1/2} - F\Psi < p\, R_{oSl}\left(u_g - u_l\right) >_{i-1/2} \right] +$$

$$+ \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos\beta}\right)_{k+1/2} p\, R_{oSl}\left(v_g - v_l\right) >_{k+1/2} - \left(\frac{\xi}{\cos\beta}\right)_{k-1/2} < p\, R_{oSl}\left(v_g - v_l\right) >_{k-1/2} \right].$$

Equation ((10.21) can be written

$$\left(\frac{\varepsilon}{\Delta t}\right)_{i\,j\,k}\left[\left(\rho_m\;h_m\right)^{n+1}_{i\,j\,k}-\left(\rho_m\;h_m\right)^{n}_{i\,j\,k}\right]+ \tag{10.22}$$

$$+\left[0,\,\widetilde{F}^{E}_{i+1/2}+\frac{\widetilde{G}^{E}_{i+1/2}}{h_{m,\,i\,j\,k}}\right]\cdot\;h^{n+1}_{m,\,i\,j\,k}-\left[0,-\left(\widetilde{F}^{E}_{i+1/2}+\frac{\widetilde{G}^{E}_{i+1/2}}{h_{m,\,i+1}}\right)\right]h^{n+1}_{m,\,i+1}-$$

$$-\left\{\left[0,\widetilde{F}^{E}_{i-1/2}+\frac{\widetilde{G}^{E}_{i-1/2}}{h_{m,\,i-1}}\right]h^{n+1}_{m,\,i-1}-\left[0,-\left(\widetilde{F}^{E}_{i-1/2}+\frac{\widetilde{G}^{E}_{i-1/2}}{h_{m,\,i\,j,\,k}}\right)\right]h^{n+1}_{m,\,i\,j\,k}\right\}+$$

$$+\left[0,\,\widetilde{F}^{E}_{j+1/2}+\frac{\widetilde{G}^{E}_{j+1/2}}{h_{m,\,i\,j\,k}}\right]h^{n+1}_{m,\,i\,j\,k}-\left[0,-\left(\widetilde{F}^{E}_{j+1/2}+\frac{\widetilde{G}^{E}_{j+1/2}}{h_{m,\,j+1}}\right)\right]h^{n+1}_{m,j+1}-$$

$$-\left\{\left[0,\widetilde{F}^{E}_{j-1/2}+\frac{\widetilde{G}^{E}_{j-1/2}}{h_{m,\,j-1}}\right]h^{n+1}_{m,j-1}-\left[0,-\left(\widetilde{F}^{E}_{j-1/2}+\frac{\widetilde{G}^{E}_{j-1/2}}{h_{m,\,i\,j,\,k}}\right)\right]h^{n+1}_{m,\,i\,j\,k}\right\}+$$

$$+\left[0,\,\widetilde{F}^{E}_{k+1/2}+\frac{\widetilde{G}^{E}_{k+1/2}}{h_{m,\,i\,j\,k}}\right]h^{n+1}_{m,\,i\,j\,k}-\left[0,-\left(\widetilde{F}^{E}_{k+1/2}+\frac{\widetilde{G}^{E}_{k+1/2}}{h_{m,\;k+1}}\right)\right]h^{n+1}_{m,\,k+1}-$$

$$-\left\{\left[0,\widetilde{F}^{E}_{k-1/2}+\frac{\widetilde{G}^{E}_{k-1/2}}{h_{m,\;k-1}}\right]h^{n+1}_{m,\,k-1}-\left[0,-\left(\widetilde{F}^{E}_{k-1/2}+\frac{\widetilde{G}^{E}_{k-1/2}}{h_{m,\,i\,j,\,k}}\right)\right]h^{n+1}_{m,\,i\,j\,k}\right\}=$$

$$=\;\varepsilon_{i\,j\,k}\cdot\;<Q>^{n+1}_{3}\;+$$

$$+\frac{1}{\Delta z_j}\left[\left(\zeta\right)_{j+1/2}<\lambda_m\;\frac{\partial T}{\partial z}>^{n}_{i,j+1/2,\,k}-\left(\zeta\right)_{j-1/2}<\lambda_m\;\frac{\partial T}{\partial z}>^{n}_{i,j-1/2,\,k}\right]+$$

$$+\frac{1}{\Delta r_i}\left[\left(F\,\Psi\right)<\lambda_m\;\frac{\partial T}{\partial r}>^{n}_{i+1/2,j,\,k}-\left(F\,\Psi\right)<\lambda_m\;\frac{\partial T}{\partial r}>^{n}_{i-1/2,j,\,k}\right]+$$

$$+\frac{1}{\Delta s_k}\left[\left(\frac{\xi}{\cos\,\beta}\right)<\lambda_m\;\frac{\partial T}{\partial s}>^{n}_{i,j,\,k+1/2}-\left(\frac{\xi}{\cos\,\beta}\right)<\lambda_m\;\frac{\partial T}{\partial s}>^{n}_{i,j.\,k-1/2}\right]+$$

$$+\left(\frac{\varepsilon}{\Delta t}\right)_{i\,j\,k}\left(p^{n+1}_{i\,j\,k}-p^{n}_{i\,j\,k}\right)+$$

$$+ \frac{1}{\Delta z_j} \left[< \zeta p\, w_m >_{j+1/2} - < \zeta p\, w_m >_{j-1/2} \right] +$$

(10.22) cont.

$$+ \frac{1}{\Delta r_i} \left[< F \Psi p\, u_m >_{i+1/2} - < F \Psi p\, u_m >_{i-1/2} \right] +$$

$$+ \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos \beta} \right)_{k+1/2} < p\, v_m >_{k+1/2} - \left(\frac{\xi}{\cos \beta} \right)_{k-1/2} < p\, v_m >_{k-1/2} \right] -$$

$$- p^{n+1}_{ijk} \left\{ \frac{1}{\Delta z_j} \left[\zeta < w_m + R_{o\,Sl} \left(w_g - w_l \right) >_{j+1/2} - \zeta < w_m + R_{o\,Sl} \left(w_g - w_l \right) >_{j-1/2} \right] + \right.$$

$$+ \frac{1}{\Delta r_i} \left[\Psi F < u_m + R_{o\,Sl} \left(u_g - u_l \right) >_{i+1/2} - \Psi F < u_m + R_{o\,Sl} \left(u_g - u_l \right) >_{i-1/2} \right] +$$

$$\left. + \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos \beta} \right)_{k+1/2} < v_m + R_{o\,Sl} \left(v_g - v_l \right) >_{k+1/2} - \left(\frac{\xi}{\cos \beta} \right)_{k-1/2} < v_m + R_{o\,Sl} \left(v_g - v_l \right) >_{k-1/2} \right] \right\} +$$

$$+ \frac{1}{\Delta z_j} \left[< \zeta\, p\, R_{o\,Sl} \left(w_g - w_l \right) >_{j+1/2,} - < \zeta p\, R_{o\,Sl} \left(w_g - w_l \right) >_{j-1/2} \right] +$$

$$+ \frac{1}{\Delta r_i} \left[F \Psi < p\, R_{o\,Sl} \left(u_g - u_l \right) >_{i+1/2} - F \Psi < p\, R_{o\,Sl} \left(u_g - u_l \right) >_{i-1/2} \right] +$$

$$+ \frac{1}{\Delta s_k} \left[\left(\frac{\xi}{\cos \beta} \right)_{k+1/2} p\, R_{o\,Sl} \left(v_g - v_l \right) >_{k+1/2} - \left(\frac{\xi}{\cos \beta} \right)_{k-1/2} < p\, R_{o\,Sl} \left(v_g - v_l \right) >_{k-1/2} \right],$$

with the following definition of the fluxes:

$$\widetilde{F}^{E}_{i \pm 1/2} = \left(F_c\ \Psi\ \rho_m\ u_m \right)_{i \pm 1/2}, \tag{10.23a}$$

$$\widetilde{F}^{E}_{j \pm 1/2} = \left(\zeta\ \rho_m\ w_m \right)_{j \pm 1/2}, \tag{10.23b}$$

$$\widetilde{F}^{E}_{k \pm 1/2} = \left(\frac{\xi}{\cos \beta}\ \rho_m\ v_m \right)_{k \pm 1/2}, \tag{10.23c}$$

$$\widetilde{G}^{E}_{i \pm 1/2} = \left[F_c\ \Psi\ x \left(1 - x \right) \rho_m \left(h_g - h_l \right) u_m\ \widetilde{H}_r \right]_{i \pm 1/2}, \tag{10.24a}$$

$$\widetilde{G}^{E}_{j\pm 1/2} = \left[\zeta \; x \left(1-x\right) \rho_m \left(h_g - h_l\right) w_m \; \widetilde{H}_z \right]_{j\pm 1/2} , \qquad (10.24b)$$

$$\widetilde{G}^{E}_{k\pm 1/2} = \left[\frac{\xi}{\cos \beta} \; x \left(1-x\right) \rho_m \left(h_g - h_l\right) v_m \; \widetilde{H}_s \right]_{k\pm 1/2} . \qquad (10.24c)$$

Eventually equations formally identical with (10.15) to (10.17) are obtained, just replacing the definitions of F^E, G^E with those of $\widetilde{F}^E$, $\widetilde{G}^E$.

The analytical expressions of the coefficients of the enthalpy equation are summarized in Appendix I.B.

11. Fully implicit treatment of the energy equation

In the most recent code version diffusive terms are also treated implicitly. The numerical treatment proceeds from eq. (10.5) as follows.

We express the heat flux in terms of the enthalpy gradient $\bar{q} = -\rho_m \tilde{a}_m \nabla h_m$, with $\tilde{a}_m = \lambda_m / (\rho_m c_{pm})$ and introduce the following definitions:

$$\bar{J}^E_m = \rho_m h_m \bar{v}_m - p \bar{v}_m + H_{SL} \bar{V}_{SL} - p R_{oSL} \bar{V}_{SL} - \rho_m \tilde{a}_m \nabla h_m , \tag{11.1}$$

$$\bar{J}^P_m = \bar{v}_m + R_{oSL} \bar{V}_{SL} . \tag{11.2}$$

Equation (10.5) can then be written

$$\frac{\partial \left(\rho_m h_m\right)}{\partial t} + \nabla \cdot \bar{J}^E_m + p \left(\nabla \cdot \bar{J}^P_m\right) = \frac{\partial p}{\partial t} + Q . \tag{11.3}$$

Integrating over the control cell occupied by the fluid volume $V_f = \varepsilon V$ and denoting L_j ($j = r, s, z$) any of the coordinate directions one derives

$$\int_{V_f} \frac{\partial}{\partial t} \left(\rho_m h_m\right) dV + \int_{V_f} \frac{\partial}{\partial L_j} J^E_{mj} \, dV + \int_{V_f} p \frac{\partial}{\partial L_j} J^P_{mj} \, dV = \tag{11.4}$$

$$= \int_{V_f} \frac{\partial p}{\partial t} dV + \int_{V_f} Q \, dV .$$

Let the symbol $< p >_3$ denote pressure mean value over the cell volume. Denoting $\bar{n}$ an outward directed unit vector normal to the cell boundary surfaces and replacing the volume integrals of the divergence terms by means of surface fluxes one derives

$$\int_{V_f} \frac{\partial}{\partial t} \left(\rho_m h_m\right) dV + \int_{A_f} \bar{J}^E_m \cdot \bar{n} \, dA + < p >_3 \int_{A_f} \bar{J}^P_m \cdot \bar{n} \, dA = \tag{11.5}$$

$$= \int_{V_f} \frac{\partial p}{\partial t} dV + \int_{V_f} Q \, dV .$$

The surface fluxes are evaluated at time level n + 1 with an upwind scheme as follows:

$$\int_{A_{f\,i+1/2}} \bar{J}_m^E \cdot \bar{n}\, dA + <p>_3 \int_{A_{f\,i+1/2}} \bar{J}_m^P \cdot \bar{n}\, dA = \tag{11.6}$$

$$= < J_{mr}^{E,n+1} A_f >_{i+1/2} + <p>_3 < J_{mr}^P A_f >_{i+1/2} =$$

$$= \left[0, F_{i+1/2}^{E,n+1} + \frac{\bar{G}_{i+1/2}^{E,n+1}}{h_{m,i}^{n+1}}\right] h_{m,i}^{n+1} - \left[0, -\left(F_{i+1/2}^{E,n+1} + \frac{\bar{G}_{i+1/2}^{E,n+1}}{h_{m,i+1}^{n+1}}\right)\right] h_{m,i+1}^{n+1} -$$

$$- D_{i+1/2}^{E,n+1} \left(h_{m,i+1}^{n+1} - h_{m,i}^{n+1}\right),$$

where

$$F_{i+1/2}^{E,n+1} = \left(A_f\, \rho_m\, u_m\right)_{i+1/2}^{n+1}$$

has been defined by eq. (10.12) and

$$\bar{G}_{i+1/2}^{E,n+1} = \left(A_f\, H_{SL}\, u_m\, \tilde{H}_r\right)_{i+1/2} + A_f \left(<p>_3 - p_{i+1/2}\right) \left[\left(1 + R_{oSL}\, \tilde{H}_r\right) u_m\right]_{i+1/2}, \tag{11.7}$$

$$\tilde{H}_r = \left(u_g / u_l - 1\right) / \left[1 + x\left(u_g / u_l - 1\right)\right], \tag{11.8}$$

$$D_{i+1/2}^{E,n+1} = \rho_m\, \tilde{\alpha}_m \,/\, \Delta r_{i+1/2}\ , \tag{11.9}$$

and similarly for the other fluxes. $\tilde{H}_r$, and similarly $\tilde{H}_s$, $\tilde{H}_z$, is obtained expressing the components of the slip velocity as a function of the mixture velocity, by means of

$$V_{LS\,j} = u_{gj} - u_{lj} = u_{mj} \frac{\dfrac{u_{gj}}{u_{lj}} - 1}{1 + x\left(\dfrac{u_{gj}}{u_{lj}} - 1\right)} = u_{mj}\, \tilde{H}_j \qquad \left(j = r, s, z\right) \tag{11.10}$$

where u is a general velocity component.

We distinguish between two solution methods: the first consists in discretizing as usual the time dependent term $\partial\,(\rho_m\, h_m) / \partial t$ and yields a Poisson-like equation which can be solved numerically by means of standard elliptic solvers; the second consists in retaining the time dependent term and yields a system of ordinary first order differential equations which can be integrated with the Runge-Kutta scheme.

11.1 Derivation of a Poisson-like equation

We now i) introduce the fluxes defined by (11.6) (and similarly for the other boundary surfaces) into equation (11.5), ii) discretize the time dependent term by

$$\int_{V_f} \frac{\partial}{\partial t} \left(\rho_m h_m\right) dV \simeq \varepsilon V \left[\left(\rho_m h_m\right)^{n+1} - \left(\rho_m h_m\right)^{n} \right], \tag{11.11}$$

and iii) divide the equation (11.5) by the cell volume, taking into account the relationships

$$A_{f\ i\pm 1/2} / V = \left(\Psi F_c\right)_{i\pm 1/2} / \Delta r , \tag{11.12a}$$

$$A_{f\ j\pm 1/2} / V = \zeta_{j\pm 1/2} / \Delta z , \tag{11.12b}$$

$$A_{f\ k\pm 1/2} / V = \xi_{k\pm 1/2} / \left(\Delta s \cos\beta_{k\pm 1/2}\right). \tag{11.12c}$$

Thus equation (11.5) yields

$$\frac{\varepsilon}{\Delta t} \left[\left(\rho_m h_m\right)^{n+1} - \left(\rho_m h_m\right)^{n} \right] + \left\{ \left[0,\ F^E_{i+1/2} + \overline{G}^E_{i+1/2} \cdot \frac{1}{h^{n+1}_m} \right] h^{n+1}_m - \right. \tag{11.13}$$

$$- \left[0, - \left(F^E_{i+1/2} + \overline{G}^E_{i+1/2} \frac{1}{h^{n+1}_{m,i+1}} \right) \right] h^{n+1}_{m,i+1} - D^E_{i+1/2} \left. \left(h^{n+1}_{m,i+1} - h^{n+1}_m \right) \right\} -$$

$$- \left\{ \left[0,\ F^E_{i-1/2} + \overline{G}^E_{i-1/2} \frac{1}{h^{n+1}_{m,i-1}} \right] h^{n+1}_{m,i-1} - \left[0, - \left(F^E_{i-1/2} + \overline{G}^E_{i-1/2} \frac{1}{h^{n+1}_m} \right) \right] h^{n+1}_m - \right.$$

$$- D^E_{i-1/2} \left. \left(h^{n+1}_m - h^{n+1}_{m,i-1} \right) \right\} +$$

$$+ \left[0,\ F^E_{j+1/2} + \overline{G}^E_{j+1/2} \frac{1}{h^{n+1}_m} \right] h^{n+1}_m - \left[0, - \left(F^E_{j+1/2} + \overline{G}^E_{j+1/2} \frac{1}{h^{n+1}_{m,j+1}} \right) \right] h^{n+1}_{m,j+1} -$$

$$- D^E_{j+1/2} \left(h^{n+1}_{m,j+1} - h^{n+1}_m \right) -$$

$$- \left\{ \left[0,\ F^E_{j-1/2} + \overline{G}^E_{j-1/2} \frac{1}{h^{n+1}_{m,j-1}} \right] h^{n+1}_{m,j-1} - \left[0, - \left(F^E_{j-1/2} + \overline{G}^E_{j-1/2} \frac{1}{h^{n+1}_m} \right) \right] h^{n+1}_m - \right.$$

$$- D^E_{j-1/2} \left. \left(h^{n+1}_m - h^{n+1}_{m,j-1} \right) \right\} +$$

$$+ \left[0, F^E_{k+1/2} + \overline{G}^E_{k+1/2} \frac{1}{h^{n+1}_m} \right] h^{n+1}_m - \left[0, -\left(F^E_{k+1/2} + \overline{G}^E_{k+1/2} \frac{1}{h^{n+1}_{m,k+1}} \right) \right] h^{n+1}_{m,k+1} -$$

$$- D^E_{k+1/2} \left(h^{n+1}_{m,k+1} - h^{n+1}_m \right) -$$

$$- \left\{ \left[0, F^E_{k-1/2} + \overline{G}^E_{k-1/2} \frac{1}{h^{n+1}_{m,k-1}} \right] h^{n+1}_{m,k-1} - \left[0, -\left(F^E_{k-1/2} + \overline{G}^E_{k-1/2} \frac{1}{h^{n+1}_m} \right) \right] h^{n+1}_m - \right.$$

$$\left. - D^E_{k-1/2} \left(h^{n+1}_m - h^{n+1}_{m,k-1} \right) \right\} = \frac{\varepsilon}{\Delta t} \left(p^{n+1} - p^n \right) + \varepsilon < Q >_3 .$$

All convective and diffusive fluxes (F, G and D's) are evaluated at time level n+1, and relative superscripts have been omitted. Rearranging, equation (11.13) can be written as a discretized Poisson equation in the form

$$A^{n+1} h^{n+1}_m - B^{n+1} h^{n+1}_{m,j-1} - C^{n+1} h^{n+1}_{m,j+1} - D^{n+1} h^{n+1}_{m,i-1} - E^{n+1} h^{n+1}_{m,i+1} -$$

$$- J^{n+1} h^{n+1}_{m,k-1} - K^{n+1} h^{n+1}_{m,k+1} = R^{n+1} , \tag{11.14}$$

with

$$A^{n+1} = \varepsilon \ \rho^{n+1}_m / \Delta t + \tag{11.15}$$

$$+ \left[0, F^E_{i+1/2} + G^E_{i+1/2} \cdot \frac{1}{h^{n+1}_m} \right] + \left[0, -\left(F^E_{i-1/2} + \overline{G}^E_{i-1/2} \frac{1}{h^{n+1}_m} \right) \right] +$$

$$+ \left[0, F^E_{j+1/2} + G^E_{j+1/2} \cdot \frac{1}{h^{n+1}_m} \right] + \left[0, -\left(F^E_{j-1/2} + \overline{G}^E_{j-1/2} \frac{1}{h^{n+1}_m} \right) \right] +$$

$$+ \left[0, F^E_{k+1/2} + G^E_{k+1/2} \cdot \frac{1}{h^{n+1}_m} \right] + \left[0, -\left(F^E_{k-1/2} + \overline{G}^E_{k-1/2} \frac{1}{h^{n+1}_m} \right) \right] +$$

$$+ D^{E,n+1}_{i+1/2} + D^{E,n+1}_{i-1/2} + D^{E,n+1}_{j+1/2} + D^{E,n+1}_{j-1/2} + D^{E,n+1}_{k+1/2} + D^{E,n+1}_{k-1/2} ,$$

$$B^{n+1} = \left[0, F^E_{j-1/2} + \frac{\overline{G}^E_{j-1/2}}{h^{n+1}_{m,j-1}} \right] + D^{n+1}_{j-1/2} , \tag{11.16}$$

$$C^{n+1} = \left[0, -\left(F^E_{j+1/2} + \frac{\overline{G}^E_{j+1/2}}{h^{n+1}_{m,j+1}} \right) \right] + D^{n+1}_{j+1/2} , \tag{11.17}$$

$$D^{n+1} = \left[0,\ F^E_{i-1/2} + \overline{G}^E_{i-1/2} \cdot \frac{1}{h^{n+1}_{m,i-1}} \right] + D^{E,n+1}_{i-1/2} \ , \tag{11.18}$$

$$E^{n+1} = \left[0, -\left(F^E_{i+1/2} + \overline{G}^E_{i+1/2} \cdot \frac{1}{h^{n+1}_{m,i+1}} \right) \right] + D^{n+1}_{i+1/2} , \tag{11.19}$$

$$J^{n+1} = \left[0,\ F^E_{k-1/2} + \frac{\overline{G}^E_{k-1/2}}{h^{n+1}_{m,k-1}} \right] + D^{n+1}_{k-1/2} \ , \tag{11.20}$$

$$K^{n+1} = \left[0, -\left(F^E_{k+1/2} + \frac{\overline{G}^E_{k+1/2}}{h^{n+1}_{m,k+1}} \right) \right] + D^{n+1}_{k+1/2} , \tag{11.21}$$

$$R^{n+1} = \left(\frac{\varepsilon}{\Delta t} \right) \left(p^{n+1} - p^n \right) + \varepsilon < Q >^E_3 + \frac{\varepsilon}{\Delta t} \left(\rho_m h_m \right)^n . \tag{11.22}$$

11.2 Derivation of a system of ordinary first order differential equations

Without discretizing the time dependent term but expanding it with the chain rule

$$\frac{\partial \left(\rho_m h_m \right)}{\partial t} = \rho_m \frac{\partial h_m}{\partial t} + h_m \frac{\partial \rho_m}{\partial t} , \tag{11.23}$$

and introducing into equation (11.5), we derive

$$\frac{d h_m}{d t} = \frac{1}{\varepsilon \rho^{n+1}_m} \left\{ - \tilde{A}^{n+1} h^{n+1}_m + B^{n+1} h^{n+1}_{m,j-1} + C^{n+1} h^{n+1}_{m,j+1} + D^{n+1} h^{n+1}_{m,i-1} + \right.$$

$$\left. + E^{n+1} h^{n+1}_{m,i+1} + J^{n+1} h^{n+1}_{m,k-1} + K^{n+1} h^{n+1}_{m,k+1} \right\} + \tilde{R}^{n+1} , \tag{11.24}$$

where all coefficients coincide with those defined previously, but

$$\tilde{A}^{n+1} = + \left[0,\ F^E_{i+1/2} + G^E_{i+1/2} \cdot \frac{1}{h^{n+1}_m} \right] + \left[0, -\left(F^E_{i-1/2} + \overline{G}^E_{i-1/2} \frac{1}{h^{n+1}_m} \right) \right] +$$

$$+ \left[0,\ F^E_{j+1/2} + G^E_{j+1/2} \cdot \frac{1}{h^{n+1}_m} \right] + \left[0, -\left(F^E_{j-1/2} + \overline{G}^E_{j-1/2} \frac{1}{h^{n+1}_m} \right) \right] + \tag{11.25}$$

$$+ \left[0,\ F^E_{k+1/2} + G^E_{k+1/2} \cdot \frac{1}{h^{n+1}_m} \right] + \left[0, -\left(F^E_{k-1/2} + \overline{G}^E_{k-1/2} \frac{1}{h^{n+1}_m} \right) \right] +$$

$$+ D^{E,n+1}_{i+1/2} + D^{E,n+1}_{i-1/2} + D^{E,n+1}_{j+1/2} + D^{E,n+1}_{j-1/2} + D^{E,n+1}_{k+1/2} + D^{E,n+1}_{k-1/2} ,$$

$$\tilde{R}^{n+1} = \frac{1}{\rho^{n+1}_m} \left\{ \left(p^{n+1} - p^n \right) / \Delta t + < Q >^E_3 - h^{n+1}_m \left(\frac{\partial \rho_m}{\partial t} \right)^n \right\} . \tag{11.26}$$

Equation (11.24) yields a system of ordinary first order differential equations

$$\left\{ \frac{d h_m}{d t} \right\} = \left\{ f \left(h_m \right) \right\} \tag{11.27}$$

which can be integrated with usual ODE solvers. We use Runge-Kutta algorithms of order four [4] (see also section V.3). Alternatively, a more precise, though time costly, scheme of order seven [5] might also be used. Experience suggests, however, that the Runge-Kutta scheme of order four gives nearly the same accuracy as the scheme of order seven but that it is less computer time consuming. Therefore only the Runge-Kutta scheme of order four is implemented in the code.

12. Constitutive equations and thermodynamic disequilibrium

i) Cladding to coolant heat transfer

The cladding to coolant heat transfer coefficient σ_{HK} is calculated from the Nusselt number

$$Nu = \frac{\sigma_{HK} D_h}{\lambda_m} = c_1 + c_2 \; Re^{c3} \; Pr^{c4} , \tag{12.1}$$

where the Reynolds and Prandtl numbers $Re = v_m D_h / \nu_m$ and $Pr = \mu_m c_{p_m} / \lambda_m$ are computed using the mixture physical properties. The coefficients in (12.1) are:
i) For sodium, $c_1 = 7, c_2 = 0.025, c_3 = c_4 = 0.8$;
ii) For water, $c_1 = 0, c_2 = 0.023, c_3 = 0.8, c_4 = 0.4$.

When the thermodynamic quality is larger than 0.3 dryout is simulated and σ_{HK} is assumed to drop to 5000 W/m2 K. This assumption is based upon experimental information.

The heat transfer coefficient σ between the coolant in the outermost radial control volume and the hexagonal canning is calculated by means of the formula

$$\frac{1}{\sigma} = \frac{1}{\sigma_{SK}} + \frac{1}{\sigma_c} . \tag{12.2}$$

σ_{SK} is the heat transfer coefficient structure to coolant due to convection given by (12.1) and σ_c is the heat transfer coefficient due to conduction in the hexagonal canning.σ_c is calculated under the assumption of a linear temperature distribution along the thickness of the hexagonal canning.

ii) Effective dynamic viscosity

The components of the turbulent stress tensor are computed by using the following half-empirical definitions:

$$\tau^t_{m,ij} = \overline{\rho_m u'_{mi} u'_{mj}} = c_o \rho_m \left[\left(L_i \bar{u}_{mj} \right)^2 + \left(L_j \bar{u}_{mi} \right)^2 \right]^{1/2} \left(\frac{\partial \bar{u}_{mi}}{\partial l_j} + \frac{\partial \bar{u}_{mj}}{\partial l_i} \right) \left(i,j = v,s,z \right) \tag{12.3}$$

where primes and bars denote turbulent fluctuations and time mean values, respectively. Subscripts i, j refer to the coordinate directions. The dimensionless coefficient ($c_o = 0.06$) has been calibrated by comparison with experimental results of turbulent velocity distributions. The mixing lengths are defined by $L_i = \gamma_i \Delta\ell_i$, where γ and $\Delta\ell$ are surface permeability and mesh length, respectively. Thus an effective turbulent dynamic viscosity of the mixture is defined by

$$\mu^t_{m,i,j} = c_o \rho_m \left[\left(L_i \, \bar{u}_{mj} \right)^2 + \left(L_j \, \bar{u}_{mi} \right)^2 \right]^{1/2} \tag{12.4}$$

and takes into account the anisotropy of the porous medium.

iii) Effective thermal diffusivity

A turbulent energy flux vector is defined for the coolant mixture by

$$q^t_{m,i} = - \overline{\rho_m \, h'_m \, u'_{mi}} = \rho_m \, \alpha^t_{mi} \left(\frac{\partial \bar{h}_m}{\partial l_i} \right) , \qquad \left(i = r,s,z \right) \tag{12.5}$$

with the definition of the eddy diffusivities for heat transfer

$$\alpha^t_{mi} = c_{oT} \; L_i \left(u^2_{mj} + u^2_{mk} \right)^{1/2} . \qquad \left(j, k \neq i \right) \tag{12.6}$$

The dimensionless constant c_{oT} ($c_{oT} = 0.01$) has been likewise evaluated by experimental comparison of temperature distributions in turbulent flow fields.

iv) Single- and two-phase pressure drops

a) <u>Single-phase friction pressure drops and pressure drops due to grid spacers</u>

The frictional pressure drops are calculated by means of the relationship by Novendstern [6] which also takes into account the contribution due to the wire wraps. The friction coefficient is given by

$$f = f_o \cdot f_m , \tag{12.7}$$

with

$$f_o = a \cdot Re^{-b} , \tag{12.8a}$$

$$f_m = CFM = \left(CFM1 + CFM2 \cdot Re^{CFME1} \right)^{CFME2} , \tag{12.8b}$$

$$CFM1 = \frac{1.034}{(P/D)^{0.124}} , \tag{12.8c}$$

$$CFM2 = \frac{29.7 \cdot \left(P/D \right)^{6.94}}{(\lambda/D)^{2.239}} . \tag{12.8d}$$

Re is the Reynolds number of the undisturbed flow. P is the pitch, D the diameter of the pins, λ the pitch length of the wire wraps. For turbulent flow the following values of the coefficients are suggested: a = 0.316, b = 0.25, CFME1 = 0.086, CFME2 = 0.855.

In case wire wraps are not to be simulated, the input parameter λ (= HELIC) is set to a large value, thus giving CFM2 $\approx$ 0.

If grid spacers must be simulated, the pressure drops in the grids are calculated as the sum of two contributions: an irreversible pressure drop at the grid entry and frictional pressure drop along the grid. The pressure recovery at the downstream edge of the grid is considered as negligible. Within the grids mass flows in transverse directions are suppressed, therefore only pressure drops in axial directions are taken into account. These are given by

$$\Delta p_g = \left(\Delta p \right)_{entry} + \left(\Delta p \right)_{friction} =$$

$$= \frac{\rho}{2} \; w_o^2 \left(1 - \frac{1}{A} \right)^2 + \frac{f_r \, \rho \, L_g \, w_o^2}{2 \, D_{hg} \, A^2} = \frac{\rho}{2} \, K_e \, w_o^2 + \frac{f_r \, \rho \, L_g \, w_o^2}{2 \, D_{hg} \, A^2} , \tag{12.9}$$

where:

A	=	$S_g/S = w_o/w_g$ ratio of reduced to undisturbed flow area
D_{h_g}	=	hydraulic diameter of the grid (m)
f_r	=	friction coefficient for the grid
K_e	=	$(1 - S_o/S_g)^2 = (1 - 1/A)^2$ resistance coefficient at grid inlet
L_g	=	grid axial length (m) ($L_g \leqq \Delta z$)
S_o	=	flow area upstream of the grid (m^2)
S_g	=	flow area through the grid (m^2)
w_o	=	flow velocity upstream of the grid (undistrubed bundle) (m/s)
w_g	=	flow velocity through the grid (m/s)

ρ = coolant density (kg/m3).

An equivalent resistance coefficient for the grid is defined by

$$K_g = K_e + \frac{f_r\, L_g}{D_{hg}\, A^2} = \left(1 - \frac{1}{A}\right)^2 + \frac{f_r\, L_g}{D_{hg}\, A^2} = \left[\Delta p_g \;/\; \left(\frac{\rho\, w_o^2}{2}\right)\right] \qquad (12.10)$$

and an equivalent friction coeffcient by

$$f_g = K_g \cdot \frac{D_h}{\Delta z} \; . \qquad (12.11)$$

D_h is the hydraulic diameter of the channel flow without grid and Δz is the mesh length. The programme user can choose between modelling the grid spacers in their actual position, as explained above, or simulating the pressure drop by smearing the local contribution uniformly over all axial meshes. In the latter case, the friction coefficient due to the grid is

$$f_g = K_g \cdot \frac{D_h}{DABST} \; , \qquad (12.12)$$

where DABST is the distance between two consecutive grids.

The roughness of the upstream edge of the grid is taken into account by replacing the flow areas ratio in $K_e = (1 - 1/A)^2$ by

$$A' = \left[c\left(A^2 - 1\right) + 1\right] A \qquad (12.13)$$

where c is an input coefficient ranging from 0 to 0.4.

Taking into account the contribution to the pressure drop due to the grid spacers, the total friction coefficient is calculated as

$$f_t = f + f_g \qquad (12.14)$$

which is introduced into the term $(V_f/2\, D_h)\, f_t\, |\, w_l\, |^n\, (\rho_l\, w_l)^{n+1}$ of equation (5.8).

b) Two-Phase pressure drop

The two-phase pressure drops are calculated by

$$\frac{\Delta p}{\Delta l_i} = \frac{f}{2D_h} \rho_m u_{mi} \mid u_{mi} \mid \left(1 + K_i\right) . \qquad \left(i = 1, 2, 3\right) \tag{12.15}$$

The factor (1 + K) is thus interpreted as a two phase multiplier. The "drag function" K is assumed to be proportional to the slip velocity

$$K_i = c \mid u_{gi} - u_{li} \mid = c \mid u_{mi} \mid U^N_{Sli} \left(\alpha\right) \tag{12.16}$$

where c is a constant and $U^N_{Sli} = \mid u_{gi} - u_{li} \mid / u_{mi}$, the normalized slip velocity, is a monotonous and increasing function of the void fraction α. Indices g, l refer to the vapour and liquid phase, respectively. In the applications we choose c = 1 - 1.5 and $U^N_{SLi}(\alpha) = 18\alpha$ independent of i. This approach to the problem of calculating the two-phase pressure drop turned out to be more convenient for large void fractions than the application of the well known Lockhart-Martinelli two-phase multipliers. However the factor $(1+K_i)$ in formula (12.15) can be interpreted as a two-phase multiplier for the slip model. For small void fractions the two approaches yield comparable results. This depends on the fact that the method by Lockhardt and Martinelli is applicable for bubbly flow (when strictly the Slip Model holds) but not for separated flow at large void fractions. Thus the use of relationships (12.15) and 12.16) allows for the application of the Slip Model, with reasonable results, beyond its normal range of validity.

v) **Thermodynamic disequilibrium between the phases**

Formal differentiation of the equation of state $\rho_m = \rho_m(p, h_m)$ yields

$$\frac{d\rho_m}{dt} = \left(\frac{\partial \rho_m}{\partial h_m}\right)_p \frac{dh_m}{dt} + \left(\frac{\partial \rho_m}{\partial p}\right)_{h_m} \frac{dp}{dt} . \tag{12.17}$$

The partial derivatives are evaluated at time level t_n by means of the analytical expressions given in section 9. Besides to allow for a smooth transition from single to two-phase flow conditions at boiling inception the derivatives of the rhs in eq. (12.17) are multiplied by smoothing coefficients c_1, c_2, respectively, which have been chosen empirically with a numerical value 0.01. The first of these two coefficients has a direct impact upon the relationship between the thermodynamic quality and the void fraction given by

$$\alpha = \frac{x\beta}{1 + x(\beta - 1)} \tag{12.18}$$

with $\beta = c_l\,(\rho_l/\rho_g)$. The assumption $c_l = 1$ would imply a thermodynamic equilibrium between the phases while the assumed plot $\alpha = \alpha\,(x)$, corresponding to $c_l = 0.01$, implies a thermodynamic disequilibrium, i.e. a relaxation of the vapour production rate. Fig. 1 shows the void fraction as a function of the quality with c_l as a parameter.

The numerical solution of the enthalpy equation (1.3) yields the updated value of h_m, hence the thermodynamic quality

$$x = \frac{\left(h_m - h_{ls}\right)}{\left(h_{gs} - h_{ls}\right)} \quad . \tag{12.19}$$

The mixture density ρ_m, hence the updated value of the void fraction α, are derived by solving numerically the mixture continuity equation, eq. (4.1).

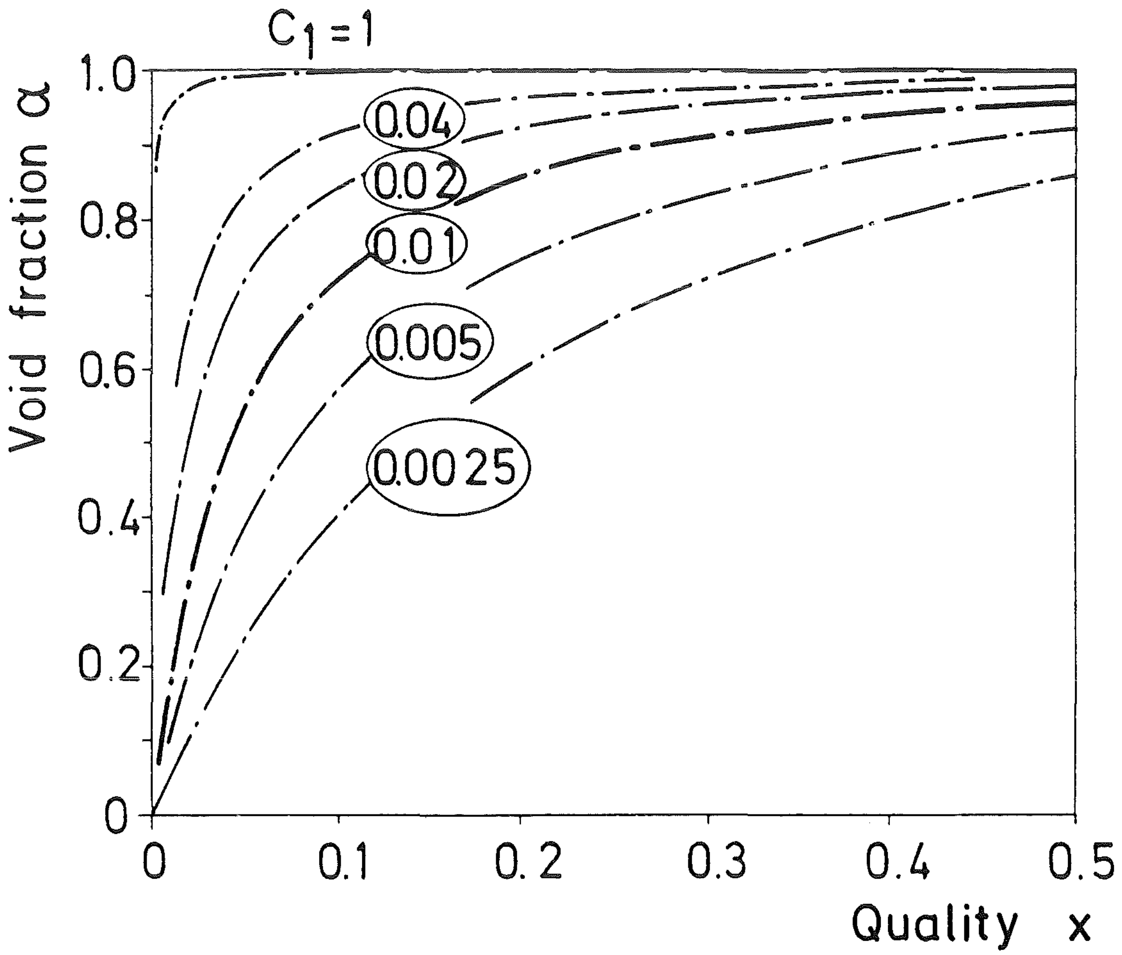

Fig. 1: Vapour volume fraction α as a function of thermodynamic quality x with c_l as parameter.

Appendix I.A. Coefficients and right hand side of the Poisson equation (6.15) describing the coolant pressure distribution (implicit formulation)

The following conventions are used

(1) Surface permeabilities are referred to as Ψ, ζ and ξ for the radial, axial and azimuthal directions, respectively. ε denotes the volume porosity.

(2) Mesh lengths are Δr, Δz, Δs.

(3) The geometry coefficients c_α are defined as follows:

(a) for the radial direction: $F = c_r = S_b/S_m$, where S_b is the area of the inner or outer boundary surface, S_m the mid area. We use the FORTRAN symbols FACCM and FACCP for the area ratios of the inner and outer surfaces of centered cells and the symbols FACRM, FACRP for the inner and outer surfaces of radially displaced cells.

(b) for the axial direction: $c_z = 1$

(c) for the azimuthal direction: $c_s = 1/\cos\beta$; β = angle between r-axis and azimuthal boundary surface of control volume.

(4) Only indices different from i or j or k are given.

(5) The bundle axis is assumed to be vertical.
The Poisson eq. (6.15) can be written:

$$A^{n+1} \cdot p^{n+1} - B^{n+1} p_{j-1}^{n+1} - C^{n+1} \cdot p_{j+1}^{n+1} - D^{n+1} \cdot p_{i-1}^{n+1} - E^{n+1} \cdot p_{i+1}^{n+1}$$

$$- J^{n+1} \cdot p_{k-1}^{n+1} - K^{n+1} \cdot p_{k+1}^{n+1} = R^{n+1} . \tag{I.A.1}$$

When both convective and diffusive terms in the momentum equation are treated implicitly, the coefficients of the Poisson equation (A.1) are as follows:

$$B^{n+1} = CKS \cdot FWZ_{j-1/2}^{n+1} , \tag{I.A.2}$$

$$C^{n+1} = CKN \cdot FWZ_{j+1/2}^{n+1} , \tag{I.A.3}$$

$$D^{n+1} = CKW \cdot FWR^{n+1}_{i-1/2} , \tag{I.A.4}$$

$$E^{n+1} = CKE \cdot FWR^{n+1}_{i+1/2} , \tag{I.A.5}$$

$$J^{n+1} = CKTM \cdot FWT^{n+1}_{k-1/2} , \tag{I.A.6}$$

$$K^{n+1} = CKTP \cdot FWT^{n+1}_{k+1/2} , \tag{I.A.7}$$

$$A^{n+1} = \left(\varepsilon / \Delta t\right)\left(\partial \rho_m / \partial p\right)^n_{h_m} + B^{n+1} + C^{n+1} + D^{n+1} + E^{n+1} + J^{n+1} + K^{n+1} , \tag{I.A.8}$$

with the definitions:

$$CKS = \zeta_{j-1/2}\left(\varepsilon V\right)_{j-1/2} / \left(\Delta z \cdot \Delta z_{j-1/2}\right) , \tag{I.A.9}$$

$$CKN = \zeta_{j+1/2}\left(\varepsilon V\right)_{j+1/2} / \left(\Delta z \cdot \Delta z_{j+1/2}\right) , \tag{I.A.10}$$

$$CKW = \Psi_{i-1/2} \cdot FACCM \cdot \left(\varepsilon V\right)_{i-1/2} / \left(\Delta r \cdot \Delta r_{i-1/2}\right) , \tag{I.A.11}$$

$$CKE = \Psi_{i+1/2} \cdot FACCP \cdot \left(\varepsilon V\right)_{i+1/2} / \left(\Delta r \cdot \Delta r_{i+1/2}\right) , \tag{I.A.12}$$

$$CKTM = \xi_{k-1/2}\left(\varepsilon V\right)_{k-1/2} / \left(\Delta s \cdot \Delta s_{k-1/2} \cdot \cos \beta_{k-1/2}\right) , \tag{I.A.13}$$

$$CKTP = \xi_{k+1/2}\left(\varepsilon V\right)_{k+1/2} / \left(\Delta s \cdot \Delta s_{k+1/2} \cdot \cos \beta_{k+1/2}\right) , \tag{I.A.14}$$

$$FWZ^{n+1}_{j\pm 1/2} = 1 / a^{w}_{j\pm 1/2} , \tag{I.A.15}$$

$$FWR^{n+1}_{i\pm 1/2} = 1 / a^{u}_{i\pm 1/2} , \tag{I.A.16}$$

$$FWT^{n+1}_{k\pm 1/2} = 1 / a^{v}_{k\pm 1/2} , \tag{I.A.17}$$

with

$$\alpha^{w}_{j+1/2} = \left(\varepsilon V\right)_{j+1/2} / \Delta t + \left(\varepsilon V f |w|^{n} / \left(2 D_h\right)\right)_{j+1/2} + \left[0, F^{n+1}_{i+1/2,j+1/2} + G^{n+1}_{i+1/2,j+1/2} \left(\widetilde{H}_z / \rho_m\right)_{j+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1}_{i-1/2,j+1/2} + G^{n+1}_{i-1/2,j+1/2} \left(\widetilde{H}_z / \rho_m\right)_{j+1/2}\right)\right] + \left[0, F^{n+1}_{j+1} + G^{n+1}_{j+1} \left(\widetilde{H}_z / \rho_m\right)_{j+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1} + G^{n+1} \left(\widetilde{H}_z / \rho_m\right)_{j+1/2}\right)\right] + \left[0, F^{n+1}_{j+1/2,\,k+1/2} + G^{n+1}_{j+1/2,\,k+1/2} \left(\widetilde{H}_z / \rho_m\right)_{j+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1}_{j+1/2,\,k-1/2} + G^{n+1}_{j+1/2,\,k-1/2} \left(\widetilde{H}_z / \rho_m\right)_{j+1/2}\right)\right] + D^{n+1}_{i+1/2,j+1/2} + D^{n+1}_{i-1/2,j+1/2} + \qquad \textbf{(I.A.18)}$$

$$+ D^{n+1}_{j+1} + D^{n+1} + D^{n+1}_{j+1/2,\,k+1/2} + D^{n+1}_{j+1/2,\,k-1/2} ,$$

$$\alpha^{u}_{i+1/2} = \left(\varepsilon V\right)_{i+1/2} / \Delta t + \left(\varepsilon V f |u|^{n} / \left(2 D_h\right)\right)_{i+1/2} + \left[0, F^{n+1}_{i+1} + G^{n+1}_{i+1} \left(\widetilde{H}_r / \rho_m\right)_{i+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1} + G^{n+1} \left(\widetilde{H}_r / \rho_m\right)_{i+1/2}\right)\right] + \left[0, F^{n+1}_{i+1/2,j+1/2} + G^{n+1}_{i+1/2,j+1/2} \left(\widetilde{H}_r / \rho_m\right)_{i+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1}_{i+1/2,j-1/2} + G^{n+1}_{i+1/2,j-1/2} \left(\widetilde{H}_r / \rho_m\right)_{i+1/2}\right)\right] +$$

$$+ \left[0, \left(F^{n+1}_{i+1/2,\,k+1/2} + G^{n+1}_{i+1/2,\,k+1/2} \left(\widetilde{H}_r / \rho_m\right)_{i+1/2}\right)\right] +$$

$$+ \left[0, -\left(F^{n+1}_{i+1/2,\,k-1/2} + G^{n+1}_{i+1/2,\,k-1/2} \left(\widetilde{H}_r / \rho_m\right)_{i+1/2}\right)\right] +$$

$$+ D^{n+1}_{i+1} + D^{n+1} + D^{n+1}_{i+1/2,j+1/2} + D^{n+1}_{i+1/2,j-1/2} + D^{n+1}_{i+1/2,\,k+1/2} + D^{n+1}_{i+1/2,\,k-1/2} , \qquad \textbf{(I.A.19)}$$

$$\alpha^{v}_{k+1/2} = \left(\varepsilon V\right)_{k+1/2} / \Delta t + \left(\varepsilon V f |v|^{n} / \left(2 D_h\right)\right)_{k+1/2} + \left[0, F^{n+1}_{i+1/2,\,k+1/2} + G^{n+1}_{i+1/2,\,k+1/2} \left(\widetilde{H}_s / \rho_m\right)_{k+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1}_{i-1/2,\,k+1/2} + G^{n+1}_{i-1/2,\,k+1/2} \left(\widetilde{H}_s / \rho_m\right)_{k+1/2}\right)\right] +$$

$$+ \left[0, F^{n+1}_{j+1/2,\,k+1/2} + G^{n+1}_{j+1/2,\,k+1/2} \left(\widetilde{H}_s / \rho_m\right)_{k+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1}_{j-1/2,\,k+1/2} + G^{n+1}_{j-1/2,\,k+1/2} \left(\widetilde{H}_s / \rho_m\right)_{k+1/2}\right)\right] + \left[0, F^{n+1}_{k+1} + G^{n+1}_{k+1} \left(\widetilde{H}_s / \rho_m\right)_{k+1/2}\right] +$$

$$+ \left[0, -\left(F^{n+1} + G^{n+1} \left(\widetilde{H}_s / \rho_m\right)_{k+1/2}\right)\right] +$$

$$+ D^{n+1}_{i+1/2,\,k+1/2} + D^{n+1}_{i-1/2,\,k+1/2} + D^{n+1}_{j+1/2,\,k+1/2} + D^{n+1}_{j-1/2,\,k+1/2} + D^{n+1}_{k+1} + D^{n+1} \quad . \tag{I.A.20}$$

The definitions of $\alpha w_{j-1/2}$, $\alpha u_{i-1/2}$, $\alpha v_{k-1/2}$ are similar. The symbol [a, b] denotes the maximum of the two real numbers a and b. Auxiliary symbols F, G, D and $\widetilde{H}$ are defined as follows:

$$F_\alpha = A_f\, u_{m_\alpha} \quad \left(\alpha = r, z, s\right), \quad \left(u_{m_\alpha} = u_m\,, w_m\,, v_m\right), \tag{I.A.21}$$

$$G_\alpha = A_f\, G_{Sl}\left(u_{g\alpha} - u_{l\alpha}\right) = A_f\, x\left(1-x\right)\rho_m\left(u_{g\alpha} - u_{l\alpha}\right), \tag{I.A.22}$$

$$D_\alpha = A_f\, \widetilde{\mu}_m / \left(\rho_m\, \Delta l_\alpha\right) \quad \left(\Delta l_\alpha = \Delta r,\, \Delta z,\, \Delta s\right), \quad \left(\widetilde{\mu}_m = \mu^l_m + \mu^t_m\right), \tag{I.A.23}$$

$$\widetilde{H}_\alpha = \left(H_\alpha - 1\right) / \left(1 + x\left(H_\alpha - 1\right)\right) \quad \left(H_\alpha = u_{g\alpha} / u_{l\alpha}\right). \tag{I.A.24}$$

The right hand side of eq. (A.1) is given by

$$R^{n+1} = \left(\varepsilon / \Delta t\right)\left(\left(\partial \rho_m / \partial p\right)^n_{h_m} p^n - \left(\partial \rho_m / \partial h_m\right)_p \left(h^{n+1}_m - h^n_m\right)\right) -$$

$$- \zeta_{j+1/2}\, \hat{w}_{j+1/2} / \Delta z + \zeta_{j-1/2}\, \hat{w}_{j-1/2} / \Delta z -$$

$$\tag{I.A.25}$$

$$- \Psi_{i+1/2} \cdot FACCP\ \hat{u}_{i+1/2} / \Delta r + \Psi_{i-1/2}\, FACCM\ \hat{u}_{i-1/2} / \Delta r -$$

$$- \xi_{k+1/2}\, \hat{v}_{k+1/2} / \left(\Delta s \cdot \cos\beta_{k+1/2}\right) + \xi_{k-1/2}\, \hat{v}_{k-1/2} / \left(\Delta s \cdot \cos\beta_{k-1/2}\right),$$

with

$$\hat{w}_{j+1/2} = 1 / \alpha^w_{j+1/2}\left(\sum_{1^\beta}^{6} \overline{\alpha^w_\beta}\left(\rho_m\, w_m\right)^{n+1}_\beta + b^w_{j+1/2}\right), \tag{I.A.26}$$

$$\hat{u}_{i+1/2} = 1 / \alpha^u_{i+1/2}\left(\sum_{1^\beta}^{6} \overline{\alpha^u_\beta}\left(\rho_m\, u_m\right)^{n+1}_\beta + b^u_{i+1/2}\right), \tag{I.A.27}$$

$$\hat{v}_{k+1/2} = 1 / \alpha^v_{k+1/2}\left(\sum_{1^\beta}^{6} \overline{\alpha^v_\beta}\left(\rho_m\, v_m\right)^{n+1}_\beta + b^v_{k+1/2}\right), \tag{I.A.28}$$

and

$$b^{w}_{j+1/2} = \left(\varepsilon V\right)_{j+1/2} \left(\rho_m w_m\right)_{j+1/2} /\Delta t - \left(\varepsilon V \rho_m g_z\right)_{j+1/2}, \tag{I.A.29}$$

$$b^{u}_{i+1/2} = \left(\varepsilon V\right)_{i+1/2} \left(\rho_m u_m\right)_{i+1/2} /\Delta t, \tag{I.A.30}$$

$$b^{v}_{k+1/2} = \left(\varepsilon V\right)_{k+1/2} \left(\rho_m v_m\right)_{k+1/2} /\Delta t, \tag{I.A.31}$$

and similarly for $w_{j-1/2}$, $u_{i-1/2}$, $v_{k-1/2}$. The coefficients of the sums in (I.A.26), (I.A.27) and (I.A.28) are given by:

$$\bar{a}^{w}_{1} = \bar{a}^{w}_{i-1,j+1/2} = \left[0, F^{n+1}_{i-1/2,j+1/2} + G^{n+1}_{i-1/2,j+1/2} \left(\tilde{H}_z/\rho_m\right)_{i-1,j+1/2}\right] + D^{n+1}_{i-1/2,j+1/2}, \tag{I.A.32}$$

$$\bar{a}^{w}_{2} = \bar{a}^{w}_{i+1,j+1/2} = \left[0, -\left(F^{n+1}_{i+1/2,j+1/2} + G^{n+1}_{i+1/2,j+1/2} \left(\tilde{H}_z/\rho_m\right)_{i+1,j+1/2}\right)\right] + D^{n+1}_{i+1/2,j+1/2}, \tag{I.A.33}$$

$$\bar{a}^{w}_{3} = \bar{a}^{w}_{j+1/2,k-1} = \left[0, F^{n+1}_{j+1/2,k-1/2} + G^{n+1}_{j+1/2,k-1/2} \left(\tilde{H}_z/\rho_m\right)_{j+1/2,k-1}\right] + D^{n+1}_{j+1/2,k-1/2}, \tag{I.A.34}$$

$$\bar{a}^{w}_{4} = \bar{a}^{w}_{j+1/2,k+1} = \left[0, -\left(F^{n+1}_{j+1/2,k+1/2} + G^{n+1}_{j+1/2,k+1/2} \left(\tilde{H}_z/\rho_m\right)_{j+1/2,k+1}\right)\right] + D^{n+1}_{j+1/2,k+1/2}, \tag{I.A.35}$$

$$\bar{a}^{w}_{5} = \bar{a}^{w}_{j-1/2} = \left[0, F^{n+1} + G^{n+1} \left(\tilde{H}_z/\rho_m\right)_{j-1/2}\right] + D^{n+1}, \tag{I.A.36}$$

$$\bar{a}^{w}_{6} = \bar{a}^{w}_{j+3/2} = \left[0, -\left(F^{n+1}_{j+1} + G^{n+1}_{j+1} \left(\tilde{H}_z/\rho_m\right)_{j+3/2}\right)\right] + D^{n+1}_{j+1}, \tag{I.A.37}$$

$$\bar{a}^{u}_{1} = \bar{a}^{u}_{i-1/2} = \left[0, F^{n+1} + G^{n+1} \left(\tilde{H}_r/\rho_m\right)_{i-1/2}\right] + D^{n+1}, \tag{I.A.38}$$

$$\bar{a}^{u}_{2} = \bar{a}^{u}_{i+3/2} = \left[0, -\left(F^{n+1}_{i+1} + G^{n+1}_{i+1} \left(\tilde{H}_r/\rho_m\right)_{i+3/2}\right)\right] + D^{n+1}_{i+1}, \tag{I.A.39}$$

$$\bar{a}^{u}_{3} = \bar{a}^{u}_{i+1/2,k-1} = \left[0, F^{n+1}_{i+1/2,k-1/2} + G^{n+1}_{i+1/2,k-1/2} \left(\tilde{H}_r/\rho_m\right)_{k-1}\right] + D^{n+1}_{i+1/2,k-1/2}, \tag{I.A.40}$$

$$\bar{a}^{u}_{4} = \bar{a}^{u}_{i+1/2,k+1} = \left[0, -\left(F^{n+1}_{i+1/2,k+1/2} + G^{n+1}_{i+1/2,k+1/2} \left(\tilde{H}_r/\rho_m\right)_{k+1}\right)\right] + D^{n+1}_{i+1/2,k+1/2}, \tag{I.A.41}$$

$$\bar{a}^{u}_{5} = \bar{a}^{u}_{i+1/2,j-1} = \left[0, F^{n+1}_{i+1/2,j-1/2} + G^{n+1}_{i+1/2,j-1/2} \left(\tilde{H}_r/\rho_m\right)_{j-1}\right] + D^{n+1}_{i+1/2,j-1/2}, \tag{I.A.42}$$

$$\bar{\alpha}_6^u = \bar{\alpha}^u_{i+1/2,j+1} = \left[0, -\left(F^{n+1}_{i+1/2,j+1/2} + G^{n+1}_{i+1/2,j+1/2}\left(\tilde{H}_r/\rho_m\right)_{j+1}\right)\right] + D^{n+1}_{i+1/2,j+1/2}, \quad \text{(I.A.43)}$$

$$\bar{\alpha}_1^v = \bar{\alpha}^v_{i-1,k+1/2} = \left[0, F^{n+1}_{i-1/2,k+1/2} + G^{n+1}_{i-1/2,k+1/2}\left(\tilde{H}_s/\rho_m\right)_{i-1}\right] + D^{n+1}_{i-1/2,k+1/2}, \quad \text{(I.A.44)}$$

$$\bar{\alpha}_2^v = \bar{\alpha}^v_{i+1,k+1/2} = \left[0, -\left(F^{n+1}_{i+1/2,k+1/2} + G^{n+1}_{i+1/2,k+1/2}\left(\tilde{H}_s/\rho_m\right)_{i+1}\right)\right] + D^{n+1}_{i+1/2,k+1/2}, \quad \text{(I.A.45)}$$

$$\bar{\alpha}_3^v = \bar{\alpha}^v_{k-1/2} = \left[0, F^{n+1} + G^{n+1}\left(\tilde{H}_s/\rho_m\right)_{k-1/2}\right] + D^{n+1}, \quad \text{(I.A.46)}$$

$$\bar{\alpha}_4^v = \bar{\alpha}^v_{k+3/2} = \left[0, -\left(F^{n+1}_{k+1} + G^{n+1}_{k+1}\left(\tilde{H}_s/\rho_m\right)_{k+3/2}\right)\right] + D^{n+1}_{k+1}, \quad \text{(I.A.47)}$$

$$\bar{\alpha}_5^v = \bar{\alpha}^v_{j-1,k+1/2} = \left[0, F^{n+1}_{j-1/2,k+1/2} + G^{n+1}_{j-1/2,k+1/2}\left(\tilde{H}_s/\rho_m\right)_{j-1}\right] + D^{n+1}_{j-1/2,k+1/2}, \quad \text{(I.A.48)}$$

$$\bar{\alpha}_6^v = \bar{\alpha}^v_{j+1,k+1/2} = \left[0, -\left(F^{n+1}_{j+1/2,k+1/2} + G^{n+1}_{j+1/2,k+1/2}\left(\tilde{H}_s/\rho_m\right)_{j+1}\right)\right] + D^{n+1}_{j+1/2,k+1/2}. \quad \text{(I.A.49)}$$

When the diffusion terms in the momentum equation are treated explicitly, the diffusion coefficients (D's) cancel from the following expressions

$a^w_{j+1/2}$		eq. (I.A.18)
$a^u_{i+1/2}$		eq. (I.A.19)
$a^v_{k+1/2}$		eq. (I.A.20)
$\bar{\alpha}^w_\beta$	$(\beta = 1, 2, \ldots 6)$	eq. (I.A.32) to (I.A.37)
$\bar{\alpha}^u_\beta$	$(\beta = 1, 2, \ldots 6)$	eq. (I.A.38) to (I.A.43)
$\bar{\alpha}^v_\beta$	$(\beta = 1, 2, \ldots 6)$	eq. (I.A.44) to (I.A.49).

The diffusion terms appear then in the definitions of the b's coefficients eqs. (I.A.29) to (I.A.31) which become:

$$b^{w}_{j+1/2} = \left(\varepsilon V\right)_{j+1/2}\left(\rho_m\, w_m\right)_{j+1/2}/\Delta t - \left(\varepsilon V \rho_m g_z\right)_{j+1/2} + \left(\zeta A < \tilde{\mu}_m \partial w/\partial z >\right)_{j+1} -$$

$$- \zeta A < \tilde{\mu}_m \partial w/\partial z > + \left(\Psi A < \tilde{\mu}_m \partial w/\partial r >\right)_{i+1/2,j+1/2} - \left(\Psi A < \tilde{\mu}_m \partial w/\partial r >\right)_{i-1/2,j+1/2} + \quad \text{(I.A.50)}$$

$$+ \left(\xi A < \tilde{\mu}_m \partial w/\partial s >\right)_{j+1/2,\,k+1/2} - \left(\xi A < \tilde{\mu}_m \partial w/\partial s >\right)_{j+1/2,\,k-1/2},$$

$$b^{u}_{i+1/2} = \left(\varepsilon V\right)_{i+1/2}\left(\rho_m\, u_m\right)_{i+1/2}/\Delta t + \left(\zeta A < \tilde{\mu}_m \partial u/\partial z >\right)_{i+1/2,j+1/2} -$$

$$- \left(\zeta A < \tilde{\mu}_m \partial u/\partial z >\right)_{i+1/2,j-1/2} + \left(\Psi A < \tilde{\mu}_m \partial u/\partial r >\right)_{i+1} - \Psi A < \tilde{\mu}_m \partial u/\partial r > + \quad \text{(I.A.51)}$$

$$+ \left(\xi A < \tilde{\mu}_m \partial u/\partial s >\right)_{i+1/2,\,k+1/2} - \left(\xi A < \tilde{\mu}_m \partial u/\partial s >\right)_{i+1/2,\,k-1/2},$$

$$b^{v}_{k+1/2} = \left(\varepsilon V\right)_{k+1/2}\left(\rho_m\, v_m\right)_{k+1/2}/\Delta t + \left(\zeta A < \tilde{\mu}_m \partial v/\partial z >\right)_{j+1/2,\,k+1/2} -$$

$$- \left(\zeta A < \tilde{\mu}_m \partial v/\partial z >\right)_{j-1/2,\,k+1/2} + \left(\Psi A < \tilde{\mu}_m \partial v/\partial r >\right)_{i+1/2,\,k+1/2} - \quad \text{(I.A.52)}$$

$$- \left(\Psi A < \tilde{\mu}_m \partial v/\partial r >\right)_{i-1/2,\,k+1/2} + \left(\xi A < \tilde{\mu}_m \partial v/\partial s >\right)_{k+1} - \xi A < \tilde{\mu}_m \partial v/\partial s > .$$

Appendix I.B. Coefficients and right-hand side of the Poisson equation describing the coolant specific enthalpy distribution (implicit formulation)

We use the same conventions as in Appendix I.A. The Poisson equation for the coolant enthalpy distribution is

$$A^{E,n+1}\, h_{m}^{n+1} + B^{E,n+1}\, h_{m,j-1}^{n+1} + C^{E,n+1}\, h_{m,j+1}^{n+1} + D^{E,n+1}\, h_{m,i-1}^{n+1} +$$

$$+ E^{E,n+1}\, h_{m,i+1}^{n+1} + J^{E,n+1}\, h_{m,k-1}^{n+1} + K^{E,n+1}\, h_{m,k+1}^{n+1} = R^{E,n+1} \quad , \tag{I.B.1}$$

with

$$A^{E,n+1} = \varepsilon V \rho_{m}^{n+1}/\Delta t + \sum_{\alpha} \left\{ \left[0,\, F_{\alpha+1/2}^{E,n+1} + G_{\alpha+1/2}^{E,n+1} / h_{m}^{n+1} \right] - \right.$$

$$\left. - \left[0, -\left(F_{\alpha-1/2}^{E,n+1} + G_{\alpha-1/2}^{E,n+1} / h_{m}^{n+1} \right) \right] \right\} \qquad \left(\alpha = i, j, k \right), \tag{I.B.2}$$

$$B^{E,n+1} = \left[0,\, F_{j-1/2}^{E,n+1} + G_{j-1/2}^{E,n+1} / h_{m,j-1}^{n+1} \right] \quad , \tag{I.B.3}$$

$$C^{E,n+1} = \left[0,\, -\left(F_{j+1/2}^{E,n+1} + G_{j+1/2}^{E,n+1} / h_{m,j+1}^{n+1} \right) \right] \quad , \tag{I.B.4}$$

$$D^{E,n+1} = \left[0,\, F_{i-1/2}^{E,n+1} + G_{i-1/2}^{E,n+1} / h_{m,i-1}^{n+1} \right] \quad , \tag{I.B.5}$$

$$E^{E,n+1} = \left[0,\, -\left(F_{i+1/2}^{E,n+1} + G_{i+1/2}^{E,n+1} / h_{m,i+1}^{n+1} \right) \right] \quad , \tag{I.B.6}$$

$$J^{E,n+1} = \left[0,\, F_{k-1/2}^{E,n+1} + G_{k-1/2}^{E,n+1} / h_{m,k-1}^{n+1} \right] \quad , \tag{I.B.7}$$

$$K^{E,n+1} = \left[0,\, -\left(F_{k+1/2}^{E,n+1} + G_{k+1/2}^{E,n+1} / h_{m,k+1}^{n+1} \right) \right] \quad , \tag{I.B.8}$$

$$R^{E,n+1} = \varepsilon V \ <Q>_3^{n+1} + \left(A_f < \lambda_m \ \partial T/\partial l_\alpha >\right)^n_{\alpha+1/2} - \left(A_f < \lambda_m \ \partial T/\partial l_\alpha >\right)^n_{\alpha-1/2} +$$

$$+ \ \varepsilon V\left(p^{n+1} - p^n\right) / \Delta t + \left(A_f < pu_{m\alpha} >\right)^n_{\alpha+1/2} - \left(A_f < pu_{m\alpha} >\right)^n_{\alpha-1/2} - \tag{I.B.9}$$

$$- \ p^{n+1} \left[\left(A_f < u_m + R_{oSl} \left(u_g - u_l\right) >\right)^n_{\alpha+1/2} - \left(A_f < u_m + R_{oSl} \left(u_g - u_l\right) >\right)^n_{\alpha-1/2}\right] +$$

$$+ \left(A_f < p R_{oSl} \left(u_g - u_l\right) >\right)^n_{\alpha+1/2} - \left(A_f < p R_{oSl} \left(u_g - u_l\right) >\right)^n_{\alpha-1/2} \quad \left(\alpha = i,j,k\right), \ \left(l_\alpha = r,z,s\right).$$

In equation (I.B.9) summation upon index α is implied. Furthermore we defined:

$$F^E_{\alpha\pm 1/2} = \left(A_f \ \rho_m u_m\right)_{\alpha\pm 1/2} , \tag{I.B.10}$$

$$G^E_{\alpha\pm 1/2} = \left(A_f \, x \left(1-x\right) \rho_m \ \left(h_g - h_l\right) u_m \ H\right)_{\alpha\pm 1/2} , \tag{I.B.11}$$

$$\widetilde{H}_\alpha = \left(u_{g\alpha} / u_{l\alpha} - 1\right) / \left(1 - x\left(u_{g\alpha} / u_{l\alpha} - 1\right)\right), \tag{I.B.12}$$

$$R_{oSl} = \alpha_g \, \alpha_l \left(\rho_l - \rho_g\right) / \rho_m . \tag{I.B.13}$$

Part II

Separated Phases Model (SPM)

by M. Bottoni

1. Governing equations for the separated phases model

The model of separated phases relies upon the following modelling of the two-phase flow regime. In each control volume for which the conservation equations are applied in the local form and then volume-averaged, three "fields" are defined: a solid field consisting of the fuel pins and, if any, of the hexagonal can, a liquid coolant field and a vapour field. The calculation of the temperature distribution in the solid field is described in reference [1].

The simulation of a coolant liquid film at cladding and structure surfaces allows a description of dryout and rewetting sequences and the correct calculation of the cladding to coolant heat transfer coefficient which depends strongly on the liquid film thickness. The fraction of the liquid coolant which does not adhere as a film to the walls, is assumed to consist of droplets carried on by the vapour flow. The dynamics of these droplets is described by the momentum equation for the liquid phase and by an ordinary differential equation for the collision rate between droplets. As a result we get the droplet size and concentration.

The flow regimes which are simulated in this way include: (a) slug flow for void fractions in the range 0.6 - 0.8; (b) annular flow in which the heat transfer between wall and coolant occurs through the liquid film at the wall; (c) drop-annular flow, in which dryout has occurred and liquid droplets are driven by a vapour flow; (d) vapour flow, after complete vaporization of the liquid droplets.

The volume $V_f = \varepsilon V$ occupied by the coolant is distributed between liquid and vapour according to the following relations:

$$\alpha + \alpha_f + \alpha_b = 1, \tag{1.1}$$

$$\alpha_l = \alpha_f + \alpha_b = 1 - \alpha, \tag{1.2}$$

where α_f, α_b are the volume fractions occupied by the liquid film and liquid droplets, respectively.

It is assumed that only the liquid phase is in contact with the cladding up to a void fraction α_d which corresponds to dryout. For $\alpha < \alpha_d$ heat transferred to the vapour phase comes from evaporation of the liquid film, and the vapour phase always remains at saturation temperature. Conversely, condensation occurs when heat is transferred to the cladding through the liquid film and the vapour phase always condenses at saturation temperature.

When $\alpha > \alpha_d$ (hence, the liquid film is completely evaporated) the vapour is in contact with the wall and liquid droplets are driven by the vapour flow. The frequency of the collisions of liquid droplets with each other determines their size and concentration, while the frequency of impacts of droplets with the surface of the cladding determines the amount of rewetting of the walls. This implies an additional cooling effect after the first dryout. Therefore, the heat transfer to the coolant is due to evaporation of the liquid also during this phase.

When the liquid droplets have been completely evaporated, or their concentration has become so small that the frequency of impacts with the walls cannot sustain a liquid film any longer, it is only the vapour which experiences the gain or loss of energy. At this stage the residual liquid droplets are driven in an environment of superheated vapour and evaporate rapidly. The void fraction reaches the limit $\alpha = 1$, and from this time on the superheated vapour is treated as a perfect gas.

In the present code version flow regimes a) and b) (slug and annular flow) are fully implemented. The code development for drop-annular flow has been made on the theoretical basis but not yet coded.

This physical situation can be modelled by means of a six-equations Unequal phase Velocity, Equal phase Temperature (UVET) seriated two-phase continuum, which we refer to as the Separated Phase Model (SPM). It relies upon the following governing equations [2].

i) Continuity equations

$$\left(\frac{\partial \rho_l'}{\partial t}\right) + \nabla \cdot \left(\rho_l' \mathrm{v}_l\right) = - M, \tag{1.3}$$

$$\left(\frac{\partial \rho_g'}{\partial t}\right) + \nabla \cdot \left(\rho_g' \mathrm{v}_g\right) = + M; \tag{1.4}$$

ii) Momentum equations

$$\frac{\partial\left(\rho_l^{'}\,\mathbf{v}_l\right)}{\partial t} + \nabla\cdot\left(\rho_l^{'}\,\mathbf{v}_l\mathbf{v}_l\right) = -\left\{\left[0, M\right]\mathbf{v}_l - \left[0, -M\right]\mathbf{v}_g\right\} + \tag{1.5}$$

$$+ \nabla\cdot\left(\mu_l\nabla\mathbf{v}_l\right) - (1-\alpha)\,\nabla p + \rho_l^{'}g - K^M\left(\mathbf{v}_l - \mathbf{v}_g\right) - \mathbf{R}_l\,,$$

$$\frac{\partial\left(\rho_g^{'}\,\mathbf{v}_g\right)}{\partial t} + \nabla\cdot\left(\rho_g^{'}\,\mathbf{v}_g\mathbf{v}_g\right) = +\left\{\left[0, M\right]\mathbf{v}_l - \left[0, -M\right]\mathbf{v}_g\right\} + \tag{1.6}$$

$$+ \nabla\cdot\left(\mu_g\nabla\mathbf{v}_g\right) - \alpha\,\nabla p + \rho_g^{'}g + K^M\left(\mathbf{v}_l - \mathbf{v}_g\right) - \mathbf{R}_g\,;$$

iii) Energy equations

$$\frac{\partial\left(\rho_l^{'}\,h_{ls}\right)}{\partial t} + \nabla\cdot\left(\rho_l^{'}\,h_{ls}\mathbf{v}_l\right) = \phi_l + U_l + \nabla\cdot\left(\lambda_l\,(1-\alpha)\,\nabla T_s\right) - \tag{1.7}$$

$$- K^E\left(\left|\mathbf{v}_l - \mathbf{v}_g\right|\right)^2 + (1-\alpha)\,\frac{\partial p}{\partial t} + (1-\alpha)\,\mathbf{v}_l\cdot\nabla p\,,$$

$$\frac{\partial\left(\rho_g^{'}\,h_{gs}\right)}{\partial t} + \nabla\cdot\left(\rho_g^{'}\,h_{gs}\mathbf{v}_g\right) = \phi_g + U_g + \nabla\cdot\left(\lambda_g\,\alpha\,\nabla T_s\right) + \tag{1.8}$$

$$+ K^E\left(\left|\mathbf{v}_l - \mathbf{v}_g\right|\right)^2 + \alpha\,\frac{\partial p}{\partial t} + \alpha\,\mathbf{v}_g\cdot\nabla p\,.$$

In these equations ρ'_l, ρ'_g are the macroscopic liquid and vapour densities defined by

$$\rho_l^{'} = \left(1-\alpha\right)\,\rho_l \tag{1.9}$$

$$\rho_g^{'} = \alpha\,\rho_g \tag{1.10}$$

where ρ_l, ρ_g are the microscopic (physical) densities.

The symbol [a, b] represents the maximum of the two real numbers a, b.

U_l and U_g are the power sources arising from viscous dissipation, given by terms of the type ($\underline{\underline{T}}$: ∇v). They are negligible compared with the input power sources.

ϕ_l and ϕ_g, the power sources to the liquid and vapour phases, respectively, are calculated by assuming that a fraction $Q_g = \eta Q$ ($0 \leqq \eta \leqq 1$) of the total power Q released to the coolant vaporizes a mass $M = \eta Q/h_{fg}$ of vapour per unit volume and time, while the remaining power fraction $Q_l = (1 - \eta)\, Q$ is released to the liquid. Thus the power sources to be inserted into eqs. (1.7) and (1.8) are

$$\Phi_l = - Mh_{ls} + Q_l / V_f , \tag{1.11}$$

$$\Phi_g = Mh_{ls} + Mh_{fg} = Mh_{gs} \tag{1.12}$$

for the liquid and vapour phase, respectively. These equations are justified in detail in section 7.2. In a first approximation we assumed $\eta = \alpha_g$. However, the calculation experience showed that it is more convenient, after solving the liquid enthalpy equation and deriving the updated liquid saturation temperature $T_l = T_s$, to use the vapour energy equation to calculate the vapour production M under the constraint $T_g = T_s$. It turns out that the assumption $\eta = \alpha_g$ tends to be correct for large void fractions, while at boiling inception the fraction η which implies a thermodynamic equilibrium between the phases is smaller than α_g.

The terms containing the function K^E represent the power generated by drag dissipation at the phase interface. This contribution is generally modelled as lost by the liquid and acquired by the vapour.

The assumption of thermodynamic equilibrium between the phase ($T_g = T_l = T_s$) implies that the two energy eqs (1.7) and (1.8) can be replaced by the energy equation for the mixture thus reducing the model to five equations. In a separate code version we have coded the energy equations separately for both phases in view of code developments to simulation of superheated vapour with thermodynamic disequilibrium between the phases ($T_l = T_s$, $T_g > T_l$). However in the following of this report we refer to the enthalpy equation for the mixture given by equation (1.3) of Part I. The numerical treatment is as explained in Section 11 of Part I.

2. Finite difference form of continuity equations

We treat the convective terms in equations (1.3) and (1.4) fully implicitly. Integrating these equations over a centred cell, replacing the volume integral of the divergence term by means of surface fluxes one derives the following finite difference forms for the liquid and vapour phases, respectively.

i) Liquid phase

$$\varepsilon_{ijk}\left(\frac{\partial \rho_l'}{\partial t}\right)_{ijk}^{n+1} + \frac{1}{\Delta z_j}\left[\zeta_{j+1/2}\left(\rho_l' w_l\right)_{i,j+1/2,k}^{n+1} - \zeta_{j-1/2}\left(\rho_l' w_l\right)_{i,j-1/2,k}^{n+1}\right] +$$

$$+\frac{1}{\Delta r_i}\left[\left(\psi F_c \rho_l' \upsilon_l\right)_{i+1/2,j,k}^{n+1} - \left(\psi F_c \rho_l' \upsilon_l\right)_{i-1/2,j,k}^{n+1}\right] + \tag{2.1}$$

$$+\frac{1}{\Delta s_k}\left[\left(\frac{\xi \rho_l' v_l}{\cos\beta}\right)_{i,j,k+1/2}^{n+1} - \left(\frac{\xi \rho_l' v_l}{\cos\beta}\right)_{i,j,k-1/2}^{n+1}\right] = -\,\varepsilon_{ijk}\quad M_{ijk}\ ;$$

ii) Vapour phase

$$\varepsilon_{ijk}\left(\frac{\partial \rho_g'}{\partial t}\right)_{ijk}^{n+1} + \frac{1}{\Delta z_j}\left[\zeta_{j+1/2}\left(\rho_g' w_g\right)_{i,j+1/2,k}^{n+1} - \zeta_{j-1/2}\left(\rho_g' w_g\right)_{i,j-1/2,k}^{n+1}\right] +$$

$$+\frac{1}{\Delta r_i}\left[\left(\psi F_c \rho_g' \upsilon_g\right)_{i+1/2,j,k}^{n+1} - \left(\psi F_c \rho_g' \upsilon_g\right)_{i-1/2,j,k}^{n+1}\right] + \tag{2.2}$$

$$+\frac{1}{\Delta s_k}\left[\left(\frac{\xi \rho_g' v_g}{\cos\beta}\right)_{i,j,k+1/2}^{n+1} - \left(\frac{\xi \rho_g' v_g}{\cos\beta}\right)_{i,j,k-1/2}^{n+1}\right] = \varepsilon_{ijk}\quad M_{ijk}\ .$$

3. Implicit treatment of momentum conservation equations

3.1 Liquid phase

The scalar component of the momentum conservation equation (1.5) for the liquid phase in the z-coordinate direction can be written

$$\frac{\partial}{\partial t}\left(\rho_l' w_l\right) + \frac{\partial}{\partial L_\alpha}\left[\left(\rho_l' V_{l_\alpha}\right) w_l\right] - \frac{\partial}{\partial L_\alpha}\left(\mu_l \frac{\partial w_l}{\partial L_\alpha}\right) = -(1-\alpha)\frac{\partial p}{\partial z} - \rho_l' g_z - \quad (3.1.1)$$

$$- R_{lz} - K^M\left(w_l - w_g\right) - \left(\left[0, M\right] w_l - \left[0, -M\right] w_g\right) \qquad (L_\alpha = r,s,z).$$

L_α represent any of the coordinate directions (r, s, z in bundle geometry) and V_α is the respective velocity component.

Letting

$$S_{lz} = -(1-\alpha)\frac{\partial p}{\partial z} - \rho_l' g_z - R_{lz} - \quad (3.1.2)$$

$$- K^M\left(w_l - w_g\right) - \left(\left[0, M\right] w_l - \left[0, -M\right] w_g\right) \qquad \textit{(source term)},$$

$$Jw_{l_\alpha} = \left(\rho_l' V_{l_\alpha}\right) w_l - \mu_l \frac{\partial w_l}{\partial L_\alpha} \quad (3.1.3)$$

(convective plus diffusive flux of momentum),

equation (3.1.1) can be written

$$\frac{\partial}{\partial t}\left(\rho_l' w_l\right) + \frac{\partial}{\partial L_\alpha}\left(Jw_{l\alpha}\right) = S_{lz}. \quad (3.1.4)$$

Integration over the volume V_f of the fluid in a control cell yields

$$\int_{V_f} \frac{\partial}{\partial t}\left(\rho_l' w_l\right) dV + \int_{V_f} \frac{\partial}{\partial L_\alpha}\left(Jw_{l\alpha}\right) dV = \int_{V_f} S_{lz}\, dV. \quad (3.1.5)$$

The control volume for the z-component of the momentum equation is obtained displacing a centred control cell (i j k) by half-mesh in the z direction. Replacing the volume integral of the divergence term by means of the fluxes through the cell bounding surfaces one derives:

$$\int_{V_f} \frac{\partial}{\partial t}\left(\rho_l^{'} w_l\right) dV + \int_{A_{f\ i+1/2,j+1/2,k}} \left(J w_l\right)_r dA - \int_{A_{f\ i-1/2,j+1/2,k}} \left(J w_l\right)_r dA +$$

$$+ \int_{A_{f\ i,j+1,k}} \left(J w_l\right)_z dA - \int_{A_{f\ i,j,k}} \left(J w_l\right)_z dA + \int_{A_{f\ i,j+1/2,k+1/2}} \left(J w_l\right)_s dA - \quad (3.1.6)$$

$$- \int_{A_{f\ i,j+1/2,k-1/2}} \left(J w_l\right)_s dA = \int_{V_f} S_{lz}\, dV \ .$$

We discretize this equation with respect to time treating convective, diffusive, and the pressure gradient terms fully implicitly and the friction term half-implicitly. Replacing the surface integrals by the mean values over the surfaces, denoted by the symbols $< \ >$, one obtains:

$$\frac{\left(\varepsilon V\right)_{i,j+1/2,k}}{\Delta t} \left[\left(\rho_l^{'} w_l\right)^{n+1} - \left(\rho_l^{'} w_l\right)^{n}\right]_{i,j+1/2,k} +$$

$$+ < \left(J w_l\right)_r A_f >^{n+1}_{i+1/2,j+1/2,k} - < \left(J w_l\right)_r A_f >^{n+1}_{i-1/2,j+1/2,k} +$$

$$+ < \left(J w_l\right)_z A_f >^{n+1}_{i,j+1,k} - < \left(J w_l\right)_z A_f >^{n+1}_{i\,j\,k} + \quad (3.1.7)$$

$$+ < \left(J w_l\right)_s A_f >^{n+1}_{i,j+1/2,k+1/2} - < \left(J w_l\right)_s A_f >^{n+1}_{i,j+1/2,k-1/2} =$$

$$= - \frac{\left(\varepsilon V (1-\alpha)\right)_{i,j+1/2,k}}{\Delta z} \left(p^{n+1}_{i,j+1,k} - p^{n+1}_{i\,j\,k}\right) - \left(\varepsilon V \rho_l^{'} g_z\right)^{n}_{i,j+1/2,k} -$$

$$- \left[\frac{\varepsilon V}{2 D_h} f_l \, |w_l|^n \left(\rho_l^{'} w_l\right)^{n+1}\right]_{i,j+1/2,k} -$$

$$- \left(\varepsilon V\right)_{i,j+1/2,k} K^M \left(w_l - w_g\right)_{i,j+1/2,k}$$

$$- \left(\varepsilon V\right)_{i,j+1/2,k} \cdot \left(\left|0, M\right| w_l - \left|0, -M\right| w_g \right)_{i,j+1/2,k}$$

The averaged fluxes of the vector Jw_m are evaluated with the upwind discretization scheme given in eq. (3.1.11).

$$Jr+ = \int_{A_{f\, i+1/2,j+1/2,k}} \left(Jw_l\right)_r dA = < Jw_l \cdot A_f >_{i+1/2,j+1/2,k} = \tag{3.1.8}$$

$$= \left\{A_f\, \rho_l^{'}\, u_l\, w_l - \frac{A_f\, \mu_l}{\rho_l^{'} \Delta r}\, \Delta\left(\rho_l^{'}\, w_l\right)\right\}_{i+1/2,j+1/2,k} =$$

$$= \left\{F^l \cdot \rho_l^{'}\, w_l - D^l \cdot \Delta\left(\rho_l^{'}\, w_l\right)\right\}_{i+1/2,j+1/2,k} ,$$

with the definitions:

$$F^l_{i+1/2,j+1/2,k} = \left(A_f\, u_l\right)_{i+1/2,j+1/2,k} , \tag{3.1.9}$$

$$D^l_{i+1/2,j+1/2,k} = \left(A_f\, \frac{\mu_l}{\rho_l^{'} \Delta r}\right)_{i+1/2,j+1/2,k} . \tag{3.1.10}$$

For both $u_{l,i+1/2,j+1/2,k}$ positive and negative, formula (3.1.8) can be written

$$Jr+ = \left[0, F^l_{i+1/2,j+1/2,k}\right] \left(\rho_l^{'}\, w_l\right)_{i,j+1/2,k} - \tag{3.1.11}$$

$$- \left[0, -F^l_{i+1/2,j+1/2,k}\right] \left(\rho_l^{'}\, w_l\right)_{i+1,j+1/2,k} +$$

$$+ D^l_{i+1/2,j+1/2,k} \left\{ \left(\rho_l^{'}\, w_l\right)_{i,j+1/2,k} - \left(\rho_l^{'}\, w_l\right)_{i+1,j+1/2,k} \right\} .$$

Using again the following subscripts to index the central node considered and the six neighbouring nodes in the three coordinate directions:

0	for	i, j + 1/2, k
1	for	i - 1, j + 1/2, k
2	for	i + 1, j + 1/2, k
3	for	i, j + 1/2, k - 1
4	for	i, j + 1/2, k + 1
5	for	i, j - 1/2, k
6	for	i, j + 3/2, k,

the flux Jr+ and, similarly, the other ones in eq. (3.1.7) can be written:

$$Jr+ = \int_{A_{f\ i+1/2,j+1/2,k}} \left(Jw_l\right)_r dA = < \left(Jw_l\right)_r \cdot A_f >_{i+1/2,j+1/2,k} = \tag{3.1.12a}$$

$$= \left[0, F^l_{i+1/2,j+1/2,k}\right] \left(\rho_l^{'} w_l\right)_0 - \left[0, -F^l_{i+1/2,j+1/2,k}\right] \left(\rho_l^{'} w_l\right)_2 +$$

$$+ D^l_{i+1/2,j+1/2,k} \left\{ \left(\rho_l^{'} w_l\right)_0 - \left(\rho_l^{'} w_l\right)_2 \right\} ,$$

$$Jr- = \int_{A_{f\ i-1/2,j+1/2,k}} \left(Jw_l\right)_r dA = < \left(Jw_l\right)_r \cdot A_f >_{i-1/2,j+1/2,k} = \tag{3.1.12b}$$

$$= \left[0, F^l_{i-1/2,j+1/2,k}\right] \left(\rho_l^{'} w_l\right)_1 - \left[0, -F^l_{i-1/2,j+1/2,k}\right] \left(\rho_l^{'} w_l\right)_0 +$$

$$+ D^l_{i-1/2,j+1/2,k} \left\{ \left(\rho_l^{'} w_l\right)_1 - \left(\rho_l^{'} w_l\right)_0 \right\} ,$$

$$Jz+ = \int_{A_{f\ i,j+1,k}} \left(Jw_l\right)_z dA = < \left(Jw_l\right)_z \cdot A_f >_{i,j+1,k} = \tag{3.1.12c}$$

$$= \left[0, F^l_{i,j+1,k}\right] \left(\rho_l^{'} w_l\right)_0 - \left[0, -F^l_{i,j+1,k}\right] \left(\rho_l^{'} w_l\right)_6 +$$

$$+ D^l_{i,j+1,k} \left\{ \left(\rho_l^{'} w_l\right)_0 - \left(\rho_l^{'} w_l\right)_6 \right\} ,$$

$$Jz- = \int_{A_{f\ i,j\,k}} \left(Jw_l\right)_z \, dA = < \left(Jw_l\right)_z \cdot A_f >_{i,j\,k} = \tag{3.1.12d}$$

$$= \left[0, F^l_{i\,j\,k}\right] \left(\rho_l' \, w_l\right)_5 - \left[0, -F^l_{i\,j\,k}\right] \left(\rho_l' \, w_l\right)_0 +$$

$$+ D^l_{i\,j\,k} \left\{ \left(\rho_l' \, w_l\right)_5 - \left(\rho_l' \, w_l\right)_0 \right\} ,$$

$$Js+ = \int_{A_{f\ i,j+1/2,\,k+1/2}} \left(Jw_l\right)_s \, dA = < \left(Jw_l\right)_s \cdot A_f >_{i,j+1/2,k+1/2} = \tag{3.1.12e}$$

$$= \left[0, F^l_{i\,,j+1/2,\,k+1/2}\right] \left(\rho_l' \, w_l\right)_0 - \left[0, -F^l_{i\,,j+1/2,\,k+1/2}\right] \left(\rho_l' \, w_l\right)_4 +$$

$$+ D^l_{i\,,j+1/2,\,k+1/2} \left\{ \left(\rho_l' \, w_l\right)_0 - \left(\rho_l' \, w_l\right)_4 \right\} ,$$

$$Js- = \int_{A_{f\ i,j+1/2,\,k-1/2}} \left(Jw_l\right)_s \, dA = < \left(Jw_l\right)_s \cdot A_f >_{i,j+1/2,k-1/2} = \tag{3.1.12f}$$

$$= \left[0, F^l_{i\,,j+1/2,\,k-1/2}\right] \left(\rho_l' \, w_l\right)_3 - \left[0, -F^l_{i\,,j+1/2,\,k-1/2}\right] \left(\rho_l' \, w_l\right)_0 +$$

$$+ D^l_{i\,,j+1/2,\,k-1/2} \left\{ \left(\rho_l' \, w_l\right)_3 - \left(\rho_l' \, w_l\right)_0 \right\} .$$

The full expressions of the convection terms F^l in the previous equations are

$$F^l_{i\,\pm\,1/2,\ j+1/2,\,k} = \left(A_f \, u_l\right)_{i\,\pm\,1/2,\ j+1/2,\,k} = \left(\psi \, \Delta s \, \Delta z \, u_l\right)_{i\,\pm\,1/2,\ j+1/2,\,k} , \tag{3.1.13}$$

$$F^l_{i,\ j+1,\,k} = \left(A_f \, w_l\right)_{i,j+1,\,k} = \left(\zeta \Delta r \, \Delta s \, w_l\right)_{i,j+1,\,k} , \tag{3.1.14a}$$

$$F^l_{i,\ j,\,k} = \left(A_f \, w_l\right)_{i,j,\,k} = \left(\zeta \Delta r \, \Delta s \, w_l\right)_{i,j,\,k} , \tag{3.1.14b}$$

$$F^l_{i,\ j+1/2,\,k\,\pm\,1/2} = \left(A_f \, v_l\right)_{i,\ j+1/2,\,k\,\pm\,1/2} = \left(\frac{\xi}{\cos\beta} \, \Delta r \, \Delta z \, v_l\right)_{i,\ j+1/2,\,k\,\pm\,1/2} . \tag{3.1.15}$$

The diffusion coefficients are given by

$$D^{l}_{i\pm 1/2,\ j+1/2,\ k} = \left(\frac{A_f\ \mu_l}{\rho_l^{'}\,\Delta r}\right)_{i\pm 1/2, j+1/2, k} = \left(\frac{\psi\ \Delta z\ \Delta s\ \mu_l}{\rho_l^{'}\ \Delta r}\right)_{i\pm 1/2, j+1/2, k}, \tag{3.1.16}$$

$$\underset{(j)}{D^{l}_{i,j+1,k}} = \left(\frac{A_f\ \mu_l}{\rho_l^{'}\,\Delta z}\right)_{\underset{(j)}{i,j+1,k}} = \left(\frac{\zeta\ \Delta r\ \Delta s\ \mu_l}{\rho_l^{'}\ \Delta z}\right)_{\underset{(j)}{i,j+1,k}}, \tag{3.1.17}$$

$$D^{l}_{i,\ j+1/2,\ k\pm 1/2} = \left(\frac{A_f\ \mu_l}{\rho_l^{'}\,\Delta s}\right)_{i,j+1/2,\ k\pm 1/2} = \left(\frac{\xi\ \Delta z\ \Delta r\ \mu_l}{\rho_l^{'}\ \Delta s}\right)_{i,j+1/2, k\pm 1/2}. \tag{3.1.18}$$

Introducing the convective and diffusive fluxes (3.1.12) evaluated at time level n + 1 into (3.1.7) and rearranging, one derives

$$\begin{aligned}
&\left(\rho_l^{'}\,w_l\right)_0^{n+1}\Bigg\{\frac{(\varepsilon V)_0}{\Delta t} + \left(\frac{\varepsilon V}{2D_h}\,f_l\,|w_l|^n\right)_0 + \left[0, F^{l,n+1}_{i+1/2,j+1/2,k}\right] + \left[0, -\left(F^{l,n+1}_{i-1/2,j+1/2,k}\right)\right] + \\
&+ \left[0, F^{l,n+1}_{i,j+1,k}\right] + \left[0, -\left(F^{l,n+1}_{i\,j\,k}\right)\right] + \left[0, F^{l,n+1}_{i,j+1/2,k+1/2}\right] + \left[0, -\left(F^{l,n+1}_{i,j+1/2,k-1/2}\right)\right] + \\
&+ D^{l,n+1}_{i+1/2,j+1/2,k} + D^{l,n+1}_{i-1/2,j+1/2,k} + D^{l,n+1}_{i,j+1,k} + D^{l,n+1}_{i\,j\,k} + D^{l,n+1}_{i,j+1/2,k+1/2} + D^{l,n+1}_{i,j+1/2,k-1/2}\Bigg\} - \\
&- \left(\rho_l^{'}\,w_l\right)_1^{n+1}\left\{\left[0, F^{l,n+1}_{i-1/2,j+1/2,k}\right] + D^{l,n+1}_{i-1/2,j+1/2,k}\right\} - \\
&- \left(\rho_l^{'}\,w_l\right)_2^{n+1}\left\{\left[0, -F^{l,n+1}_{i+1/2,j+1/2,k}\right] + D^{l,n+1}_{i+1/2,j+1/2,k}\right\} - \\
&- \left(\rho_l^{'}\,w_l\right)_5^{n+1}\left\{\left[0, F^{l,n+1}_{i\,j\,k}\right] + D^{l,n+1}_{i\,j\,k}\right\} - \\
&- \left(\rho_l^{'}\,w_l\right)_6^{n+1}\left\{\left[0, -F^{l,n+1}_{i,j+1,k}\right] + D^{l,n+1}_{i,j+1,k}\right\} - \\
&- \left(\rho_l^{'}\,w_l\right)_3^{n+1}\left\{\left[0, F^{l,n+1}_{i,j+1/2,k-1/2}\right] + D^{l,n+1}_{i,j+1/2,k-1/2}\right\} - \\
&- \left(\rho_l^{'}\,w_l\right)_4^{n+1}\left\{\left[0, -F^{l,n+1}_{i,j+1/2,k+1/2}\right] + D^{l,n+1}_{i,j+1/2,k+1/2}\right\} =
\end{aligned} \tag{3.1.19}$$

$$= \frac{(\varepsilon V)_0}{\Delta t} \left(\rho_l' w_l\right)_0^n - \left(\varepsilon V \rho_l' g_z\right)_0^n - \left(1-\alpha\right)\left(\frac{\varepsilon V}{\Delta z}\right)_0 \left(p^{n+1}_{i,j+1,k} - p^{n+1}_{i\,j\,k}\right) -$$

$$- \left[\varepsilon V K^M \left(w_l - w_g\right)\right]^{n+1}_{i,j+1/2,k} - \varepsilon V \left(\left[0, M\right] w_l - \left[0, -M\right] w_g\right)^{n+1}_{i,j+1/2,k} .$$

This equation can be written in the compact form

$$a^w_{l0} \left(\rho_l' w_l\right)^{n+1}_0 - \sum_{1}^{6}{}_\beta \; a^w_{l\beta} \left(\rho_l' w_l\right)^{n+1}_\beta = b^w_{l0} - d^w_{l0} \left(p^{n+1}_{i,j+1,k} - p^{n+1}_{i\,j\,k}\right) \tag{3.1.20}$$

with the following definitions of the coefficients :

$$a^w_{l0} = \frac{(\varepsilon V)_0}{\Delta t} + \left(\frac{\varepsilon V}{2D_h} f_l \,|w_l|^n\right)_0 + \left[0, F^{l,n+1}_{i+1/2,j+1/2,k}\right] + \left[0, -F^{l,n+1}_{i-1/2,j+1/2,k}\right] + \tag{3.1.21a}$$

$$+ \left[0, F^{l,n+1}_{i,j+1,k}\right] + \left[0, -F^{l,n+1}_{i\,j\,k}\right] + \left[0, F^{l,n+1}_{i,j+1/2,k+1/2}\right] + \left[0, -F^{l,n+1}_{i,j+1/2,k-1/2}\right] +$$

$$+ D^{l,n+1}_{i+1/2,j+1/2,k} + D^{l,n+1}_{i-1/2,j+1/2,k} + D^{l,n+1}_{i,j+1,k} + D^{l,n+1}_{i\,j\,k} + D^{l,n+1}_{i,j+1/2,k+1/2} + D^{l,n+1}_{i,j+1/2,k-1/2} ,$$

$$a^w_{l1} = \left\{\left[0, F^{l,n+1}_{i-1/2,j+1/2,k}\right] + D^{l,n+1}_{i-1/2,j+1/2,k}\right\} , \tag{3.1.21b}$$

$$a^w_{l2} = \left\{\left[0, -F^{l,n+1}_{i+1/2,j+1/2,k}\right] + D^{l,n+1}_{i+1/2,j+1/2,k}\right\} , \tag{3.1.21c}$$

$$a^w_{l3} = \left\{\left[0, F^{l,n+1}_{i,j+1/2,k-1/2}\right] + D^{l,n+1}_{i,j+1/2,k-1/2}\right\} , \tag{3.1.21d}$$

$$a^w_{l4} = \left\{\left[0, -F^{l,n+1}_{i,j+1/2,k+1/2}\right] + D^{l,n+1}_{i,j+1/2,k+1/2}\right\} , \tag{3.1.21e}$$

$$a^w_{l5} = \left\{\left[0, F^{l,n+1}_{i\,j\,k}\right] + D^{l,n+1}_{i\,j\,k}\right\} , \tag{3.1.21f}$$

$$a^w_{l6} = \left\{\left[0, -F^{l,n+1}_{i,j+1,k}\right] + D^{l,n+1}_{i,j+1,k}\right\} , \tag{3.1.21g}$$

$$b^w_{l0} = \frac{\left(\varepsilon V\right)_0}{\Delta t} \left(\rho_l' w_l\right)^n_0 - \left(\varepsilon V \rho_l' g_z\right)^n_0 - \tag{3.1.21h}$$

$$- \left[\varepsilon V K^M \left(w_l - w_g\right) \right]^{n+1}_{i,j+1/2,k} - \varepsilon V \left(\left[0, M\right] w_l - \left[0, -M\right] w_g \right)^{n+1}_{i,j+1/2,k},$$

$$d^w_{l0} = \left(\frac{(1-\alpha)\,\varepsilon V}{\Delta z} \right)_0 . \tag{3.1.22}$$

Defining

$$\hat{w}_{l6} = \frac{1}{a^w_{l0}} \left\{ \sum_1^6 {}_\beta \; a^w_{l\beta} \left(\rho_l' w_l\right)^{n+1}_\beta + b^w_{l0} \right\}, \tag{3.1.23}$$

$$d^w_{l6} = \frac{d^w_{l0}}{a^w_{l0}} = \frac{1}{a^w_{l0}} \left(\frac{(1-\alpha)\,\varepsilon V}{\Delta z} \right)_0 , \tag{3.1.24}$$

equation (3.1.20) can be written

$$\left(\rho_l' w_l\right)^{n+1}_{i,j+1/2,k} = \hat{w}_{l6} - d^w_{l6} \left(p^{n+1}_{i,j+1,k} - p^{n+1}_{i\,j\,k} \right). \tag{3.1.25a}$$

Similarly one derives for the radial and azimuthal components of the momentum equation for the liquid phase

$$\left(\rho_l' u_l\right)^{n+1}_{i+1/2,j,k} = \hat{u}_{l2} - d^u_{l2} \left(p^{n+1}_{i+1,j,k} - p^{n+1}_{i,j\,k} \right), \tag{3.1.25b}$$

$$\left(\rho_l' v_l\right)^{n+1}_{i,j,k+1/2} = \hat{v}_{l4} - d^v_{l4} \left(p^{n+1}_{i,j,k+1} - p^{n+1}_{i\,j\,k} \right), \tag{3.1.25c}$$

with

$$\hat{u}_{l2} = \frac{1}{a^u_{l0}} \left\{ \sum_1^6 {}_\beta \; a^u_{l\beta} \left(\rho_l' u_l\right)^{n+1}_\beta + b^u_{l0} \right\}, \tag{3.1.26}$$

$$\hat{v}_{l4} = \frac{1}{a^{v}_{l0}} \left\{ \sum_{1}^{6}{}_{\beta}\; a^{v}_{l\beta} \left(\rho'_l\, v_l\right)^{n+1}_{\beta} + b^{v}_{l0} \right\} , \tag{3.1.27}$$

$$d^{u}_{l2} = \frac{1}{a^{u}_{l,\, i+1/2, j, k}} \left(\frac{(1-\alpha)\, \varepsilon\, V}{\Delta r} \right)_{i+1/2, j, k} , \tag{3.1.28}$$

$$d^{v}_{l4} = \frac{1}{a^{v}_{l,\, i, j, k+1/2}} \left(\frac{(1-\alpha)\, \varepsilon\, V}{\Delta s} \right)_{i, j, k+1/2} . \tag{3.1.29}$$

For the three components of the momentum equations, written for control volumes displaced by half-cell in the respective backward direction, one has (with similar definitions of symbols):

$$\left(\rho'_l\, u_l\right)^{n+1}_{i-1/2, j, k} = \hat{u}_{l1} - d^{u}_{l1} \left(p^{n+1}_{i j k} - p^{n+1}_{i-1, j\, k} \right) , \tag{3.1.30a}$$

$$\left(\rho'_l\, v_l\right)^{n+1}_{i, j, k-1/2} = \hat{v}_{l3} - d^{v}_{l3} \left(p^{n+1}_{i j k} - p^{n+1}_{i, j, k-1} \right) , \tag{3.1.30b}$$

$$\left(\rho'_l\, w_l\right)^{n+1}_{i, j-1/2, k} = \hat{w}_{l5} - d^{w}_{l5} \left(p^{n+1}_{i j k} - p^{n+1}_{i, j-1, k} \right) . \tag{3.1.30c}$$

3.2 Vapour phase

The scalar component of the momentum conservation equation (1.6) for the vapour phase in the z-coordinate direction can be written

$$\frac{\partial}{\partial t}\left(\rho_g' w_g\right) + \frac{\partial}{\partial L_\alpha}\left[\left(\rho_g' V_{g_\alpha}\right) w_g\right] - \frac{\partial}{\partial L_\alpha}\left(\mu_g \frac{\partial w_g}{\partial L_\alpha}\right) = -\alpha \frac{\partial p}{\partial z} - \rho_g' g_z - \quad (3.2.1)$$

$$- R_{gz} + K^M\left(w_l - w_g\right) + \left(\left[0, M\right] w_l - \left[0, -M\right] w_g\right) \qquad (L_\alpha = r,s,z).$$

Letting

$$S_{gz} = -\alpha \frac{\partial p}{\partial z} - \rho_g' g_z - R_{gz} + \quad (3.2.2)$$

$$+ K^M\left(w_l - w_g\right) + \left(\left[0, M\right] w_l - \left[0, -M\right] w_g\right) \qquad \textit{(source term)},$$

$$Jw_{g_\alpha} = \left(\rho_g' V_{g_\alpha}\right) w_g - \mu_g \frac{\partial w_g}{\partial L_\alpha} \quad (3.2.3)$$

(convective plus diffusive flux of momentum),

equation (3.2.1) can be written

$$\frac{\partial}{\partial t}\left(\rho_g' w_g\right) + \frac{\partial}{\partial L_\alpha}\left(Jw_{g\alpha}\right) = S_{gz}. \quad (3.2.4)$$

Integration over the volume V_f of the fluid in a control cell yields

$$\int_{V_f} \frac{\partial}{\partial t}\left(\rho_g' w_g\right) dV + \int_{V_f} \frac{\partial}{\partial L_\alpha}\left(Jw_{g\alpha}\right) dV = \int_{V_f} S_{gz}\, dV. \quad (3.2.5)$$

The control volume for the z-component of the momentum equation is obtained displacing a centred control cell (i j k) by half-mesh in the z direction. Replacing the volume integral of the divergence term by means of the fluxes through the cell bounding surfaces one derives:

$$\int_{V_f} \frac{\partial}{\partial t}\left(\rho_g^{'} w_g\right) dV + \int_{A_{f\ i+1/2,j+1/2,k}} \left(Jw_g\right)_r \ dA - \int_{A_{f\ i-1/2,j+1/2,k}} \left(Jw_g\right)_r \ dA +$$

$$+ \int_{A_{f\ i,j+1,k}} \left(Jw_g\right)_z \ dA - \int_{A_{f\ i,j,k}} \left(Jw_g\right)_z \ dA + \int_{A_{f\ i,j+1/2,k+1/2}} \left(Jw_g\right)_s \ dA - \quad (3.2.6)$$

$$- \int_{A_{f\ i,j+1/2,k-1/2}} \left(Jw_g\right)_s \ dA = \int_{V_f} S_{gz}\, dV \ .$$

We discretize this equation with respect to time treating convective, diffusive, and the pressure gradient terms fully implicitly and the friction term half-implicitly. Replacing the surface integrals by the mean values over the surfaces, denoted by the symbols $< >$, one obtains:

$$\begin{aligned}
&\frac{\left(\varepsilon V\right)_{i,j+1/2,k}}{\Delta t} \left[\left(\rho_g^{'}\, w_g\right)^{n+1} - \left(\rho_g^{'}\, w_g\right)^{n}\right]_{i,j+1/2,k} + \\
&+ < \left(Jw_g\right)_r \ A_f >^{n+1}_{i+1/2,j+1/2,k} - < \left(Jw_g\right)_r \ A_f >^{n+1}_{i-1/2,j+1/2,k} + \\
&+ < \left(Jw_g\right)_z \ A_f >^{n+1}_{i,j+1,k} - < \left(Jw_g\right)_z \ A_f >^{n+1}_{i\,j\,k} + \qquad\qquad (3.2.7) \\
&+ < \left(Jw_g\right)_s \ A_f >^{n+1}_{i,j+1/2,k+1/2} - < \left(Jw_g\right)_s \ A_f >^{n+1}_{i,j+1/2,k-1/2} = \\
&= - \frac{\left(\varepsilon V \alpha\right)_{i,j+1/2,k}}{\Delta z} \left(p^{n+1}_{i,j+1,k} - p^{n+1}_{i\,j\,k}\right) - \left(\varepsilon V \rho_g^{'}\, g_z\right)^{n}_{i,j+1/2,k} - \\
&- \left[\frac{\varepsilon V}{2D_h}\ f_g\ |w_g|^n \left(\rho_g^{'}\, w_g\right)^{n+1}\right]_{i,j+1/2,k} + \\
&+ \left(\varepsilon V\right)_{i,j+1/2,k}\ K^M \left(w_l - w_g\right)_{i,j+1/2,k} + \\
&+ \left(\varepsilon V\right)_{i,j+1/2,k} \cdot \left(\left|0, M\right| w_l - \left|0, -M\right| w_g\right)_{i,j+1/2,k} .
\end{aligned}$$

The averaged fluxes of the vector Jw_m are evaluated with the following upwind discretization scheme:

$$Jr+ = \int_{A_{f\ i+1/2,j+1/2,k}} \left(Jw_g\right)_r\ dA = < Jw_g \cdot A_f >_{i+1/2,j+1/2,k} = \tag{3.2.8}$$

$$= \left\{ A_f\ \rho_g'\ u_g\ w_g - \frac{A_f\ \mu_g}{\rho_g'\ \Delta r}\ \Delta\left(\rho_g'\ w_g\right)\right\}_{i+1/2,j+1/2,k} =$$

$$= \left\{ F^g \cdot \rho_g'\ w_g - D^g \cdot \Delta\left(\rho_g'\ w_g\right)\right\}_{i+1/2,j+1/2,k} ,$$

with the definitions:

$$F^g_{i+1/2,j+1/2,k} = \left(A_f\ u_g\right)_{i+1/2,j+1/2,k} , \tag{3.2.9}$$

$$D^g_{i+1/2,j+1/2,k} = \left(A_f\ \frac{\mu_g}{\rho_g'\ \Delta r}\right)_{i+1/2,j+1/2,k} . \tag{3.2.10}$$

For both $u_{g,i+1/2,j+1/2,k}$ positive and negative, formula (3.2.8) can be written

$$Jr+ = \left[0, F^g_{i+1/2,j+1/2,k}\right]\left(\rho_g'\ w_g\right)_{i,j+1/2,k} - \tag{3.2.11}$$

$$- \left[0, -F^g_{i+1/2,j+1/2,k}\right]\left(\rho_g'\ w_g\right)_{i+1,j+1/2,k} +$$

$$+ D^g_{i+1/2,j+1/2,k}\left\{\left(\rho_g'\ w_g\right)_{i,j+1/2,k} - \left(\rho_g'\ w_g\right)_{i+1,j+1/2,k}\right\} .$$

With the usual indexing conventions the fluxes can be written:

$$Jr+ = \int_{A_{f\ i+1/2,j+1/2,k}} \left(Jw_g\right)_r\ dA = < \left(Jw_g\right)_r \cdot A_f >_{i+1/2,j+1/2,k} = \tag{3.2.12a}$$

$$= \left[0, F^g_{i+1/2,j+1/2,k}\right]\left(\rho_g'\ w_g\right)_0 - \left[0, -F^g_{i+1/2,j+1/2,k}\right]\left(\rho_g'\ w_g\right)_2 +$$

$$+ D^g_{i+1/2,j+1/2,k}\left\{\left(\rho_g'\ w_g\right)_0 - \left(\rho_g'\ w_g\right)_2\right\} ,$$