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Coolant Channel Module CCM. An Universally Applicable Thermal-Hydraulic Drift-Flux Based Separate-Region Mixture-Fluid Model

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1. Introduction

The development of LWR Nuclear Power Plants (NPP) and the question after their safety behaviour have enhanced the need for adequate theoretical descriptions of these plants. Thus thermal-hydraulic models and, based on them, effective computer codes played already very early an important role within the field of NPP safety research. The models and codes should have the potential to describe the steady state and transient behaviour of characteristic key parameters of a single- or two-phase fluid flowing along the corresponding loops of such a plant and thus also along any type of heated or non-heated coolant channels.

Obviously many discussions have and will continue to take place among experts as to which type of theoretical approach should be chosen for the correct description of thermal-hydraulic two-phase problems when looking at the wide range of applications. Very comprehensive reviews and critical discussions of different possible methods have been published already very early in the book of Ishii (1990), in the workshop presentations of Wulff (1987) and by Banerjee and Yadigaroglu (1990). Due to the presence of discontinuities in the first principle of mass conservation in a two-phase flow model, caused at the transition from single- to two-phase flow and vice versa, it turns out that the direct solution of the basic conservation equations for mixture fluid along such a coolant channel gets very complicated. What is thus the most appropriate way to deal with such a special thermal-hydraulic problem?

With the introduction of the **'Separate-Phase Model'** concept it could already very early a very successful way be shown how to avoid upcoming difficulties in finding solution methods to treat such a two-phase flow situation under the assumption of separating the two-phases of such a mixture-flow completely from each other. This yields a system of 4-, 5- or sometimes even 6-equations defined by splitting each of the conservation equations into two so-called 'field equations'. Hence, compared to the four independent parameters characterising the mixture fluid, the separate-phase systems demand a much higher number of additional variables and special assumptions. This has the consequence that an enormous

amount of CPU-time has to be expended for the solution of the resulting sets of differential and analytical equations in a computer code. It is clear that, based on such assumptions, the interfacial relations both between each phase and the (heated or cooled) wall but also between each of the two phases are completely rearranged, raising the difficult question of how to describe in a realistic way the direct heat input into and between the phases and the movement resp. the friction of the phases between them. This problem is solved in such an approach by introducing corresponding exchange (=closure) terms between the equations based on special transfer (= closure) laws. Since they can, however, not be based on fundamental laws or at least on experimental measurements this approach requires a significant effort to find a correct formulation of the exchange terms between the phases. It must therefore be recognised that the quality of these basic equations (and especially their boundary conditions) will be intimately related to the (rather artificial and possibly speculative) assumptions adopted if comparing them with the original conservation laws of the 3-equation system and their constitutive equations as well. The problem of a correct description of the interfacial reaction between the phases and the wall remains. Hence, very often no consistency between different models due to their underlying assumptions can be stated. Another problem arises from the fact that special methods have to be foreseen to describe the moving boiling or mixture level boundaries (or at least to estimate their 'condensed' levels) in such a mixture fluid (see, for example, the 'Level Tracking' method in TRAC). Additionally, these methods show often deficiencies in describing extreme situations such as the treatment of single- and two-phase flow at the ceasing of natural circulation, the power situations if decreasing to zero etc. The codes are sometimes very inflexible, especially if they have to provide to a very complex physical system also elements which belong not to the usual class of 'thermal-hydraulic coolant channels'. These can, for example, be nuclear kinetic considerations, heat transfer out of a fuel rod or through a tube wall, pressure build-up within a compartment, time delay during the movement of an enthalpy front along a downcomer, natural circulation along a closed loop, parallel channels, inner loops etc.

Despite of these difficulties the 'Separate-Phase Models' have become increasingly fashionable and dominant in the last decades of thermal-hydraulics as demonstrated by the widely-used codes TRAC (Lilles et al.,1988, US-NRC, 2001a), CATHENA (Hanna, 1998), RELAP (US-NRC,2001b, Shultz,2003), CATHARE (Bestion,1990), ATHLET (Burwell et al.,1989, Austregesilo et al., 2003, Lerchl et al., 2009).

Several reasons can be named why this method is preferred by many authors and users:

- Advantages due the unique formulation of the up to 6 basic partial differential eqs. which allows then also to apply a unique mathematical solution method,
- the possibility to circumvent discontinuities (Wulff, 1987) in simulating the transitions from single- to two-phase flow and vice versa, thus avoiding difficulties in describing the movement of phase boundaries along a coolant channel,
- avoiding the very difficult direct theoretical treatment of a mixture-fluid approach,
- allowing establishing within the resulting 'modular' codes the necessary set of solution equations (ODE-s and constitutive equations in dependence of corresponding perturbation parameters) by combining them by means of an adequate input data set, i.e. outside of the code, with the advantage that the user does not need to be familiar with the construction of digital codes.

- giving the possibility to assume further-on that, in the case of two-phase flow situations, the water-phase can adopt temperatures below, the steam phase above saturation conditions. This means, the model can also take care of 'thermal-hydraulic non-equilibrium' situations, an important advantage for the application of this class of codes (as this is for example the case if cold water is injected into a steam dome or steam into a sub-cooled water plenum etc.).

It is on the other hand clear that as an alternative for the description of two-phase phenomena by splitting them into different phases the direct solution of the basic equations of a **mixture-fluid technique** could be regarded as a very appropriate approach, provided that despite of the above mentioned difficulties an exact solution can be found. This direct method could therefore be seen as a real counterpart to the currently preferred and dominant 'separate-phase models'.

However, in the past the difficulties in the direct treatment of a 'mixture-fluid approach' have been responsible for the fact that only approximate and very simplified solutions for special situations could be provided, thus demanding severe restrictions in their field of application. As pointed-out by (Fabic, 1996) in the early seventies such simplified 'homogenous equilibrium models (HEM-s)' have been derived under the assumption of a homogeneous fluid, a mixture where water and steam phase are assumed to move with the same velocity, i.e. the slip remains equal to 1 and the relative and thus also drift velocities equal to 0. Since for most purposes this is too far from reality, it is obvious that such simplified 'homogeneous' approaches (see for example Dunn, 1998) could only be applied to special cases, for example where the speed of the calculation has to be enhanced in order to be usefully applied in comprehensive two-phase flow studies. Their shortcomings are mainly responsible for the seemingly widespread misunderstanding of the quality of 'mixture-fluid' models, their poor image and the subsequent unfair treatment of this class of models.

Zuber et al. (1965) and Wulff (1987) proposed already very early a concept called (a bit imprecisely) **'drift-flux model'** which has been continuously expanded according to the rising demands in reactor safety research. In fact it is a 'four-equation non-homogeneous non-equilibrium two-phase flow model' with mass-, energy- and momentum balances for the mixture and a separate mass balance for the vapour phase based on a specially developed 'drift-flux theory'. It has been successfully applied in a number of post-calculations of reactor transients (with up to ten times real-times simulation speed) including BWR instability simulations with large power and flow oscillations.

At the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) at Garching/Munich very early activities have been started too to develop thermal-hydraulic models and digital codes which have the potential to describe in a detailed way the overall transient and accidental behaviour of fluids flowing along the core but also the main components of different Nuclear Power Plants (NPP) types. For one of these components, namely the natural circulation U-tube steam generator together with its main steam system, an own theoretical model has been derived. The resulting digital code UTSG (Hoeld, 1978) could be used both in a stand-alone way but also as part of more comprehensive transient codes, such as the thermal-hydraulic GRS system code ATHLET (Burwell et al., Austregesilo, 2003) with an high level simulation language GCSM (General Control Simulation Module) to take care of the balance-of-plant (BOP) actions. Based on the experience of many years of application both at the GRS and a number of other institutes in different countries but also due to the

rising demands coming from the safety-related research studies this UTSG theory and code has been continuously extended, yielding finally a very satisfactory and mature code version UTSG-2 (Hoeld, 1990a).

During the research work for the development of the code UTSG-2 it arose finally the idea to establish an own basic element which is able to simulate the thermal-hydraulic mixture-fluid situation within any type of cooled or heated channel in an as general as possible way, having the aim to be applicable for any modular construction of complex thermal-hydraulic assemblies of pipes and junctions. Thereby, as described in detail in this paper, in contrast to the above mentioned class of 'separate-phase' modular codes instead of separating the phases of a mixture fluid within the entire coolant channel an alternative theoretical approach has been chosen, differing both in its form of application but also in its theoretical background. To circumvent the above mentioned difficulties due to discontinuities resulting from the spatial discretization of a coolant channel, resulting eventually in nodes with a transition from single- to two-phase flow and vice versa, a special and unique concept has been derived assuming that a (basic) coolant channel (BC) should be subdivided into a number of sub-channels (SC-s) with the imposition that each of these SC-s can consist of only two types of flow regimes, an SC with just a single-phase fluid, containing exclusively either sub-cooled water (setting $L_{FTYPE}=1$) or superheated steam ($L_{FTYPE}=2$), or an SC with a two-phase mixture ($L_{FTYPE}=0$). The theoretical considerations of this **'separate-region approach'** (within the class of mixture-fluid models) can then be restricted to only these two regimes. Hence, for each SC type, the 'classical' 3 conservation equations for mass, energy and momentum can be treated in a direct way. In case of a sub-channel with mixture flow these basic equations have to be supported by a drift flux correlation yielding an additional relation for the appearing fourth variable, namely the steam mass flow. This can, eventually, be achieved by any two-phase correlation (for example also a slip correlation). But, to take care also of stagnant or counter-current flow situations, an effective drift-flux correlation seems to be more effective. For separate-phase models no such direct experimentally based correlations are available. It has to be noted that, different to the 'drift-flux model' where a 4-th mass balance equation for the vapour phase is introduced, the fundamental mixture-fluid equations are based on an adequate drift-flux correlation in an analytical form.

It is obvious that this procedure has, however, the consequence that varying SC entrance and outlet boundaries have to be considered too. As demonstrated in this paper an adequate way to solve this essential problem could be found and a corresponding procedure been established.

As a result of these theoretical considerations an universally applicable 1D thermal-hydraulic drift-flux based separate-region **c**oolant **c**hannel **m**odule (and code) CCM could be constructed. Its aim is to make it possible to calculate automatically the steady state and transient behaviour of all characteristic parameters of a single- and two-phase fluid within the entire coolant channel. It represents thus a valuable tool for the establishment of complex codes and can contribute even in the case of complex thermal-hydraulic systems which may consist of a number of different types of (basic) coolant channels to the overall set of equations by determining automatically the different differential and constitutive equations needed for each of these sub- and thus basic channels.

To check the performance and validity of the code package CCM, to verify and validate it (see Hoeld, 1978, 1990b, 2002a, 2007a, 2007b) the digital code UTSG-2 has been extended to a new version, called UTSG-3. It is based, similarly as in the previous code UTSG-2, on the

same U-tube, main steam and downcomer (with feedwater injection) system layout, but now, among other essential improvements, the three characteristic channel elements of the code UTSG-2 (i.e. the primary and secondary side of the heat exchange region and the riser region) have been replaced by adequate CCM modules. Naturally, during the application of UTSG-3 and thus CCM both codes have been continuously expanded to a now very mature form (Hoeld, 1998b, 1999, 2000).

It is obvious that such a theoretical 'separate-region' approach can disclose a new way in describing thermal-hydraulic problems, regarding the resulting 'mixture-fluid' technique as a very appropriate way to circumvent the uncertainties apparent from the separation of the phases in a mixture flow. The starting equations are the direct consequence of the original fundamental physical laws for the conservation of mass, energy and momentum, supported by well-tested heat transfer and single- and two-phase friction correlation packages (and thus avoiding also the sometimes very speculative derivation of the 'closure' terms). In a very comprehensive study by (Hoeld, 2004b) a variety of arguments for the here presented type of approach is given, some of which will be discussed in the conclusions presented in chapter 6.

The very successful application of the code combination UTSG-3/CCM demonstrates the ability to find an exact and direct solution for the basic equations of a 'non-homogeneous drift-flux based thermal-hydraulic mixture-fluid coolant channel model'. The theoretical background of CCM will be described in very detail in the following chapters.

For the establishment of the corresponding (digital) module CCM, based on this theoretical model and written in double-precision (with its single-precision version CCMS) very specific methods had to be achieved, thereby taking into account the following points:

- The code should be easily applicable, demanding only a limited amount of easily available input data. It should also be able to simulate the thermal-hydraulic mixture-fluid situation along any cooled or heated channel in as general a way as possible. It should thus be able to describe any modular construction of complex thermal-hydraulic assemblies of pipes and junctions. Such an universally applicable tool can then be taken for calculating the steady state and transient behaviour of all the characteristic parameters of each of the appearing coolant channels and thus be a valuable element for the construction of complex computer codes. It should yield as output all the necessary time-derivatives and constitutive parameters of the coolant channels required for the establishment of an overall thermal-hydraulic code.
- It was the intention of CCM that it should act as a complete system in its own right, requiring only BC- (and not SC-) related, and thus easily available input parameters (geometry data, initial and boundary conditions, parameters resulting from the integration etc.). The partitioning of BC-s into SC-s is done at the begin of each recursion or time-step automatically within CCM, so no special actions are required of the user.
- Knowing now the characteristic parameters at all SC nodes (within a BC) then the single- and two-phase parameters at all node boundaries of the entire BC can be determined, but also also the corresponding time-derivatives of the averaged parameters over these nodes. This yields a final set of ODE-s and constitutive equations.
- The quality of such a model is very much dependent on the method by which the problem of the varying SC entrance and outlet boundaries can be solved, especially if they cross BC node boundaries during their movement along a channel. Hence, on the

basis of the 'Leibniz' rule (see eq.(29)), special measures had to be developed which allow the characterisation of their transient behaviour in deriving own differential equations.

- For the support of the nodalized differential equations along different SC-s a 'quadratic **p**olygon **a**pproximation' **p**rocedure (PAX) was constructed in order to interrelate the mean nodal with the nodal boundary functions. Additionally, due to the possibility of varying SC entrance and outlet boundaries, nodal entrance gradients are also required from the PAX procedure too (See section 3.3).
- Several correlation packages such as, for example, packages for the thermodynamic properties of water and steam, heat transfer coefficients, drift flux correlations and single- and two-phase friction coefficients had to be established and implemented (See sections 2.2.1 to 2.2.4).
- It order to be able to describe also thermodynamic non-equilibrium situations it can be assumed that each phase is described by an own with each other interacting BC. Then, in the model the possibility of a variable cross flow area along the entire channel had to be considered as well.

Within the CCM procedure two further aspects play an important role These are, however, not essential for the development of mixture-fluid models but can help enormously to enhance the computational speed and applicability of the resulting code in simulating a complex net of coolant pipes:

- Solution of energy and mass balance equations during each intermediate time step independently from momentum balance considerations in order to avoid the heavy CPU-time consuming solution of stiff equations (See section 3.5).
- This allows then also the introduction of an 'open' and 'closed channel' concept (see section 3.11), a special method which can be very helpful in describing complex physical systems with eventually inner loops, as this can be done for example if simulating a 3D compartment by parallel channels (Jewer et al., 2005).

The application of a direct mixture-fluid technique follows a long tradition of research efforts. Ishii (1990), a pioneer of two-fluid modelling, states with respect to the application of effective drift-flux correlation packages in thermal-hydraulic models: 'In view of the limited data base presently available and difficulties associated with detailed measurements in two-phase flow, an advanced mixture-fluid model is probably the most reliable and accurate tool for standard two-phase flow problems'. There is no new knowledge available to indicate that this view is invalid.

Generally, the mixture-fluid approach is in line with (Fabic, 1996) who names three strong points arguing in favour of this type of drift-flux based mixture-fluid models:

- They are supported by a wealth of test data,
- they do not require unknown or untested closure relations concerning mass, energy and momentum exchange between phases (thus influencing the reliability of the codes),
- they are much simpler to apply,

and, it can be added,

- discontinuities during phase changes can be avoided by deriving special solution procedures for the simulation of the movement of these phase boundaries,
- the possibility to circumvent a set of 'stiff' ODE-s saves an enormous amount of CPU time which means that the other parts of the code can be treated in much more detail.

A first version of the module CCM has already been presented in October 2005 at the NURETH-11 conference at Avignon (Hoeld, 2005), a corresponding detailed version published then in (Hoeld, 2007a). Due to the rising experiences in applying this module it has been continuously adapted during the last years resulting in the here presented final form.
The theoretical model and module CCM has the potential to be extended, in a second phase, to a 'porous' coolant channel model too, porous at each node boundary, i.e. to the more detailed case where coolant mass (water, steam and/or water/steam mixtures) is exchanged also at nodal boundaries between neighbouring channels (and not only at BC entrance or outlet).
Parallel to this paper in a second article within this 'Open Access Book' a detailed description of the last status of the resulting 'Natural-circulation U-tube Steam Generator' Code UTSG-3 (including main steam and feedwater systems) is given by (Hoeld, 2011). It demonstrates the ability to apply the 'Coolant Channel Module CCM' as an important element in a complex system of loops and branches in a successful way.

2. Thermal-hydraulic drift-flux based mixture fluid approach

2.1 Thermal-hydraulic conservation equations

Thermal-hydraulic single-phase or mixture-fluid models for coolant channels or, as presented here, for each of the sub-channels are generally based on a number of fundamental physical laws, i.e. on genuine conservation equations for mass, energy and momentum. They are supported by adequate constitutive equations (packages for thermo-dynamic and transport properties of water and steam, for heat transfer coefficients, for drift flux, for single- and two-phase friction coefficients etc.). Thereby second-order terms (representing, for example, dissipation in flow direction, drag and gravitational work) are frequently found to be quantitatively insignificant (Wulff, 1987) and will thus not be taken into account.
In view of possible applications as an element in complex thermal-hydraulic ensembles outside of CCM eventually a fourth and fifth conservation law has to be considered too. The equation for volume balance makes it possible to calculate for example the transient behaviour of the overall system pressure. Together with the local pressure differences then the absolute pressure profile along the BC can be determined. The fifth physical law is based on the (trivial) fact that the sum of all pressure decrease terms along a closed loop must be zero. It is the basis for the treatment of the thermal-hydraulics of a channel according on 'the closed channel concept'. If thus such a channel acts as a part of a closed loop (with given fixed BC entrance and outlet pressure terms) then the necessary entrance mass flow term has be determined in order to fulfil the demand from momentum balance.

2.1.1 Mass balance (for both single- and two-phase flow)

$$\frac{\partial}{\partial t}\{A[(1-\alpha)\rho_W+\alpha\rho_S]\}+\frac{\partial}{\partial z}G=0 \qquad (1)$$

containing the density terms ρ_W and ρ_S for sub-cooled or saturated water and saturated or superheated steam, the void fraction α and the cross flow area A which can eventually be changing along the coolant channel. It determines, after a nodalization, the total mass flow $G=G_W+G_S$ at node outlet in dependence of its node entrance value.

2.1.2 Energy balance (for both single- and two-phase flow)

$$\frac{\partial}{\partial t}\{A[(1-\alpha)\rho_W h_W+\alpha\rho_S h_S-P]\}+\frac{\partial}{\partial z}[G_W h_W+G_S h_S] = q_L = U\, q_F = A\, q \tag{2}$$

containing the enthalpy terms h_W and h_S for sub-cooled or saturated water and saturated or superheated steam. As boundary values either the 'linear power q_L', the 'heat flux q_F' along the heated (or cooled) tube wall (with its perimeter U_{TW}) or the local 'power density term q' are demanded to be known (See also sections 2.2.4 and 3.5). They are assumed to be directed into the coolant (then having a positive sign).

After an appropriate finite-difference nodalization procedure (see chapter 3.2) it follow in the transient case (as demonstrated in the sections 3.7 to 3.9) then differential equations

- for the mean nodal enthalpies (h_{WMn}, h_{SMn}) of either sub-cooled water (if L_{FTYPE}=1) or superheated steam (L_{FTYPE} =2) in the case of a single-phase flow situation and thus, by applying water/steam tables, corresponding coolant temperature terms (T_{WMn},T_{SMn}) too, or, at two-phase flow conditions (L_{FTYPE} =0), for the mean nodal void fraction α_{Mn} over each node n

and

- at the transition from single- to two-phase (and vice versa) for the boiling boundary z_{BB} (if α=0) or, if α=1, the mixture (or dry-out) level z_{ML} (section 3.9). Thereby it can be taken advantage of the fact that at these positions either the coolant enthalpy or temperature are limited by its saturation enthalpy or temperature (h_W =h' or h_S =h'' and T_W = T_S =T_{SAT} or T_S =T_{SAT}) or the void fraction becomes equal to 1 (or 0).

2.1.3 Momentum balance (for both single- and two-phase flow)

$$\frac{\partial}{\partial t}(G_F)+\left(\frac{\partial P}{\partial z}\right) = \left(\frac{\partial P}{\partial z}\right)_A+\left(\frac{\partial P}{\partial z}\right)_S+\left(\frac{\partial P}{\partial z}\right)_F+\left(\frac{\partial P}{\partial z}\right)_X \tag{3}$$

describing either the pressure differences (at steady state) or (in the transient case) the change in the total mass flux (G_F =G/A) along a channel.

The general pressure gradient $\left(\frac{\partial P}{\partial z}\right)$ can be determined in dependence of

- the mass acceleration

$$\left(\frac{\partial P}{\partial z}\right)_A = -\frac{\partial}{\partial z}[(G_{FW}v_W+G_{FS}v_S)] \tag{4}$$

with v_S and v_W denoting steam and water velocities given by the eqs.(9) and (10),

- the static head

$$\left(\frac{\partial P}{\partial z}\right)_S = -\cos(\Phi_{ZG})\, g_C\,[\alpha\rho_S+(1-\alpha)\rho_W] \tag{5}$$

with Φ_{ZG} representing the angle between upwards and flow direction, i.e., $\cos(\Phi_{ZG})= \pm z_{EL}/z_L$ and z_L denoting the length, z_{EL} the relative elevation height with a positive sign at upwards flow)

- the single- and/or two-phase friction term

$$\left(\frac{\partial P}{\partial z}\right)_F = -f_R\,\frac{G_F\,|G_F|}{2\,d_{HW}\,\rho} \tag{6}$$

with a friction factor derived from corresponding constitutive equations (section 2.2.2) and finally

- the direct perturbations $(\partial P / \partial z)_X$ from outside, arising either by starting an external pump or considering a pressure adjustment due to mass exchange between parallel channel.

2.2 Constitutive equations

For the exact description of the steady state and transient behaviour of single- or two-phase fluids there are needed, besides the conservation equations, a number of mostly empirical constitutive relations. Naturally, any effective correlation package can be used for this purpose. A number of such correlations have been developed at the GRS and thoroughly tested, showing very satisfactory results.

2.2.1 Thermopdynamic and transport properties of water and steam

The different thermodynamic and transport properties for water and steam demanded by the conservation and constitutive equations have to be determined by applying adequate water/steam tables. This is, for light-water systems, realized in the code package MPP (Hoeld, 1996). It yields the wanted values such as the saturation temperature T_{SAT}, densities ($\rho^{/}$, $\rho^{//}$), enthalpies ($h^{/}$, $h^{//}$) for saturated water and steam with respect to their local pressure (P) and corresponding densities (ρ) and enthalpies (h) for sub-cooled water or superheated steam (index W and S) again with respect to their independent local parameters T and P (but also h and P).

For the solution of the conservation equations also time-derivatives of these thermodynamic properties which respect to their independent local parameters are demanded. They get, for example for the case of an enthalpy term h, the form

$$\frac{d}{dt} h(z,t) = \frac{d}{dt} h[T(z,t),P(z,t)] = \left(\frac{\partial h}{\partial T}\right) \frac{d}{dt} T_{Mn}(t) + \left(\frac{\partial h}{\partial P}\right)_{Mn} \frac{d}{dt} P_{Mn}(t)$$
$$= h^{T} \frac{d}{dt} T_{Mn}(z,t) + h^{P} \frac{d}{dt} P_{Mn}(z,t) \qquad (7)$$

Hence the thermodynamic water/steam tables should provide also the derivatives (T^{P}_{SAT}, ρ'^{P}, $\rho^{//P}$, h'^{P}, h''^{P}) for saturated water and saturated steam but also the partial derivatives (ρ^{T}, ρ^{P}, $c_P = h^{T}$, h^{P}) for subcooled water or superheated steam with respect to their independent parameters T and P (but also h and P). Additionally, corresponding thermodynamic transport properties such as 'dynamic viscosity' and 'thermal heat conductivity' (and thus the 'Prantl number') are asked from some constitutive equations too as this can be stated, for example, for the code packages MPPWS and MPPETA (Hoeld, 1996). All of them have been derived on the basis of tables given by (Schmidt and Grigull, 1982) and (Haar et al., 1988).

Obviously, the CCM method is also applicable for other coolant systems (heavy water, gas) if adequate thermodynamic tables for this type of fluids are available.

2.2.2 Single- and two-phase friction factors

In the case of **single-phase flow** with regard to equation (6) the friction factor f_R will, as recommended by (Moody, 1994), be set equal to the Darcy-Weisbach single-phase friction factor f_{DW} being represented by

$$f_R = f_{DW} = \frac{1}{\xi^2} \qquad \text{(at single-phase flow)} \tag{8}$$

with the parameter ξ depending on the Reynolds number $Re = G\, d_H/(A\, \eta)$ and the relative roughness ε_{TW}/d_H of the wall surface. The factor ξ can be approximated by the relation

$$\begin{aligned} \xi &= 2 \log_{10}\left(\frac{d_H}{\varepsilon_{TW}}\right) + 1.14 \qquad \text{if } Re > Re_{CTB} = 441.19 \left(\frac{d_H}{\varepsilon_{TW}}\right)^{1.1772} \\ &= -2 \log_{10}\left(2.51 \frac{\xi}{Re} + \frac{\varepsilon_{TW}}{3.71\, d_H}\right) \qquad \text{if } Re \le Re_{CTB} \end{aligned} \tag{9}$$

For **two-phase flow** conditions this factor can be extended to

$$f_R = f_{DW}\, \Phi^{\,2}_{2PF} \qquad \text{(at two-phase flow)} \tag{10}$$

with the single-phase part f_{DW} to be determined under the assumption that the fluid moves with the total mass flow G (= 100 % liquid flow). The two-phase multiplier $\Phi^{\,2}_{2PF}$ (dependent only on steam quality and pressure) is given by (Martinelli-Nelson, 1948) as measured curves. A possible attempt to describe these curves analytically could, as proposed by (Hoeld, 1990a, 2004a), be given by the approximation function

$$\Phi^{\,2}_{2PF} = \exp \frac{f_1 X}{\sqrt{1 + f_2 X + f_3 X^2}} \qquad \rightarrow \quad \frac{\rho'}{\rho''} \frac{(f_{WD})_S}{(f_{WD})_W} \quad \text{if } X \rightarrow 1 \tag{11}$$

with the factors

$$\begin{aligned} f_1 &= 44.216 + 0.7428\, 10^{-6}\, P \\ f_2 &= 12.645 + 4.9841\, 10^{-6}\, P \\ f_3 &= 17.975 + 25.7440\, 10^{-6}\, P \qquad \text{(P in Pa)} \end{aligned} \tag{12}$$

For the special case of a steam quality X nearing 1 the friction term has to approach the single-phase steam friction factor $(f_{DW})_S$. Thus the two-phase multiplier has, as shown above, to be corrected in an appropriate way (for example, by changing the curve after a maximum of X at about 0.8).

2.2.3 Drift flux correlation

In the case of two-phase flow, the three conservation equations (1), (2) and (3) demanding four independent variables (G, α, P and G_S) have to be completed by an additional two-phase relation in order to obtain an adequate representation of the needed fourth variable G_S. This can be achieved by any two-phase correlation, e.g. also a slip correlation. However, to take care of stagnant or counter-current flow situations too an effective drift-flux correlation seemed here to be more appropriate, correlations which can be seen as a 'bridge' between G_S and α.

For this purpose an own drift-flux correlation package has been established, named MDS (Hoeld, 2001 and 2002a). It is based on the result of a very comprehensive study (Hoeld et al., 1992) and (Hoeld, 1994) comparing different slip (6) and drift-flux (3) correlations with each other and also with a number (5) of available experimental data in order to check their validity over a wide range of application. Besides them, it had to be found which of them is

most suited for incorporation into the MDS package and thus CCM code. Due to different requirements in the application of CCM it turned out that the drift-flux correlation package in the form of the 'flooding-based full-range' Sonnenburg correlation (1989) should be preferred. This correlation combines the common drift-flux procedure being formulated by (Zuber-Findlay, 1965) and expanded by (Ishii-Mishima, 1980) and (Ishii, 1990) etc. with the modern envelope theory. The correlation in the final package MDS had to be rearranged in such a way that also the special cases of $\alpha \rightarrow 0$ or $\alpha \rightarrow 1$ (where its absolute values but also their gradients are demanded by CCM) could be treated. Additionally, an inverse form had to be installed and considerations with respect to a possible entrainment be included.
For the case of a vertical channel this correlation can be represented as

$$v_D = 1.5\, v_{WLIM}\, C_0 C_{VD} \left[(1+C_{VD}^2)^{3/2} - (1.5+C_{VD}^2)\, C_{VD}\right] \quad \text{with} \quad v_D \rightarrow v_{D0} = \frac{9}{16} C_0 v_{WLIM} \quad \text{if} \quad \alpha \rightarrow 0 \tag{13}$$

where the coefficient C_{VD} is given by

$$C_{VD} = \frac{2}{3} \frac{v_{SLIM}}{v_{WLIM}} \frac{1 - C_0\alpha}{C_0\alpha} \tag{14}$$

The resulting package MDS yields in combination with an adequate correlation for the phase distribution parameter C_0 relations for the limit velocities v_{SLIM} and v_{WLIM} and thus (independently of the total mass flow G) for the drift velocity v_D in relation to the void fraction α. All of them are dependent on the given 'system pressure P', the 'hydraulic diameter d_{HW}' (with respect to the wetted surface A_{WSF}) and its inclination angle Φ_{ZG}), on specifications about the geometry type (L_{GTYPE}) and, for low void fractions, the information whether the channel is heated or not.
The drift flux theory can be expressed (by a now already on G dependent) steam mass flow term

$$G_S = \frac{\rho''}{\rho'} \frac{\alpha}{C_{GC}} (C_0 G + A\rho' v_D) = A G_{FS} \tag{15}$$

with the coefficient

$$C_{GC} = 1 - (1 - \frac{\rho''}{\rho'})\, \alpha C_0 \rightarrow 1 \text{ if } \alpha \rightarrow 0 \text{ and } \rightarrow \frac{\rho''}{\rho'} \text{ if } \alpha \rightarrow 1 \tag{16}$$

by considering the definition equations of the velocities for steam, water and drift

$$v_D = (1 - \alpha C_0)\, v_S - (1-\alpha)\, C_0 v_W \tag{17}$$

$$v_S = \frac{G_S}{A\alpha\rho''} \quad \text{with} \quad G_S = G - G_W = XG \tag{18}$$

$$v_W = \frac{G_W}{A(1-\alpha)\rho'} \quad \text{with} \quad G_W = (1\text{-}X)\, G \tag{19}$$

By means of this drift-flux correlation now the fourth variable is determined too. Then also all other characteristic two-phase parameters can be derived starting from their definition equations. Their interrelations are shown, for example, in the tables of (Hoeld, 2001 and 2002a). Such two-phase parameters could be the phase distribution parameter C_0, the water mass flow G_W, drift, water, steam and relative velocities v_D, v_W ,v_S and v_R and eventually the steam quality X. Especially the determination of the steam mass flow gradient

$$G_S^{(\alpha)} \rightarrow G_{S0}^{(\alpha)} = \frac{\rho''}{\rho'} (C_{00}\, G + A\rho' v_{D0}) = A\rho'' v_{S0} \text{ or } = 0 \qquad \text{if } \alpha \rightarrow 0 \text{ and } L_{HEATD} = 0 \text{ or } 1$$

$$\rightarrow G_{S1}^{(\alpha)} = A \frac{\rho''}{\rho'} (1 + C_{01}^{(\alpha)}) (G - \rho'' v_{SLIM}) = A\rho' v_{W1} \quad \text{if } \alpha \rightarrow 1 \tag{20}$$

will play (as shown, for example, in eq.(70)) an important part, if looking to the special situation that the entrance or outlet position of a SC is crossing a BC node boundary ($\alpha \rightarrow 0$ or $\rightarrow 1$). This possibility makes the drift-flux package MDS to an indispensable part in the nodalization procedure of the mixture-fluid mass and energy balance.

The solution of the basic (algebraic) set of steady state equations demands the steam mass flow term G_S as the independent variable, and not the void fraction α. The same is the case after an injection of a two-phase mixture coming from a 'porous' channel or an abrupt change in steam mass flux G_{FS} (as this takes place after a change in total mass flow or in the cross flow area of a following BC). Then the total and the steam mass flows G and G_S have to be taken as the basis for further two-phase considerations. The void fraction α and other two-phase parameters (v_D, C_0) can then to be determined from an inverse (INV) form of this drift-flux correlation (with G_S now as input):

$$\alpha = f_{DRIFT\,(INV)} (G_S \text{ or } v_D, G, P, \frac{z_{EL}}{z_L}, d_{HW}, ..) \tag{21}$$

As shown in (Hoeld, 2002a) counter-current flow (CCF) along the entire void fraction range can be stated if the signs of the gradients of the G_S-α curve at $\alpha = 0$ and $\alpha=1$ are opposite, i.e. if the total mass flux G_F lies within certain lower and upper limits

$$\text{If } G_{FCL} \le G_F = \frac{G}{A} \le G_{FCU} \quad \text{then CCF}$$
$$(\text{with } G_{FCL} = -\frac{9}{16}\rho' v_{WLIM} \text{ and } G_{FCU} = \rho'' v_{SLIM}) \tag{22}$$

Besides vertical up- or downwards, co-, stagnant or even counter-current two-phase flow situations (along channels of different geometry types such as rod bundles, rectangular ducts, round pipes etc.) the drift-flux correlations must have the potential to describe also two-phase flow situations through inclined or even horizontal channels in order to make the theoretical model as generally applicable as possible.

Usually correlations and thus also the drift-flux theory are based on steady state measurements. During transient calculations the correlation can thus be used only in a pseudo-stationary way, i.e., a change in void fraction results in an immediate change in drift velocity and thus in all the other characteristic two-phase parameters. There exist, however, physical phenomena (interactions of melt with water, condensation shocks, water and steam

hammer) where the delay between relative velocity and void fraction has a special importance, also if this delay lays within a range of 0.01 to 0.1 s. In the 'drift flux model' this is taken care by the fourth mass balance equation for the steam, in the separate-phase models by the (time-dependent) exchange term within the mass balance equations for the two phases water and steam. To cover thus in this approach also such transient phenomena the drift-flux considerations can be extended by providing the drift velocity v_D with respect to the void fraction with a corresponding time-delay function of 1-st order. Then the original (pseudo-steady state) drift velocity parameter $v_D = v_{DPSE}$ has to be expanded to its transient counter-part

$$v_D = v_{DPSE} - (v_{DPSE} - v_{DB}) \exp(- \frac{t - t_B}{\Theta_{VDT}}) \tag{23}$$

with $v_{DB} = v_D$ at the begin of a time interval $t = t_B$. All the other two-phase parameters are then calculated accordingly. The disadvantage of not directly knowing the time coefficient Θ_{VDT} is outweighed by the advantage of having a direct and controlled input coefficient, avoiding thus the uncertainties of the sometimes very complex separate-phase theory. There exist different possibilities to determine indirectly this coefficient, either from similar theoretical considerations as performed to establish the exchange terms, from experience or from adequate parameter studies.

2.2.4 Heat transfer coefficients

As input to the energy balance eq.(2) the linear power value q_L (or the corresponding heat flux q_F along the perimeter U_{TW}) are demanded. They describe the heat transferred into or out of the coolant channel), i.e. from a heated or cooled surface (for example from or into a U-tube wall or out of the canning of a fuel rod). These terms (but also the local surface temperature T_{TW} of the channel wall) can be determined by solving an adequate Fourier heat conduction equation with its boundary condition

$$q_F = \alpha_{TW} (T_{TW} - T) = \frac{q_L}{U} = \frac{A}{U} q \tag{24}$$

This is, for example, demonstrated for the case of heat conduction through a U-tube wall in (Hoeld, 2002b, 2011).

Hence, a method how to get the necessary heat transfer coefficients α_{TW} at different flow regimes within a coolant channel had to be established. In connection with the development of the UTSG code (and thus also of CCM) an own very comprehensive heat transfer coefficient package, called HETRAC (Hoeld 1988a), has been established. It combines, for example, especially for this purpose chosen HTC correlations for each possible flow situation within LWR-s and steam generators (i.e., into or out of heated or cooled tube walls or fuel elements) in a very effective way. Thereby adequate correlations for the cases of sub-cooled water, sub-cooled and nucleate boiling, onset of critical heat flux, transient or instable film boiling, stable film boiling, onset of superheating and superheated steam for different geometry constellations and over a wide range of input parameters (pressures, total and steam mass flows, coolant temperatures, wall temperatures or heat fluxes etc.) had to be selected. The package describes not only heat transfer from wall to the different phases but also between these phases.

This classic method is different to the 'separate-phase' models where it must be assumed that the heat is transferred both directly from the wall to each of the two possible phases but also exchanged between them. There arises then the question how the corresponding heat transfer coefficients for each phase should look like.

3. Coolant channel module CCM

3.1 Channel geometry and finite-difference nodalization

The theoretical considerations take advantage of the fact that, as sketched in fig.1, a 'basic' coolant channel (BC) can, according to their flow regimes (characterized by the logical L_{FTYPE}

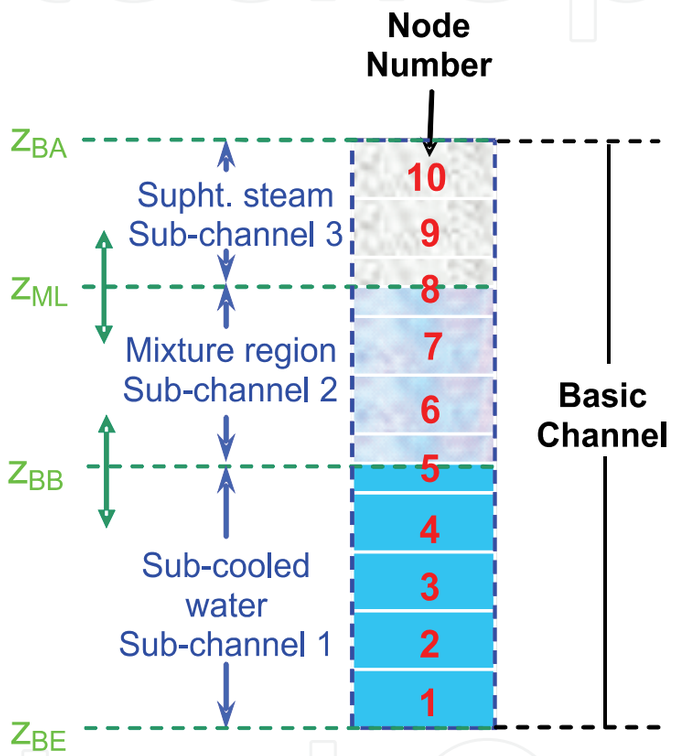

Fig. 1. Subdivision of a 'basic channel' into 'sub-channels' according to their flow regimes.

Discretization of BC and SC-s

= 0, 1 or 2), be subdivided into a number (N_{SCT}) of sub-channels (SC-s,), with the consequence of having variable entrance and outlet positions.

The BC with its total length $z_{BT} = z_{BA}-z_{BE}$ can then, for discretization purposes, be subdivided into a number of (not necessarily equidistant) N_{BT} nodes. Their nodal positions are z_{BE}, z_{Bk} (with k=1,N_{BT}), the elevation heights z_{ELBE}, z_{ELk}, the nodal length $\Delta z_{Bk}=z_{Bk}-z_{Bk-1}$, nodal elevations $\Delta z_{ELBk}=z_{ELBk}-z_{ELBk-1}$, locally varying cross flow and average areas A_{Bk} and $A_{BMk}=0.5(A_{Bk}+A_{Bk-1})$ with the slopes $A_{z_{Bk}} = (A_{Bk}-A_{Bk-1})/\Delta z_{Bk}$ and corresponding nodal volumes $V_{BMk} = \Delta z_{Bk}A_{BMk}$. All of them can be assumed to be known from input.

As a consequence, each of the sub-channels (SC-s) is then subdivided too, now into a number of N_{CT} SC nodes with geometry data being identical to the corresponding BC values, except, of course, at their entrance and outlet positions. The SC entrance position z_{CE}

and their function f_{CE} are either identical with the BC entrance values z_{BE} and f_{BE} or equal to the outlet values of the SC before. The SC outlet position (z_{CA}) is either limited by the BC outlet (z_{BA}) or characterized by the fact that the corresponding outlet function has reached an upper or lower limit (f_{LIMCA}), with the term representing either a function at the boiling boundary or a mixture level. Such a function follows from the given BC limit values and will, in the case of single-phase flow, be equal to the saturation temperature T_{SATCA} or saturation enthalpies ($h^{/}$ or $h^{//}$ if L_{FTYPE}=1 or 2), in the case of two-phase flow (L_{FTYPE}=0) equal to a void fraction of α = 1 or = 0. The moving SC inlet and outlet positions z_{CE} and z_{CA} can (together with their corresponding BC nodes N_{BCE} and N_{BCA} = N_{BCE}+N_{CT}) be determined according to the conditions ($z_{BNk-1} \leq z_{CE} < z_{BNk}$ at k = N_{BCE}) and ($z_{BNk-1} \leq z_{CA} < z_{BNk}$ at k = N_{BCA}). Then also the total number of SC nodes (N_{CT}=N_{BCA}-N_{BCE}) is given, the connection between n and k (n=k-N_{BCE} with n=1, N_{CT}), the corresponding positions (z_{Nn}, z_{ELCE}, z_{ELNn}), their lengths (Δz_{Nn}=z_{Nn}-z_{Nn-1}), elevations (Δz_{ELNn}=z_{ELNn}-z_{ELNn-1}), and volumes (V_{Mn}=$z_{Nn}A_{Mn}$) and nodal boundary and mean nodal flow areas (A_{Nn}, A_{Mn}) with

$$A_{Nn} = A_{Nn-1} + A^{z}_{Bk} \frac{\Delta z_{Nn}}{\Delta z_{Bk}}$$

$$A_{Mn} = 0.5(A_{Nn}+A_{Nn-1}) = A_{Nn-1} + 0.5\, A^{z}_{Bk} \frac{\Delta z_{Nn}}{\Delta z_{Bk}} \qquad (n=1,N_{CT},\ k=n+N_{BCE}) \qquad (25)$$

Hence, also their time-derivatives and that of the nodal volumes can be ascertained from the relations above.

3.2 Spatial discretization of PDE-s of 1-st order (Modified finite element method)

Based on this nodalization the spatial discretization of the fundamental eqs.(1) to (3) can be performed by means of a 'modified finite element method'. This means that if a partial differential equation (PDE) of 1-st order having the general form with respect to a general solution function f(z,t)

$$\frac{\partial}{\partial t} f(z,t) + \frac{\partial}{\partial z} H[f(z,t)] = R[f(z,t)] \qquad (26)$$

is integrated over the length of a SC node three types of discretization elements can be expected:

- Integrating a function f(z,t) over a SC node n yields the nodal mean function values f_{Mn}

$$\int_{z_{Nn-1}(t)}^{z_{Nn}(t)} R[f(z,t)\}dz = \Delta z_{Nn}(t)\, R[f_{Mn}\, t)] \qquad (n=1,\ N_{CT}) \quad (27)$$

- integrating over the gradient of the function yields to a difference of functions values at their node boundaries

$$\int_{z_{Nn-1}(t)}^{z_{Nn}(t)} \frac{\partial}{\partial z} H[f(z,t)]dz = H[f_{Nn}(t)] - H[f_{Nn-1}(t)] \qquad (n=1,\ N_{CT}) \qquad (28)$$

- and finally the integration over a time-derivative of a function (by applying the 'Leibniz' rule)

$$\int_{z_{Nn-1}(t)}^{z_{Nn}(t)} \frac{\partial}{\partial t} f(z,t)dz = \Delta z_{Nn}(t) \frac{d}{dt} f_{Mn}(t) - [f_{Nn}(t) - f_{Mn}(t)] \frac{d}{dt} z_{Nn}(t)$$

$$- [f_{Mn}(t) - f_{Nn-1}(t)] \frac{d}{dt} z_{Nn-1}(t) \qquad (n=1, N_{CT}) \quad (29)$$

This last rule plays in the case of the here presented 'separate-region' mixture-fluid approach an outstanding part, allowing determining the movement of SC boundaries within a BC in a direct way, i.e., yielding time-derivatives of parameters which represent either a boiling boundary or a mixture level. This procedure differs considerably from some of the 'separate-phase methods' where, as already pointed out, very often only the collapsed levels of a mixture fluid can be calculated.

3.3 Quadratic polygon approximation procedure PAX

Looking at the above described three different types of possible discretization elements it is obvious that appropriate methods had to be developed which can help to establish relations between such mean nodal (f_{Mn}) and node boundary (f_{Nn}) function values after a discretization procedure.

In the 'separate-phase' models mostly a method is applied (called 'upwind or donor cell differencing scheme') where the mean parameter values are shifted (in flow direction) to the node boundaries.

This is not possible for the mixture-fluid approach of CCM. There, as can be seen from the relations of the sections 3.7 to 3.9, not only the absolute nodal SC boundary or mean function values are demanded but as well also their nodal slopes and thus, if the length of the SC nodes tends to zero, gradients. For this purpose a special 'quadratic **p**olygon **a**prox**x**imation' procedure, named 'PAX', had to be developed. It plays an outstanding part in the development of 'mixture-fluid models'. In particular, the difficult task of how to take care of the varying SC boundaries (eventually crossing BC node boundaries) in an appropriate and exact way had to be solved.

3.3.1 Establishment of an adequate approximation function

The PAX procedure is based on the assumption that the solution function f(z) of a PDE is split into a number of N_{CT} nodal SC functions $f_n(z,t)$. Each of them being approximated by a specially constructed quadratic polygon

$$f_{Nn} = f_{Nn-1} + a_{Nn}\Delta z_{Nn} + b_{Nn}\Delta z_{Nn}^2 \qquad (n=1,N_{CT}) \quad (30)$$

Their nodal mean functions f_{Mn} (for all SC nodes) will thus have the form

$$f_{Mn} = \frac{1}{\Delta z_{Nn}(t)} \int_{z_{Nn-1}(t)}^{z_{Nn}(t)} f(z,t)dz = f_{Nn-1} + \frac{1}{2} a_{Nn}\Delta z_{Nn} + \frac{1}{3} b_{Nn}\Delta z_{Nn}^2 \qquad (n=1,N_{CT}) \quad (31)$$

the corresponding nodal slopes of either the mean nodal or the nodal boundary functions

$$f_{Nn}^{(s)} = \frac{(f_{Nn} - f_{Nn-1})}{\Delta z_{Nn}} = a_{Nn} + b_{Nn}\Delta z_{Nn}$$

$$\rightarrow f_{CEI}^{(z)} \text{ (at n=1)} \quad \text{or} \quad \rightarrow f_{Nn-1}^{(z)} \text{ (at n=}N_{CT}>1) \quad \text{if } \Delta z_{Nn} \rightarrow 0 \qquad (32)$$

$$f^{(s)}_{Mn} = 2\,\frac{(f_{Mn} - f_{Nn-1})}{\Delta z_{Nn}} = a_{Nn} + \frac{2}{3} b_{Nn}\Delta z_{Nn}$$

$$\rightarrow f^{(z)}_{CEI} \text{ (at n=1)} \quad \text{or} \quad \rightarrow f^{(z)}_{Nn-1} \text{ (at n=} N_{CT}\text{>1)} \quad \text{if } \Delta z_{Nn} \rightarrow 0 \tag{33}$$

and, finally, their nodal gradients (needed for the case that during a transient the length of a node tends to zero)

$$f^{(z)}_{Nn} = \left(\frac{\partial f}{\partial z}\right)_{Nn} = a_{Nn} + 2\, b_{Nn}\Delta z_{Nn} = 4\, f^{(s)}_{Nn} - 3\, f^{(s)}_{Mn} = \frac{2}{\Delta z_{Nn}}(2f_{Nn} - 3\, f_{Mn} + f_{Nn-1}) \quad (n=1, N_{CT}) \tag{34}$$

Thereby the approximation functions have to fulfil the following requirements:

- The node entrance functions (f_{Nn-1}) must be either equal to the SC entrance function ($f_{Nn-1} = f_{CE}$) (if n=1) or to the node outlet function of the node before (if n > 1). This is obviously not demanded for the gradients of the nodal entrance functions (except for the last node at n = N_{CT}).

$$f^{(z)}_{Nn-1} = a_{Nn} = \quad \text{either} = f^{(z)}_{CE} = f^{(z)}_{CEI} \quad \text{or} = f^{(z)}_{Nn} \quad \text{(of the node before)}$$

$$(n = N_{CT} \text{ if } N_{CT}=1 \text{ or} > 1)$$

$$= \frac{1}{2}(3\, f^{(s)}_{Mn} - f^{(z)}_{Nn}) = \frac{2}{\Delta z_{Nn}}(3f_{Mn} - f_{Nn} - 2f_{Nn-1}) \rightarrow f^{(s)}_{Mn} = f^{(s)}_{Mn-1} \text{ if } \Delta z_{Nn} \rightarrow 0 \tag{35}$$

$$(n=1, N_{CT}-1 \text{ if } N_{CT}>1)$$

- The mean function values f_{Mn} over all SC nodes have to be preserved (otherwise the balance equations could be hurt).
- With the objective to guarantee stable behaviours of the approximated functions (for example by excluding 'saw tooth-like' behaviour) it will, in an additional assumption, be demanded that the outlet gradients of the first N_{CT} -1 nodes should be set equal to the slopes between their neighbour mean function values. The entrance gradient of the last node (n= N_{CT}) should be either equal to the outlet gradient of the node before (if n = N_{CT} > 1) or equal to a given SC input gradient (for the special case n = N_{CT} =1). Thus

$$f^{(z)}_{Nn} = 2\,\frac{f_{Mn+1} - f_{Mn}}{\Delta z_{Nn+1} + \Delta z_{Nn}} \qquad (n=1, N_{CT}-1, \text{ if } N_{CT}>1) \tag{36}$$

$$f^{(z)}_{Nn-1} = f^{(z)}_{CE} = f^{(z)}_{CEI} \qquad (n = N_{CT} = 1)$$

$$= \frac{2}{\Delta z_{Nn}}(2f_{Nn} - 3f_{Mn} + f_{Nn-1}) \rightarrow f^{(z)}_{Nn-1} \text{ if } \Delta z_{CA} \rightarrow 0 \quad (n = N_{CT}, \text{ if } N_{CT} > 1) \tag{37}$$

This means, the corresponding approximation function reaches not only over the node n but its next higher one (n+1) has to be considered too (except, of course, for the last node). This assumption makes the PAX procedure very effective (and stable). It helps to smooth the curve, guarantees that the gradients at the upper or lower SC boundary do not show abrupt changes if these boundaries cross a BC node boundary and has the effect that perturbations at channel entrance do not directly affect corresponding parameters of the upper BC nodes.

For the special case of a SC having shrunk to a single node ($n=N_{CT}=1$) the quadratic approximation demands (instead of the now not available term f_{Mn}) as an additional input to PAX the gradient $f^{(z)}_{CEI}$ at SC entrance. It represents thereby the gradient of either the coolant temperature $T^{(z)}_{CEI}$ or void fraction $\alpha^{(z)}_{CEI}$ (in case of single- or two-phase flow entrance conditions). If this parameter is not directly available it can, for example, be estimated by combining the mass and energy balance equations at SC entrance in an adequate way (See Hoeld, 2005). This procedure allows to take care not only of SC-s consisting of only one single node but also of situations where during a transient either the first or last SC of a BC starts to disappear or to be created anew (i.e. $z_{CA} \rightarrow z_{BE}$ or $z_{CE} \rightarrow z_{BA}$), since now the nodal mean value f_{Mn} at $n = N_{CT}$ (for both $N_{CT} = 1$ or > 1) is no longer or not yet known.

3.3.2 Resulting nodal parameters due to PAX

In order to be able to determine the nodal approximation coefficients f_{Nn-1}, a_{Nn} and b_{Nn} of eq.(30) (and, in turn, then also all other characteristic functions of the PAX procedure), it must, in dependence of the available input data, be distinguished between a steady and a transient case.

The **steady state** part of the basic equations consists of a set of non-linear algebraic equations (as presented later-on in the sections 3.7 and 3.8). It can be expected that as input to PAX the following data are available:

- SC entrance (z_{CE}) and node positions (z_{Nn}) (and thus also the SC outlet boundary position z_{CA} as explained in section 3.9) determining then in PAX the number of SC nodes (N_{CT}),
- the nodal function limit values f_{LIMNn} (usually saturation temperature values at single-phase flow resp. f_{LIMNn} =1 or =0 at mixture flow conditions),
- the SC entrance function $f_{N0} = f_{CE}$ and (at least for the special case $n=N_{CT}=1$) its gradient $f^{(z)}_{CEI}$

and

- the nodal boundary functions f_{Nn} ($n=1,N_{CT}$) with $f_{CA} = f_{Nn}$ at $n = N_{CT}$ and $f_{CA}= f_{LIMCA}$ if $z_{CA} < z_{BA}$.

These inputs act within the PAX procedure as basic points of the polygon approximation curves, yielding then the nodal mean function values f_{Mn} (at $n=1,N_{CT}$) which are needed as initial values for the transient case. Hence, after rearranging eqs. (30) and (31) it follows (including the special case of $N_{CT} = 1$)

$$f_{Mn} = \frac{(\Delta z_{Nn+1} + \Delta z_{Nn})(2f_{Nn} + f_{Nn-1}) - \Delta z_{Nn} f_{Mn+1}}{3\Delta z_{Nn+1} + 2\Delta z_{Nn}}$$

($n = 1, N_{CT}-1, N_{CT} > 1$ if $z_{CA} = z_{BA}$ or $n = 1, N_{CT}-2, N_{CT} > 2$ if $z_{CA} < z_{BA}$)

$$= \frac{1}{3}(f_{CA} + 2 f_{CE}) + \frac{1}{6}\Delta z_{CA} f^{(z)}_{CEI} \qquad (n = N_{CT} = 1)$$

$$= \frac{1}{3}(f_{CA} + 2f_{Nn-1}) + \frac{1}{6}\frac{\Delta z_{Nn-1}}{\Delta z_{CA} + \Delta z_{Nn-1}}(f_{CA} - f_{Nn-2}) \qquad (n = N_{CT} > 1) \quad (38)$$

In the **transient case** the discretization of the PDE-s yields (for each SC) a set of N_{CT} ordinary differential equations (ODE-s) (as to be shown again in the sections 3.7, 3.8 and 3.9).

From their integration it follow then

- the SC outlet position $z_{CA}(=z_{Nn})$ < or =z_{BA} (at n=N_{CT}) and thus also the total number N_{CT} of SC nodes

and either

- if $z_{CA}=z_{BA}$ (i.e. if the now known SC outlet position is identical with the BC outlet) the mean nodal function values f_{Mn} for all N_{CT} nodes (n=1,N_{CT})

or

- if $z_{CA} < z_{BA}$ (i.e., if this SC outlet position moves within the BC) the mean nodal function values f_{Mn} of only N_{CT}-1 nodes (n=1, N_{CT}-1), but now, instead of the missing last SC mean node function f_{Mn}, knowing that the outlet function f_{Nn} must be equal to f_{CA} = f_{LIMCA} at z_{Nn} = z_{CA}.

Knowing now N_{CT} these nodal input function values can then be taken (together with its input parameter f_{CE} and the nodal positions z_{BE} and z_{Bn} at n=1, N_{CT}) as basic points for the PAX procedure yielding, after rearranging the eqs.(30) to (34) in an adequate way, the other characteristic nodal function parameters of the SC.

Hence, it follows for the special situation of a SC being the last one within the BC (i.e., if z_{CA} = z_{BA})

$$f_{Nn} = \frac{1}{2}(3f_{Mn} - f_{Nn-1}) + \frac{1}{2}\frac{\Delta z_{Nn}}{\Delta z_{Nn+1}+\Delta z_{Nn}}(f_{Mn+1} - f_{Mn}) \quad (n=1, N_{CT}-1 \text{ with } N_{CT}>1 \text{ if } z_{CA}=z_{BA})$$

$$= 3f_{Mn} - 2f_{CE} - \frac{1}{2}\Delta z_{CA} f^{(z)}_{CEI} \quad (n = N_{CT} = 1 \quad \text{if } z_{CA}=z_{BA})$$

$$= f_{CA} = 2(f_{Mn} - f_{Mn-1}) + f_{Nn-2} \quad (n = N_{CT} > 1 \quad \text{if } z_{CA}=z_{BA}) \quad (39)$$

resp. for the case $z_{CA} < z_{BA}$

$$f_{Nn} = \frac{1}{2}(3f_{Mn} - f_{Nn-1}) + \frac{1}{2}\frac{\Delta z_{Nn}}{\Delta z_{Nn+1}+\Delta z_{Nn}}(f_{Mn+1} - f_{Mn}) \quad (n=1, N_{CT}-2 \text{ with } N_{CT}>2 \text{ if } z_{CA}<z_{BA})$$

$$= \frac{1}{2}(3f_{Mn} - f_{Nn-1}) + \frac{1}{4}\frac{\Delta z_{Nn}}{\Delta z_{Nn+1}+\Delta z_{Nn}}(f_{LIMCA} - f_{Nn-1}) \quad (n=N_{CT}-1 \text{ with } N_{CT}>1 \text{ if } z_{CA}<z_{BA})$$

$$= f_{CA} = f_{LIMCA} \quad (n = N_{CT} \quad \text{if } z_{CA}<z_{BA}) \quad (40)$$

The last mean nodal function value f_{Mn} (at n=N_{CT}) is for the case $z_{CA} < z_{BA}$ not yet determined (but needed). It follows if rearranging eq.(44) and replacing there f_{CA} by f_{LIMCA}

$$f_{Mn} = \frac{1}{3}(f_{LIMCA} + 2f_{CE}) + \frac{1}{6}\Delta z_{CA} f^{(z)}_{CEI} \quad (n = N_{CT} = 1 \text{ if } z_{CA}<z_{BA})$$

$$= f_{Mn-1} + \frac{1}{2}(f_{LIMCA} - f_{Nn-2}) = \frac{1}{3}(f_{LIMCA} + 2f_{Nn-1}) + \frac{1}{6}\frac{\Delta z_{Nn-1}}{\Delta z_{CA}+\Delta z_{Nn-1}}(f_{LIMCA} - f_{Nn-2}) \quad (41)$$

$$(n=N_{CT}>1 \text{ if } z_{CA}<z_{BA})$$

The corresponding time-derivative which is needed for the determination of the SC boundary time-derivative (see section 3.9) follows (for the case $z_{CA} < z_{BA}$) by differentiating the relation above

$$\frac{d}{dt} f_{Mn} = f^{t}_{PXCA} + f^{z}_{PXCA}\frac{d}{dt} z_{CA} \quad (n=N_{CT} \text{ if } z_{CA}<z_{BA}) \quad (42)$$

yielding the coefficients

$$f^{t}_{PXCA} = \frac{1}{3}\left(\frac{d}{dt} f_{LIMCA} + 2\frac{d}{dt} f_{CE}\right) - \frac{1}{6}\left(f^{(z)}_{CEI}\ \frac{d}{dt} z_{CE} - \Delta z_{CA}\ \frac{d}{dt} f^{(z)}_{CEI}\right) \quad (n = N_{CT} = 1 \text{ if } z_{CA}\ z_{BA})$$

$$= \frac{d}{dt} f_{Mn-1} + \frac{1}{2}\frac{d}{dt} f_{LIMCA} - \frac{1}{2}\frac{d}{dt} f_{Nn-2} \quad (n = N_{CT} > 1 \text{ if } z_{CA} < z_{BA})$$

$$f^{z}_{PXCA} = \frac{1}{6} f^{(z)}_{CEI} \text{ or } = 0 \quad (n = N_{CT} = 1 \text{ or } > 1 \text{ if } z_{CA} < z_{BA}) \tag{43}$$

The differentials $\frac{d}{dt} f_{Mn-1}$, $\frac{d}{dt} z_{CA}$, $\frac{d}{dt} f_{LIMCA}$ are directly available from CCM and, if N_{CT}=2, the term $\frac{d}{dt} f_{Nn-2} = \frac{d}{dt} f_{CE}$ from input. For the case that a SC contains more than two nodes only their corresponding mean values are known, the needed term $\frac{d}{dt} f_{Nn-2}$ has thus to be estimated by establishing the time-derivatives of all the boundary functions at the nodes below $N_{CT} < 2$. These can be derived in an iterative way by differentiating eq.(40)

$$\frac{d}{dt} f_{Nn} = \frac{d}{dt} f_{CE} \quad (n = 0)$$

$$= \frac{d}{dt} f_{CA} = \frac{d}{dt} f_{LIMCA} \quad (n = N_{CT} \text{ if } z_{CA} < z_{BA})$$

$$= \frac{d}{dt} f_{CA} = 2\left(\frac{d}{dt} f_{Mn} - \frac{d}{dt} f_{Mn-1}\right) + \frac{d}{dt} f_{Nn-2} \quad (n = N_{CT} > 1 \text{ if } z_{CA} = z_{BA})$$

$$= \frac{d}{dt} f_{Mn} + \frac{1}{2}\left(\frac{d}{dt} f_{Mn+1} - \frac{d}{dt} f_{Nn-1}\right)$$

$$+ \frac{1}{2}\frac{\Delta z_{Nn+1}}{\Delta z_{Nn+1} + \Delta z_{Nn}}\left[\frac{d}{dt} f_{Mn} - \frac{d}{dt} f_{Mn+1} - \frac{f_{Mn+1} - f_{Mn}}{\Delta z_{Nn+1} + \Delta z_{Nn}}\ \frac{d}{dt} z_{Nn-1}\right] \tag{44}$$

$$(n=1, N_{CT}\text{-}2 \text{ and } N_{CT} > 2 \text{ if } z_{CA} < z_{BA}) \text{ or } (n=1, N_{CT}\text{-}1 \text{ and } N_{CT} > 1 \text{ if } z_{CA} = z_{BA})$$

with

$$\frac{d}{dt} f_{Nn-1} = \frac{3}{2}\frac{d}{dt} f_{Mn-1} - \frac{1}{2}\frac{d}{dt} f_{Nn-2} + \frac{1}{4}\frac{\Delta z_{Nn-1}}{\Delta z_{CA} + \Delta z_{Nn-1}}\left[\frac{d}{dt} f_{LIMCA} - \frac{d}{dt} f_{Nn-2} - \frac{f_{LIMCA} - f_{Nn-2}}{\Delta z_{CA} + \Delta z_{Nn-1}} \Delta z_{CA}\right] \tag{45}$$

$$(n = N_{CT} > 1 \text{ if } z_{CA} < z_{BA})$$

This term follows after differentiating eq.(44). It plays an important role for the propagation of perturbations below the last node.

The differentials $\frac{d}{dt} f_{Mn}$ (at $n = N_{CT}$ if $z_{CA} = z_{BA}$) or $\frac{d}{dt} z_{CA}$ (at $n = N_{CT}$ if $z_{CA} < z_{BA}$) can only be established if they are combined with corresponding expressions being derived within the mixture-fluid model (See chapters 3.7 and 3.8). They will then be added to the overall set of ODE-s.

Finally, with regard to the eqs.(32) and (33) the slopes, gradients and approximation coefficients can be determined.

3.3.3 Code package PAX

Based on the above established set of equations the subroutine PAX could be installed. It is derived with respect to the (automatic) calculation of the nodal mean or nodal boundary values (for a steady state or transient situation). It allows also determining the gradients and slopes at SC entrance and outlet (and thus also outlet values characterizing the entrance parameters of an eventually subsequent SC). Additionally, contributions needed for the determination of the time-derivatives of the boiling boundary or mixture level can be gained (See later-on the eqs.(87) and (88)).

Before incorporating the subroutine into the overall coolant channel module the validity of the presented PAX procedure has been thoroughly tested. With the help of a special driver code (PAXDRI) different characteristic and extreme cases have been calculated.

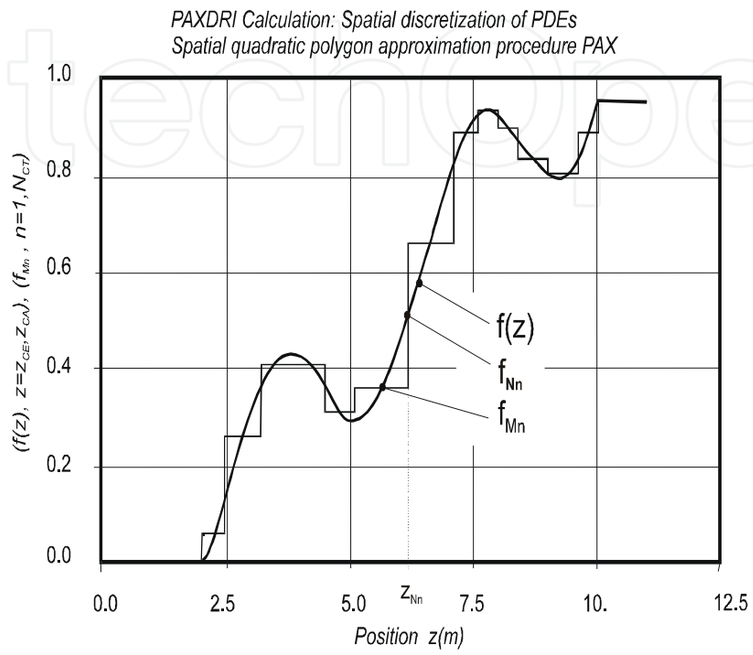

Fig. 2. Approximation function f(z) along a SC for both steady state and transient conditions after applying PAX (Example)

The resulting curves of such a characteristic example are plotted in fig.2. It presents an approximation curve of an artificially constructed void fraction distribution $f(z) = \alpha(z)$ along a SC with two-phase flow both in a steady state but also transient situation. Both curves (on the basis of f_{Mn} and f_{Nn}) should be (and are) identical.

3.4 Needed input parameters

3.4.1 Initial conditions

For the start of the transient calculations corresponding steady state parameters will be taken as initial conditions.

3.4.2 Boundary conditions

For steady state and especially for transient calculations the following input parameters are expected to be known (as boundary conditions), all of them being restricted to only (easily available) BC values (They will then, within CCM, be automatically translated into the corresponding SC values):

- Power profile along the entire BC. This means that the nodal heat flux terms q_{FBE} and q_{FBk} (at BC entrance and each node k=1,N_{BT}) are wanted, known either directly from input, calculated from corresponding power density input values q_{BE} and q_{Bk} or from

q_{BE} and the nodal power terms $Q_{Bk} = 0.5*(q_{Bk}+q_{Bk-1})\Delta z_{Bk}$. These values can be also achieved (on the basis of given nodal wall temperature values) by solving the appropriate 'Fourier heat conduction eq.' taking into account the heat transfer boundary condition of eq.(24) (see sections 2.2.4 and 3.5). This can, for example, be done by applying an own heat conduction module as demonstrated by (Hoeld, 2002b, 2004a and 2011).

- For normalization purposes at steady state conditions then, as an additional parameter, the total nominal (steady state) heat power $Q_{NOM,0}$ is asked.
- Channel entrance temperature T_{BEIN} (or enthalpy h_{BEIN})
- System pressure P_{SYS} and its time-derivative (dP_{SYS}/dt), situated at a fixed position either along the BC (entrance, outlet) or even outside of the ensemble. Due to the fast pressure wave propagation the local pressure time-derivatives can then be set equal to the change in system pressure (as described in section 3.6).
- Total mass flow G_{BEIN} at BC entrance together with pressure terms at BC entrance P_{BEIN} and outlet P_{BAIN}. These three parameters are needed for steady state considerations (partially used for normalization purposes). In the transient case only two of them are demanded as input, the third one will be determined automatically by the model. These allows then to distinguish between the situation of an 'open' or 'closed channel' concept as this will be explained in more detail in section 3.11.
- Steam mass flow G_{SBEIN} at BC entrance (=0 or = G_{BEIN} at single- or $0 < G_{SBEIN} < G_{BEIN}$ at two-phase flow conditions). The corresponding entrance void fraction α_{BE} will then be determined automatically within the code by applying the inverse drift-flux correlation (see eq.(21)).

Eventually needed time-derivatives of such entrance functions can either be expected to be known directly from input or be estimated from their absolute values.

By choosing adequate boundary conditions then also thermal-hydraulic conditions of other situations can be simulated, such as, for example, that of several channel assembles (nuclear power plants, test loops etc.) which can consist of a complex web of pipes and branches (represented by different BC-s, all of them distinguished by their key numbers KEYBC). Even if the ensemble consists of inner loops (for example in case of parallel channels) the case can be treated in an adequate way according to the concept of a 'closed' channel (see section 3.6.2).

3.4.3 Solution vector resulting from the integration procedure

The characteristic steady state parameters are determined in a direct way, i.e. calculated according to the non-linear set of equations for the SC-s (being presented in the chapters 3.7, 3.8 and 3.9), combined to BC parameters and then send again back to the main (= calling) program. However, since the constitutive equations demand parameters (coolant temperatures, void fractions, pressures, etc.) which are the result of these calculations a recursive procedure in combination with and controlled by the main program has to be applied until a certain convergence in these parameters can be stated.

For the transient case, as a result of the integration (performed within the calling program and thus outside of CCM) the solution parameters of the set of ODE-s are transferred after each intermediate time step to CCM. These are (as described in detail also in chapter 4) mainly the mean nodal SC and thus BC coolant temperatures, mean nodal void fractions and the resulting boiling or superheating boundaries. These last two parameters allow then to subdivide the BC into SC-s yielding the corresponding constitutive parameters and the total and nodal length (z_{Nn} and Δz_{Nn}) of these SC-s and thus also their total number (N_{CT}) of

SC nodes. The needed SC (and thus BC) time-derivatives are then determined in CCM (as described in the sections 3.7, 3.8 and 3.9) and then transmitted again to the calling program where the integration for the next time step takes place.

3.5 BC (and thus also SC) power profile

The power terms (Q_{Bk}) into or out of a BC node k (with corresponding positive or negative signs) can, together with a linear power term or power density term at BC entrance, be expected to be either known from input (e.g., in the case of a heated loop) or from the solution of a Fourier heat conduction equation (in connection with the energy balance equation). From this BC power profile obeying to the relation

$$\begin{aligned} Q_{Bk} &= \frac{1}{2}\Delta z_{Bk}(q_{LBk}+q_{LBk-1}) = \frac{1}{2}\Delta z_{Bk}(U_{Bk}q_{FBk}+U_{Bk-1}q_{FBk-1}) \\ &= \frac{1}{2}\Delta z_{Bk}\,(A_{Bk}q_{Bk}+A_{Bk-1}q_{Bk-1}) \text{ and thus } q_{LB} = \frac{2Q_{Bk}}{\Delta z_{Bk}} - q_{LBk-1} \qquad (k=1,N_{BT}) \end{aligned} \tag{46}$$

the corresponding SC nodal terms (q_{LNn}, Q_{Mn} and q_{Nn}) can be determined. They are usually equal to the corresponding BC terms, except for the SC entrance (if $z_{CE} > z_{BE}$) or outlet (if $z_{CA} < z_{BA}$). Hence, if assuming linear behaviour of the linear nodal power terms within the corresponding BC nodes it follows for the 'linear SC power' term

$$\begin{aligned} q_{LNn}\,(=q_{LCE}) &= q_{LBE}\,(=\text{input}) \text{ or } = (q_{LCA})_{\text{of the last node of the SC before}} \quad (n=0 \text{ if } z_{CE} = \text{or} > z_{BE}) \\ &= q_{LBk} \qquad (n=1,N_{CT} \text{ and } k=n+N_{BCE} \text{ if } L_{FTYPE}=2) \\ &= q_{LBk} \qquad (n=1,\, N_{CT-1} \text{ and, if } z_{CA} = z_{BA},\, n= N_{CT} \text{ with } k=n+N_{BCE}) \\ &= q_{LBk-1} + (q_{LBk} - q_{LBk-1})\,\frac{\Delta z_{CA}}{\Delta z_{Bk}} \qquad (n=N_{CT} \text{ and } k=N_{BCA} \text{ if } z_{CA} < z_{BA}) \end{aligned} \tag{47}$$

for the 'total power term' into the node n

$$\begin{aligned} Q_{Mn} &= Q_{Bk} \text{ or } = Q_{Bk} - (Q_{MCA})_{\text{of last node of the SC before}} \quad (n=1 \text{ with } k=1+N_{BCE} \text{ if } z_{CE} = \text{or} > z_{BE}) \\ &= Q_{Bk} \qquad (n=1,\, N_{CT} \text{ and } k=n+N_{BCE} \text{ if } L_{FTYPE}=2) \\ &= \frac{1}{2}\Delta z_{Nn}(q_{LNn}+q_{LNn-1}) = Q_{Bk} \quad (n=2,N_{CT-1} \text{ and, if } z_{CA} = z_{BA},\, n= N_{CT} \text{ with } k=n+N_{BCE}) \\ &= Q_{MCA} = \Delta z_{CA}\,[q_{LBk-1} + \frac{1}{2}\,(q_{LBk} - q_{LBk-1})\,\frac{\Delta z_{CA}}{\Delta z_{Bk}}\,] \quad (n=N_{CT} \text{ and } k=N_{BCA} \text{ if } z_{CA} < z_{BA}) \end{aligned} \tag{48}$$

and finally for the 'mean nodal' and 'nodal boundary power density' terms (q_{Mn} and q_{Nn}), being independent of Δz_{Nn} and thus also valid for the case $\Delta z_{Nn} \to 0$ (as demanded later-on by the eqs.(52) and (69))

$$\begin{aligned} q_{Mn} &= \frac{Q_{Mn}}{\Delta z_{Nn}} = \frac{1}{2A_{Mn}}\,(q_{LNn-1}+q_{LNn}) \qquad (n=1,N_{CT}) \\ q_{Nn} &= q_{CE} = q_{BE} \text{ or } = (q_{CA})_{\text{of the last node of the SC before}} \qquad (n=0 \text{ if } z_{CE} = \text{or} > z_{BE}) \\ &= 2q_{Mn} - q_{Nn-1} \qquad (n=1,N_{CT}) \end{aligned} \tag{49}$$

The SC length z_{CA} (and thus the length of its last node Δz_{CA}) are (for the case $z_{CA,0} < z_{BA}$) only in the transient case known (as a result of the integration procedure). For steady state conditions the term $Q_{MCA,0}$ follows from energy balance considerations (eqs.(61) and (80)). Then, in a reverse manner, $\Delta z_{CA,,0}$ can be calculated from eq.(86) (See section 3.10).
In special (and very seldom) situations the assumption of linearity within such a BC node may not any longer be suited. This is, for example, the case if a very steep increase or decrease in heat transfer within a BC can be expected (for example at the onset of sub-cooled boiling or at dry-out conditions of the two-phase mixture). Corresponding corrections have then to be foreseen, for example, by a denser nodalization, i.e. further subdividing the corresponding CCM node length into more 'HTC' nodes.

3.6 Decoupling of mass and energy balance from momentum balance equations

Treating the conservation equations in a direct way produces due to elements with fast pressure wave propagation (and thus being responsible for very small time constants) a set of 'stiff' ODE-s with the consequence that their solution turns out to be enormously CPU-time consuming. To avoid this costly procedure the CCM has been developed with the aim to decouple the mass and energy from their momentum balance equations. This can be achieved by determining the thermodynamic properties of water and steam in the energy and mass balance equations on the basis of an estimated pressure profile P(z,t). Thereby the pressure difference terms from a recursive (or a prior computational time step) will be added to an eventually time-varying system pressure $P_{SYS}(t)$, known from boundary conditions. After having solved the two conservation equations for mass and energy (now separately from and not simultaneously with the momentum balance) the different nodal pressure gradient terms can (by the then following momentum balance considerations) be determined according to the eqs.(4), (5) and (6).
For the time-derivatives it can additionally be assumed that according to the fast (acoustical) pressure wave propagation along a coolant channel all the local pressure time-derivatives can be set equal to a given external system pressure time-derivative, i.e.,

$$\frac{d}{dt} P(z,t) \cong \frac{d}{dt} P_{SYS} \tag{50}$$

By applying the above explained 'intelligent' (since physically justified) simplification in CCM the small, practically negligible, error in establishing the thermodynamic properties on the basis of such an estimated pressure profile can be outweighed by the enormous benefit substantiated by two facts:

- The very time-consuming solution of stiff equations can be avoided,
- the calculation of the mass flow distribution into different channels resulting from pressure balance considerations can, in a recursive way, be adapted already within each integration time step, i.e. there is no need to solve the entire set of differential equations for this purpose (See 'closed channel' concept in section 3.11).

3.7 Thermal-hydraulics of a SC with single-phase flow ($L_{FTYPE} > 0$)

The spatial integration of the two PDE-s of the conservation eqs.(1) and (2) over the (single-phase) SC nodes n (by taking into account the rules from section 3.2, the relations from the eqs.(7) and (50) and the possibility of locally changing nodal cross flow areas along the BC) yields for the transient case

- a relation for the total nodal mass flow

$$G_{Nn} = G_{Nn-1} - V_{Mn}(\rho^{T}_{Mn}\frac{d}{dt}T_{Mn} + \rho^{P}_{Mn}\frac{d}{dt}P_{SYS}) + (\rho_{Nn} - \rho_{Mn})A_{Nn}\frac{d}{dt}z_{Nn} + \\ + (\rho_{Mn} - \rho_{Nn-1})A_{Nn-1}\frac{d}{dt}z_{Nn-1}$$

$$= G_{Nn-1} - G_{1Tn} - G_{1Pn} + G_{1Zn} \qquad (n=1,N_{CT}),\ L_{FTYPE} > 0 \qquad (51)$$

and

- the time-derivatives for the mean nodal coolant temperatures (if eliminating the term G_{Nn} in the resulting equation by inserting from the equation above):

$$\frac{d}{dt}T_{Mn} = T^{t}_{Tn} + T^{z}_{TCA}\frac{d}{dt}z_{Nn} \qquad (52)$$

$$(n=1, N_{CT} \text{ and } z_{CA}=z_{BA}) \text{ or } (n=1, N_{CT}-1 \text{ and } z_{CA} < z_{BA}),\ L_{FTYPE} > 0$$

with the abbreviations

$$T^{t}_{Tn} = \frac{q_{Mn} - \frac{G_{Nn-1}}{A_{Mn}}h^{(s)}_{Nn} + q_{Pn}}{\rho_{Mn}\,h^{T}_{Mn}\,C_{TMn}} + T^{z}_{TCE}\frac{d}{dt}z_{Nn-1} \qquad (53)$$

$$T^{z}_{TCE} = \frac{1}{2}\left[T^{(s)}_{Mn} - 2\left(1 - \frac{\rho_{CE}}{\rho_{Mn}}\right)T^{(s)}_{Nn}\right]\frac{A_{CE}}{A_{Mn}C_{TMn}} \quad \text{or} \quad = 0 \quad (n = 1 \text{ or } > 1),\ L_{FTYPE} > 0 \qquad (54)$$

$$T^{z}_{TCA} = 0 \quad \text{or} \quad = \frac{1}{2}\frac{A_{Nn}}{A_{Mn}C_{TMn}}T^{(s)}_{Nn} \qquad (55)$$

$$(n < N_{CT} \text{ or } = N_{CT} \text{ if } z_{CA} < z_{BA} \text{ or } = z_{BA}),\ L_{FTYPE} > 0$$

and the coefficients

$$q_{Pn} = [1 - \rho_{Mn}h^{P}_{Mn} + \rho^{P}_{Mn}(h_{Nn} - h_{Mn})]\frac{d}{dt}P_{SYS} \qquad (56)$$

$$q_{Zn} = \frac{1}{2A_{Mn}}\{A_{Nn}\rho_{Mn}h^{(s)}_{Nn}\frac{d}{dt}z_{Nn} + A_{Nn-1}[\rho_{Mn}h^{(s)}_{Mn} - 2(\rho_{Mn} - \rho_{Nn-1})h^{(s)}_{Nn}]\frac{d}{dt}z_{Nn-1}\} \qquad (57)$$

$$C_{TMn} = 1 - \frac{\rho^{T}_{Mn}}{\rho_{Mn}}\frac{h_{Nn} - h_{Mn}}{h^{T}_{Mn}} = 1 - \frac{\rho^{T}_{Mn}}{\rho_{Mn}}(T_{Nn} - T_{Mn}) \qquad (58)$$

$$T^{z}_{TCE} = \frac{1}{2}\left[T^{(s)}_{Mn} - 2\left(1 - \frac{\rho_{CE}}{\rho_{Mn}}\right)T^{(s)}_{Nn}\right]\frac{A_{CE}}{A_{Mn}C_{TMn}} \quad \text{or} \quad = 0 \qquad (59)$$

$$(\text{if } n = 1 \text{ and } z_{CE} > z_{BE} \text{ or } = z_{BE}),\ L_{FTYPE} > 0$$

It can be expected that at the begin of each (intermediate) time step the mean nodal coolant temperature values T_{Mn} are known, either from steady state considerations (at the begin of

the transient calculations) or as a result of the integration procedure. Hence the parameters needed in the relations above can be determined too. From the PAX procedure it follow the SC nodal terms T_{Nn}, $T^{(s)}_{Nn}$ and $T^{(s)}_{Mn}$ and, demanded for the case that $\Delta z_{Nn} \rightarrow 0$, their gradients. Finally, by considering the water/steam tables (Hoeld, 1996), also their nodal enthalpies are fixed.

If, in the transient case, the SC nodal boundary temperature does not reach along the entire BC its limit value ($T_{LIMNn}=T_{SATNn}$) the total number of SC nodes is given as $N_{CT}=N_{BT}-N_{BCE}$ and z_{Nn} (at $n=N_{CT}$) $=z_{CA}=z_{BT}$. Otherwise, if this limit is (at node n) reached, then $N_{CT} = n$, $T_{Nn}=T_{SATNn}$ with z_{CA} ($< z_{BT}$) resulting from the integration. Then, from the procedure above also the time-derivative of the boiling boundary moving within this channel can be derived (as this will be discussed in section 3.9).

The **steady state** part of the total nodal mass flow (charaterized by the index 0) follows from the basic non-linear algebraic equation (resulting from setting in eq. (51) the time-derivative equal to 0)

$$G_{Nn,0} = G_{CA,0} = G_{CE,0} = G_{BA,0} = G_{BE,0} \qquad (n=1,N_{CT}),\ L_{FTYPE} >0 \qquad (60)$$

Replacing in eq.(52) $Q_{Mn,0}$ by $Q_{BK,0}$ (if $n > 1$), since N_{CT} is not yet known, yields the steady state nodal enthalpy terms

$$h_{Nn,0} = h_{Nn-1,0} + \frac{Q_{Mn,0}}{G_{BE,0}} \leq h'_{Nn,0} \text{ or } \geq h''_{Nn,0} \qquad (\text{with } h_{Nn-1,0} = h_{CE,0} \text{ at } n=1) \qquad (61)$$

$$(\text{if } L_{FTYPE} = 1 \text{ or } = 2 \text{ at } n = 1,\ N_{BT}\text{-}N_{BCE})$$

Regarding the restrictions above the total number N_{CT} of SC nodes for the steady state is then also fixed with

$$N_{CT} = n < N_{BT} - N_{BCE} \text{ and } z_{CA,0}(=z_{Nn,0}) < z_{BA} \qquad (\text{if } h_{Nn,0} = h'_{Nn,0} \text{ and } L_{FTYPE} = 1)$$

$$N_{CT} = N_{BT} - N_{BCE} \text{ and } z_{CA,0} = z_{BA} \qquad (\text{if } h_{Nn,0} < h'_{Nn,0} \text{ and } L_{FTYPE} = 1) \text{ or } (\text{if } L_{FTYPE} = 2) \qquad (62)$$

Finally, according to eq.(51), the nodal power term for the last SC node is given as

$$Q_{MCA,,0} = Q_{Mn,,0} = (h'_{CA,0} - h_{Nn-1,0})\, G_{BE,0} \qquad (\text{if } n = N_{CT} < N_{BCA} \text{ and } L_{FTYPE} = 1)$$

$$= (h_{Nn-1,0} - h''_{CA,0})\, G_{BE,0} \qquad (\text{if } n = N_{CT} < N_{BCA} \text{ and } L_{FTYPE} = 2) \qquad (63)$$

From the resulting steady state enthalpy values $h_{Nn,0}$ at their node boundaries follow then (from the thermodynamic water/steam tables) the corresponding coolant temperature values $T_{Nn,0}$ (with $T_{Nn,0} = T_{SATNn,0}$ if $n = N_{CT}$ and $z_{CA} < z_{BA}$) and by applying the PAX procedure (according to section 3.3) their mean nodal temperature and enthalpy values $T_{Mn,0}$ and $h_{Mn,0}$ (acting as start values for the transient calculations). It has to be noted that, due to the non-linearity of the basic steady state equations, this procedure has to be done in a recursive way.

It can additionally be stated that both the steady state and transient two-phase mass flow parameters get the trivial form

$$G_{SNn} = G_{SNn,0} = 0 \text{ resp. } G_{WNn} = G_{CE} \text{ and } G_{WNn,0} = G_{BE,0} \qquad (n=1, N_{CT}, \text{if } L_{FTYPE} = 1)$$

$$G_{SNn} = G_{CE} \text{ and } G_{SNn,0} = G_{BE,0} \text{ resp. } G_{WNn} = G_{WNn,0} = 0 \qquad (n=1, N_{CT}, \text{if } L_{FTYPE} = 2) \qquad (64)$$

and

$$\frac{d}{dt}\alpha_{Mn} = 0 \quad \text{and} \quad \alpha_{Nn} = \alpha_{Nn,0} = \alpha_{Mn,0} = X_{Nn} = X_{Nn,0} = 0 \quad \text{or} \quad = 1 \qquad (n=1, N_{CT}, \text{ if } L_{FTYPE} = 1 \text{ or } = 2) \tag{65}$$

3.8 Thermal-hydraulics of a SC with two-phase flow ($L_{FTYPE} = 0$)

Similar as in the section before, the spatial integration of the two PDE-s of the conservation eqs.(1) and (2) now over the (mixture-phase) SC nodes n (by taking into account the rules from section 3.2, the relations from the eqs.(7) and (50) and the possibility of locally changing nodal cross flow areas along the BC) yields for the transient case

- the total nodal mass flow terms

$$G_{Nn} = G_{Nn-1} + V_{Mn}(\rho' - \rho'')_{Mn}\left(\frac{d}{dt}\alpha_{Mn} - \alpha^{t}_{GPn} - \alpha^{t}_{GZn}\right) = G_{Nn-1} + G_{2An} - G_{2Pn} - G_{2Zn} \qquad (n=1, N_{CT}, L_{FTYPE} = 0) \tag{66}$$

by introducing (if neglecting thereby the small differences between mean and nodal saturation thermodynamic values) the coefficients

$$\alpha^{t}_{GPn} = \left(\frac{1}{(\rho' - \rho'')}\right)_{Mn}[(1-\alpha)\rho'^{P} + \alpha\rho''^{P}]_{Mn}\frac{d}{dt}P_{SYS} \tag{67}$$

$$\alpha^{t}_{GZn} = \frac{1}{2}\frac{A_{CE}}{A_{Mn}}\alpha^{(s)}_{Mn}\frac{d}{dt}z_{CE} \qquad (n = 1 \text{ and } z_{CE} > z_{BE})$$

$$= 0 \qquad (1 < n < N_{CT})$$

$$= \frac{A_{CA}}{A_{Mn}}\left(\alpha^{(s)}_{CA} - \frac{1}{2}\alpha^{(s)}_{Mn}\right)\frac{d}{dt}z_{CA} \qquad (n = N_{CT}, N_{CT}>1 \text{ and } z_{CA} < z_{BA}) \tag{68}$$

a

and

- the mean nodal void fraction time-derivatives

$$\frac{d}{dt}\alpha_{Mn} = \alpha^{t}_{ASn} - \alpha^{t}_{APn} + \alpha^{z}_{CA}\frac{d}{dt}z_{Nn} + \alpha^{z}_{CE}\frac{d}{dt}z_{Nn-1} = \alpha^{t}_{An} + \alpha^{t}_{AZn} \qquad (n=1, N_{CT} \text{ and } z_{CA}=z_{BA}) \text{ or } (n=1, N_{CT}-1, N_{CT}>1 \text{ and } z_{CA}<z_{BA}),\ L_{FTYPE}=0 \tag{69}$$

with the coefficients

$$\alpha^{t}_{ASn} = \alpha^{t}_{AQn} - \alpha^{t}_{AGn} = \frac{1}{\rho''_{Mn}}\left(\frac{q_{Mn}}{h_{SWMn}} - \frac{G^{(s)}_{SNn}}{A_{Mn}}\right) \tag{70}$$

$$\alpha^{t}_{APn} = \frac{1}{(\rho'' h_{SW})_{Mn}}[(1-\alpha)\rho' h'^{P} + \alpha(\rho' h''^{P} + \rho''^{P} h_{SW}) - 1]_{Mn}\frac{d}{dt}P_{SYS} \tag{71}$$

$$\alpha^{t}_{AZn} = \alpha^{t}_{GZn} \tag{72}$$

$$G^{(s)}_{SNn} = \frac{\Delta G_{SNn}}{\Delta z_{Nn}} \rightarrow G^{(z)}_{SNn} = G^{(\alpha)}_{SNn}\, \alpha^{(z)}_{Nn} \qquad \text{if } \alpha_{Nn} \rightarrow \alpha_{CE} = 0 \text{ (at n=1)} \quad \text{or } \alpha_{Nn} \rightarrow \alpha_{CA} = 1 \text{ (at n= } N_{CT}) \tag{73}$$

It can again be expected that at the begin of each (intermediate) time step the mean nodal void fraction values α_{Mn} are known, either from steady state considerations (at the begin of the transient calculations) or as a result of the integration procedure. Hence the parameters needed in the relations above can be determined too. From the PAX procedure it follow their nodal boundary void fraction terms α_{Nn} together with their gradients $\alpha^{(z)}_{Nn}$ and $\alpha^{(z)}_{Mn}$. The slopes $\alpha^{(s)}_{Nn}$ and $\alpha^{(s)}_{Mn}$ can be established from their definition equations and thus, as shown both in section 2.2.3 but also in the tables given by Hoeld (2001 and 2002a), all the other characteristic two-phase parameters (such as steam, water or relative velocities etc). It has again to be noted that, due to the non-linearity of the basic equation, this procedure has to be done in a recursive way.

If, in the transient case, the SC nodal boundary void fraction α_{Nn} does not reach along the entire BC its limit value (α_{LIMNn}=1 or 0) the total number of SC nodes is given as $N_{CT}=N_{BT}-N_{BCE}$ and z_{Nn} (at $n=N_{CT}$) $=z_{CA}=z_{BT}$. Otherwise, if this limit is reached (at node n), then N_{CT} = n, α_{Nn}=1 (or =0) with z_{CA} (< z_{BT}) resulting from the integration. Then, from the procedure above also the time-derivative of the boiling boundary moving within this channel can be derived (as this will be discussed in section 3.9).

Hence it follows for the steam mass flow gradients

$$\begin{aligned} G^{(\alpha)}_{SNn} &= A_{CE}\, v_{S0}\, \rho^{//}_{Nn} \quad \text{with } v_{S0} = v_S \text{ (at } \alpha_{Nn} = 0) \text{ (n=1 and } \alpha_{Nn} \rightarrow \alpha_{CE} = 0) \\ &= A_{CA} v_{W1}\, \rho^{/}_{Nn} \quad \text{with } v_{W1} = v_W \text{ (at } \alpha_{Nn} = 1) \text{ (n=} N_{CT}\text{-1 and } \alpha_{Nn} \rightarrow \alpha_{CA} = 1 \end{aligned} \tag{74}$$

The term $\frac{d}{dt}\alpha_{Mn}$ can be eliminated in eq.(66) if inserting from eq.(69) yielding a relation between G_{SNn} and G_{Nn}

$$G_{Nn} + \left(\frac{\rho'}{\rho''} - 1\right)_{Mn} G_{SNn} = G_{Xn} \qquad (n=1, N_{CT}, L_{FTYPE} = 0) \tag{75}$$

with the 'auxiliary' mass flow term G_{Xn} referring only to values known from the node below

$$G_{Xn} = G_{Nn-1} + \left(\frac{\rho'}{\rho''} - 1\right)_{Mn} G_{SNn-1} + V_{Mn} (\rho' - \rho'')_{Mn} (\alpha^{t}_{AQn} - \alpha^{t}_{APn} - \alpha^{t}_{GPn}) \qquad (n=1, N_{CT}, L_{FTYPE} = 0) \tag{76}$$

A similar relation to G_{Nn} can be established from the drift flux correlation (eq.(18)). Thereby it has been taken advantage of the fact that the needed drift velocity v_{DNn} and the phase distribution parameter C_{0Nn} can be determined independently from the total mass flow G_{Nn} (and thus before this term is known). Hence, combining the eqs.(75) and (18) results in

$$G_{Nn} = \frac{G_{Xn} - (A\,\alpha\,v_D\,\rho'\,C_{DC})_{Nn}}{1 + (\alpha\,C_0\,C_{DC})_{Nn}} \qquad (n=1,N_{CT}) \quad (77)$$

with the coefficient

$$C_{DCNn} = \left(\frac{\rho'}{\rho''} - 1\right)_{Mn} \left(\frac{\rho''}{\rho' C_{GC}}\right)_{Nn} \quad (78)$$

From the drift flux correlation package (Hoeld et al., 1992 and Hoeld, 1994, see also the eqs.(13) and (18)) follow then all the other characteristic two-phase parameters, e.g. the nodal steam mass flow G_{SNn} and, eventually, $\alpha_{Nn}^{(z)}$ and, according to eq.(74), also the slope $G_{SNn}^{(s)}$. Then, finally, from the eqs.(69) (but also (66)) the mean nodal void fraction time-derivative $\frac{d}{dt}\alpha_{Mn}$ can be derived, needed for the next integration step.
Obviously, at mixture flow the mean nodal temperature and enthalpy terms are equal to their saturation values

$$T_{Mn} = T_{SAT}(P_{Mn}) \text{ resp. } h_{Mn} = h'(P_{Mn}) \text{ or } = h''(P_{Mn}) \quad (n= 1, N_{CT} \text{ and } L_{FTYPE} = 0) \quad (79)$$

and are thus only dependent on the local resp. system pressure value.
From mass conservation considerations it is obvious that at a transient situation and in the case of a transition from one BC into another obviously only the mass flow terms remain unchanged, not the void fractions.
Setting in the eqs.(66) and (69) the time-derivatives equal to 0, one obtains relations for the **steady state case.** For the total mass flow parameters $G_{Nn,0} = G_{BE,0}$ a similar relation as already given for the single-phase flow in eq.(60) is valid. The nodal steam mass flow gets the form

$$G_{SNn,0} = G_{SNn-1,0} + \frac{Q_{Mn,0}}{h_{SWMn,0}} \leq G_{BE,0} \qquad (n= 1, N_{BT}–N_{BCE} \text{ and } L_{FTYPE} = 0) \quad (80)$$

Regarding the restrictions above the total number N_{CT} of SC nodes is fixed in the steady state case with

$$\begin{aligned} &N_{CT} = n < N_{BT} - N_{BCE} \text{ and } z_{CA,0}(=z_{Nn,0}) < z_{BA} \qquad (\text{if } G_{SNn,0} = G_{BE,0} \text{ and } L_{FTYPE} = 0) \\ &N_{CT} = N_{BT} - N_{BCE} \text{ and } z_{CA,0} = z_{BA} \qquad (\text{if } G_{SNn,0} < G_{BE,0} \text{ and } L_{FTYPE} = 0) \end{aligned} \quad (81)$$

The steady state nodal steam quality parameters are given as

$$X_{Nn,0} = \frac{G_{SMn,0}}{G_{Nn,0}} \qquad (n = 1, N_{CT} \text{ if } L_{FTYPE} = 0) \quad (82)$$

the corresponding nodal boundary void fraction values $\alpha_{Nn,0}$ by applying the inverse drift-flux correlation (eq.(21)). The corresponding mean nodal void fraction values $\alpha_{Mn,0}$ can be determined by applying the PAX procedure, parameters which are needed as starting values for the transient calculation.
Then from eq.(80) it follows for the case $N_{CT} < N_{BT} - N_{BCE}$ the corresponding nodal power for the last SC node

$$Q_{MCA,,0} = Q_{Mn,,0} = (G_{Nn,0} - G_{SNn-1,0})\, h_{SWNn,0} \quad (n = N_{CT} < N_{BCA} \text{ if } L_{FTYPE} = 0) \quad (83)$$

3.9 SC boundaries

The SC entrance position z_{CE} (= z_{Nn} at n=0) is either equal to the BC entrance z_{BE} (for the first SC within the BC) or equal to the SC outlet boundary of the SC before.

In the **steady state** case the SC outlet boundary (= boiling boundary $z_{BB,0}$ or mixture level $z_{ML,0}$) can be represented as

$$\begin{aligned} z_{CA,0} &= z_{BA} && (n = N_{CT} \text{ and } z_{CA,0} = z_{BA}) \\ &= z_{Nn-1} + \Delta z_{CA,0} && (n = N_{CT} \text{ and } z_{CA,0} < z_{BA}) \end{aligned} \quad (84)$$

The (steady state) term N_{CT} is already determined in the eqs.(62) or (81), the corresponding nodal power $Q_{MCA,0}$ given by the eqs.(63) or (80). Hence after rearranging eq.(32) one gets an algebraic quadratic equation with respect to $\Delta z_{CA,0}$

$$Q_{MCA,0} = Q_{Mn,,0} = \Delta z_{CA,0} \left[q_{LBk-1} + \frac{1}{2} \frac{q_{LBk,0} - q_{LBk-1,0}}{\Delta z_{Bk}} \Delta z_{CA,0} \right] \quad (n = N_{CT} \text{ and } k = N_{BCA} \text{ if } N_{CT} < N_{BCA}) \quad (85)$$

yielding finally as solution

$$\begin{aligned} \Delta z_{CA,0} &= \Delta z_{Bk} && (n = N_{CT} \text{ and } k = N_{BCA} \text{ if } N_{CT} = N_{BT}) \\ &= \Delta z_{Bk} \frac{q_{LBk-1,0}}{q_{LBk-1,0} - q_{LBk,0}} \left[1 - \sqrt{1 - 2\left(1 - \frac{q_{LBK,0}}{q_{LBk-1,0}}\right) \frac{Q_{CMA,0}}{\Delta z_{Bk}\, q_{LBMk-1,0}}} \right] && (k = N_{BCA} \text{ if } N_{CT} < N_{BT}) \\ \rightarrow\ & \frac{Q_{MCA,0}}{q_{LBk-1,0}} \left[1 + \frac{1}{2} \left(1 - \frac{q_{LBk,0}}{q_{LBk-1,0}}\right) \frac{Q_{CMA,0}}{\Delta z_{Bk}\, q_{LBk-1,0}} \right] && \text{if } q_{LBk,0} \rightarrow q_{LBk-1,0} \end{aligned} \quad (86)$$

From the relations in section 3.5 then also the other steady state power terms can be determined.

In the **transient case** the outlet boundary z_{CA} (=boiling boundary or mixture level) follows, as already pointed-out, directly from the integration procedure. Then also Δz_{CA} and N_{CT} are fixed. This SC outlet boundary z_{CA} can move along the entire BC and thus also cross BC node boundaries. A SC can even shrink to a single node (N_{CT} =1), start to disappear or to be created anew. This means that in PAX the slope in the vicinity of such a boundary is replaced by a gradient.

The mean nodal coolant temperature or, if L_{FTYPE}=0, void fraction of the last SC node is interrelated by the PAX procedure with the locally varying SC outlet boundary z_{CA} Hence, in a transient situation the time-derivative of only one of these parameters is demanded, after the integration then the second one follows from the PAX procedure.

If combining (in the case of single-phase flow) the eqs.(42) and (52), the wanted relation for the SC boundary time derivative can be expressed by

$$\frac{d}{dt} z_{CA} = \frac{d}{dt} z_{BB} = \frac{T^t_{PXCA} - T^t_{TCA}}{T^z_{TCA} - T^z_{PXCA}} \text{ or } = 0 \qquad (n = N_{CT},\ z_{CA} < z_{BA} \text{ or } z_{CA} = z_{BA} \text{ if } L_{FTYPE} > 0) \quad (87)$$

and, if considering the eqs. (42) and (69), for the case of mixture flow

$$\frac{d}{dt} z_{CA} = \frac{d}{dt} z_{ML} = \frac{\alpha^t_{PXCA} - \alpha^t_{ACA}}{\alpha^z_{ACA} - \alpha^z_{PXCA}} \text{ or } = 0 \qquad (n = N_{CT},\ z_{CA} < z_{BA} \text{ or } z_{CA} = z_{BA} \text{ if } L_{FTYPE} = 0) \quad (88)$$

If $z_{CA} < z_{BA}$, the corresponding time-derivatives $\frac{d}{dt} T_{Mn}$ or $\frac{d}{dt} \alpha_{Mn}$ of the last SC node (at $n=N_{CT}$) follow then by inserting the terms above into the eqs.(52) or (69). After the integration procedure then the SC outlet boundary z_{CA} (= boiling boundary z_{BB} or mixture level z_{ML}) and thus also the total number N_{CT} of SC nodes is given.
In these considerations it is excluded that a BC node can contain more than one moving boundary. Hence a SC with $N_{CT}=1$ can only appear at BC entrance ($z_{CE} = z_{BE}$) or BC outlet ($z_{CA} = z_{BA}$). For such a special case either the temperature slope (T^{z}_{CEI}) resp. (at mixture fluid conditions) the term α^{z}_{CEI} at SC entrance are needed as input to the PAX procedure (see section 3.3.1).

3.10 Pressure profile along the SC (and thus also BC)

After having solved the mass and energy balance equations separately (and not simultaneously) with the momentum balance the now exact nodal SC and BC pressure difference terms ($\Delta P_{Nn} = P_{Nn} - P_{Nn-1}$ and ΔP_{BNn}) can (for both single- or two-phase flow situations) be determined by discretizing the momentum balance eq.(3) and integrating over the corresponding SC nodes. The total BC pressure difference $\Delta P_{BT} = P_{BA} - P_{BE}$ between BC outlet and entrance follows then from the relation

$$\Delta P_{BT} = \Delta P_{PBT} - \Delta P_{GBT} \qquad \text{(with } \Delta P_{GBT,0} = 0 \text{ at steady state conditions)} \tag{89}$$

with

$$\Delta P_{PBT} = \Delta P_{SBT} + \Delta P_{ABT} + \Delta P_{XBT} + \Delta P_{FBT} + \Delta P_{DBT} \qquad \text{(with } \Delta P_{PBT,0} = \Delta P_{BTIN,0} \text{ at steady state conditions)} \tag{90}$$

comprising terms from static head (ΔP_{SBT}), mass acceleration (ΔP_{ABT}), wall friction (ΔP_{FBT}) and external pressure accelerations (ΔP_{XBT}, pump or other perturbations from outside) and (in the transient case) the pressure difference term ΔP_{GBT} which takes care of the time-dependent changes in total mass flux along a BC (caused by the direct influence of changing nodal mass fluxes) having the form

$$\Delta P_{GBT} = \int_0^{z_{BT}} \frac{d}{dt} G_{FB}(z,t)\, dz = z_{BT} \frac{d}{dt} G_{FBMT} \quad \text{at transient conditions}$$
$$= 0 \quad \text{at steady state} \tag{91}$$

Thereby the 'fictive' mean mass flux term G_{FBMT} (averaged over the entire BC) has been introduced which can be represented as

$$G_{FBMT} = \frac{1}{z_{BT}} \int_0^{z_{BT}} G_{FB}(z,t)\, dz$$

$$\cong \frac{1}{z_{BT}} \sum_{n=1}^{N_{SCT}} \sum_{n=1}^{N_{CT}} \Delta z_{Nn}\, G_{FBMn} = \frac{1}{2} \frac{1}{z_{BT}} \sum_{k=1}^{N_{BT}} \frac{\Delta z_{Bk}}{A_{BMk}} (G_{Bk} + G_{BK-1}) \tag{92}$$

Its time derivative can be estimated as

$$\frac{d}{dt} G_{FBMT} \cong \frac{G_{FBMT} - G_{FBMTB}}{\Delta t} \rightarrow \left(\frac{d}{dt} G_{FBMT}\right)_{at\ t=tB} \quad \text{if} \quad \Delta t = t - t_B \rightarrow 0 \quad \text{(Index B = begin of time-step)} \tag{93}$$

Regarding, however, the friction correlations, there arises the problem how to consider correctly contributions from spacers, tube bends, abrupt changes in cross sections etc. as well. The entire friction pressure decrease (ΔP_{FBT}) along a BC can thus never be described solely by analytical expressions in a satisfactory manner. To minimize these uncertainties a further friction term will be included into these considerations having the form

$$\Delta P_{DBT} = (f_{FMP,0} - 1)\, \Delta P_{FBT} + \Delta P_{FADD} \tag{94}$$

This means that eq.(90) is either supplemented with an additive term (index FADD) or the friction parts are provided with a multiplicative factor $f_{FMP,0}$. Which of them should prevail can be governed from outside by an input coefficient $\varepsilon_{DPZ} = \varepsilon_{DPZI}$. Thereby, the additive part will be assumed to be proportional to the square of the total coolant mass flow (e.g., at BC entrance)

$$\Delta P_{FADD} = - f_{ADD,0}\, z_{BT} \left(\frac{G_F |G_F|}{2\rho\ d_{HW}}\right)_{BE} \tag{95}$$

At steady state conditions the total BC pressure difference term ($\Delta P_{BT,0}$) is known from input ($\Delta P_{BT,0} = \Delta P_{BTIN}$). Since $\Delta P_{GBT,0} = 0$, the steady state total additional term $\Delta P_{DBT,0}$ results from eq.(90). If defining the additive steady state friction pressure difference $\Delta P_{FADD,0}$ to be the (1-ε_{DPZ})-th part of the total additional pressure difference term then

$$\Delta P_{FADD,0} = (1 - \varepsilon_{DPZ})\, \Delta P_{DBT,0} \tag{96}$$

The corresponding additive friction factor $f_{ADD,0}$ follows then directly from eq.(95), the multiplicative one $f_{FMP,0}$ from the combination of the eqs.(94) and (96)

$$f_{FMP,0} = 1 + \varepsilon_{DPZ}\ \frac{\Delta P_{DBT,0}}{\Delta P_{FBT,0}} \tag{97}$$

There arises the question how the validity of both friction factors can be expanded to transient situations too. This can, for example, be done by assuming that they should remain time-independent. Then, finally, the wanted nodal pressure decrease terms can be determined for both steady state but also transient situations. By adding now the resulting nodal BC pressure difference terms to the (time-varying) system pressure $P_{SYS}(t)$ (given from outside as boundary condition with respect to a certain position (in- or outside of the BC) then finally also the absolute nodal pressure profile P_{Bk} along the BC can be established (needed at the begin of the next time step for the determination of the constitutive equations).

3.11 BC entrance mass flow ('Open and closed channel concept')

As to be seen from the sections above in order to be able to calculate the characteristic nodal and total single- and two-phase parameters along a BC the BC entrance mass flow must be

known. This term is for the steady state case given by input ($G_{BE} = G_{BEIN}$), together with the two pressure entrance and outlet values ($P_{BE} = P_{BEIN}$, $P_{BA} = P_{BAIN}$). In the transient situation it can, however, be expected that for the normal case of an 'open' channel besides the entrance mass flow only one of these two pressure terms is known from input, either at BC entrance or outlet. The missing one follows then from the calculation of the pressure decrease parts.

Such a procedure can not be applied without problems if the channels are part of a complex set of closed loops, loops consisting of more than one coolant channel (and not driven by an outside source, such as a pump). Then the mass flow terms (and especially entrance term of at least one of the channel) has to be adjusted to the fact that the sum of the entire pressure decrease terms along such a closed circuit must be zero. Usually, in the common thermal-hydraulic codes (see for example the 'separate-phase' approaches) this problem is handled by solving the three (or more) fundamental equations for the entire complex system simultaneously, a procedure which affords very often immense computational times and costs. In the here applied module (based on a separate treatment of momentum from mass and energy balance) a more elegant method could be found by introducing an additional aspect into the theory of CCM. It allows, different to other approaches, taking care of this situation by solving this problem by means of a 'closed channel concept' (in contrast to the usual 'open channel' method).

Choosing for this purpose a characteristic 'closed' channel within such a complex loop it can be expected that its pressure difference term $\Delta P_{BT} = \Delta P_{BA} - \Delta P_{BE}$ over this channel is fix (= negative sum of all the other decrease terms of the remaining channels which can be calculated by the usual methods). Thus also the outlet and entrance BC pressure values (P_{BAIN}, ΔP_{BEIN}) are now also available as inputs to CCM. Since, according to eq.(91), then also the term ΔP_{PBT} is known, it follows from eq.(95) the 'closed channel concept criterion'

$$z_{BT}\ \frac{d}{dt}\ G_{FBMT} = \Delta P_{GBT} = \Delta P_{PBT} - \Delta P_{BTIN} \qquad \text{(at 'closed channel' conditions)} \qquad (98)$$

This means that for this purpose the total mass flow along a BC (and thus also at its entrance) must be adapted in such a way that the above for the 'closed channel' concept essential criterion remains valid at each time step, i.e., that the actual time derivative of the mean mass flux G_{FBMT} averaged over the channel must, as recommended by eq.(92), agree in a satisfactory manner with the required one from the equation above.

There exist, obviously, different methods how to deal with this complicated problem. One of them could be to determine the entrance mass flow G_{BE} by changing this value in a recursive way until the resulting term $\frac{d}{dt}\ G_{FBMT}$ agrees with the criterion above.

Another possibility is to find a relation between the time-derivatives of the mean and certain local mass flux values (e.g., at BC entrance), i.e., to establish for example a relation between the terms $\frac{d}{dt}\ G_{FBMT}$ and $\frac{d}{dt}\ G_{FBE}$. Then the wanted mass flow time-derivative at BC entrance can be determined directly from eq.(98). One practicable method to establish such a relation could follow if considering that a change of the mass flux is propagating along the channel so fast that the time derivative of its mean values could be set (in a first step) almost equal to the time-derivative at its entrance value. This term can, eventually, be provided with a form factor which can be adapted by an adequate recursion procedure until the condition of eq.(98) is fulfilled. The so won entrance mass flow is then governing the mass flow behaviour of the entire loop.

This method has been applied within the UTSG-3 code (Hoeld, 2011) for the simulation of the natural-circulation behaviour of the secondary steam generator loop. Similar considerations have been undertaken for a 3D case where the automatic mass flow distribution into different entrances of a set of parallel channels is asked (See e.g. Hoeld, 2004a and Jewer et al., 2005). The experience of such calculations should help to decide which of the different possible procedures should finally be given preference.
The 'open/closed channel concept' makes sure that measures with regard to the entire closed loop do not need to be taken into account simultaneously but (for each channel) separately. Its application can be restricted to only one 'characteristic' channel of a sequence of channels within a complex loop. This additional tool of CCM can in such cases help to handle the variety of closed loops within a complex physical system in a very comfortable way.

4. Code package CCM

Starting from the above presented 'drift-flux based mixture-fluid theory' the (1D) thermal-hydraulic coolant channel module CCM could be established. It was derived with the intention to provide the authors of different and sometimes very complex thermal-hydraulic codes with a general and easily applicable tool needed for the simulation of the steady state and transient behaviours of the most important single- and two-phase parameters along any type of heated or cooled coolant channel.
The subdivision of such a (basic) channel (BC), characterized by an own key number (KEYBC), into different sub-channels (SC-s), characterized by its fluid type (L_{FTYPE}), is done automatically within the module. Thereby the different SC-s will change from one SC type to another, i.e. two-phase flow follows single-phase flow and vice versa. SC-s can shrink to a single node or even disappear but also be created anew. The SC inlet boundary conditions are either identical to the entrance conditions of the BC or to the outlet parameters of the SC before.
The module CCM has been constructed in such a way that only input data with regard to the BC are demanded. These input data (for each channel KEYBC) will be transferred to the CCM by only two types of commons containing data established in the calling overall program, allowing thus a very easy handling of the code:

- The first common is only occupied by fixed BC geometry data (such as channel length, elevation heights, fixed or varying cross sections, hydraulic diameters).
- The second one has to contain
  resulting data coming from the (overall) integration procedure (such as mean nodal coolant temperature or mean nodal steam void fraction values, boiling boundary and mixture level along the BC) and (in the case of a closed loop) the total mass flow term at BC entrance
  and moreover
  parameters representing the initial and boundary conditions of the system such as the nodal power profile (entrance power density q_{BCE} and mean nodal mean power values Q_{BMk}),the coolant temperature, mass flow and pressure terms at BC entrance (T_{BE}, G_{BE}, P_{BE}) and, in the case of steady state conditions or at transient situations with a BC being a part of an 'open channel', also the pressure term (P_{BE} or P_{BA}) at BC entrance or outlet.

At the end of a recursion- or time-step characteristic parameters of all SC-s are transferred to the corresponding BC positions, thus yielding, for example, a final set of (non-linear) algebraic or (in the transient case) non-linear ordinary differential equations (ODE-s) of 1-st order together with the parameters following from the constitutive equations of CCM. The resulting sets of equations for different channels appearing in a complex physical system can be combined with other sets of algebraic equations or ODE-s coming from additional parts of such a complex model (considerations with respect to heat transfer, nuclear kinetics, top plenum, downcomer etc.). The final overall sets can then be solved by applying adequate algebraic solution methods or an appropriate time-integration routine (See, for example, Hoeld, 2011).
As output CCM will then yield all the wanted and needed characteristic thermal-hydraulic single- and two-phase BC (and thus also SC) parameters of such a general coolant channel. These are:

- Time-derivatives of the mean nodal coolant fluid temperatures
- time-derivatives of the mean nodal void fractions
- time-derivatives describing the movements of the boiling boundary or mixture level within the BC
- time-derivative of the total mass flow entering the BC (at least for the case that the BC is a part of a closed loop and thus being, for example, of interest for a thermal-hydraulic 3D representation),
- other constitutive nodal BC boundary parameters such as terms for total, water and steam mass flow, for pressure and pressure drop, coolant temperatures, void fraction etc.

The module CCM has been continuously expanded into a very efficient and mature version. To analyze transient situations at normal operational conditions sometimes also very simple codes ('pen' codes) can be applied. The quality of a code has, however, to be proved in the context of how reliably complex or limit cases can be handled. Thus much weight and effort has been placed on the question of how the performance of CCM, especially at extreme situations, can be judged, i.e., in cases where the mass flow ceases to stagnant conditions, the power input decreases to zero, abrupt pressure changes (for example due to a fast opening or closing of valves), the boiling boundary or mixture level disappear, the coolant channel starts to dry-out etc.
The special case of water or steam mass flow terms being exchanged at node boundaries between two parallel 'porous' coolant channels (with pressure differences as driving forces) has not yet been taken into account.

5. Verification and validation (V & V) procedures

During the course of development of the different versions of the code combination UTSG-3/CCM has gone through an appropriate verification and validation (V&V) procedure (with continuous feedbacks being considered in the continual formulation of the theoretical model).
CCM is (similar as done in the separate-phase models) constructed with the objective to be used only as an element within an overall code. Hence, further V&V steps could be performed only in an indirect way, i.e. in combination with such overall codes. This has been done in a very successful way by means of the U-tube steam generator code UTSG-3. Thereby the module CCM could profit from the experiences been gained in decades of years

work with the construction of an effective non-linear one-dimensional theoretical model and, based on it, corresponding digital code UTSG-2 for vertical, natural-circulation U-tube steam generators (Hoeld, 1978 and 1990) and now also the new advanced code version UTSG-3 (Hoeld 2002b, 2004).
The good agreement of the test calculations with similar calculations of earlier versions applied to the same transient cases demonstrates that despite of the continuous improvements of the code UTSG and the incorporation of CCM into UTSG-3 the newest and advanced version has still preserved its validity.
A more detailed description over these general V&V measures demonstrated on one characteristic test case can be found in (Hoeld, 2011).

6. Conclusions

The universally applicable coolant channel module CCM allows describing the thermal-hydraulic situation of fluids flowing along up-, horizontal or downwards channels with fluids changing between sub-cooled, saturated and superheated conditions. It must be recognized that CCM represents a complete system in its own right, which requires only BC-related, and thus easily available, input values (geometry data, initial and boundary conditions, resulting parameters from integration). The partitioning into SC-s is done automatically within the module, without requiring any special actions on the part of the user. At the end of a time-step the characteristic parameters of all SC-s are transferred to the corresponding BC positions, thus yielding the final set of ODE-s together with the parameters following from the constitutive equations of CCM.
In contrast to the currently very dominant separate-phase models, the existing theoretical inconsistencies in describing a two-phase fluid flowing along a coolant channel if changing between single-phase and two-phase conditions and vice versa can be circumvented in a very elegant way in the 'separate-region' mixture-fluid model presented here. A very unique technique has been established built on the concept of subdividing a basic channel (BC) into different subchannels (SC-s), thus yielding exact solutions of the basic drift-flux supported conservation equations. This type of approach shows, as discussed in (Hoeld, 2004b), distinct advantages vs. 'separate phase' codes, especially if taking into account

- the quality of the fundamental equations (basic conservation equations following directly from physical laws supported by experimentally based constitutive equations vs. split 'field' equations with artificial closure terms),
- the special solution methods due to the detailed interpolation procedure from PAX allowing to calculate the exact movement of boiling boundaries and mixture (or dry-out) levels (different to the 'donor-cell averaging' methods yielding mostly only 'condensed' levels),
- the possibility to take advantage of the 'closed-channel concept' (needed for example for thermal- hydraulic 3D considerations) allowing thus to decouple a characteristic ('closed') channel from other parts of a complex system of loops,
- the speed of the computation,
- the derivation of the theory in close connection with the establishment of the code by taking advantage of feedbacks coming from both sides,
- the considerable effort that has been made in verifying and checking the CCM (besides an extensive V & V procedure), with respect to the applicability and adjustment and also for very extreme situations,

- its easy applicability,
- the maturity of the module, which is continuously enhanced by new application cases.
- taking advantage of the fact that most of the development work for the coolant channel thermal-hydraulics has already been shifted to this module (including the special provisions for extreme situations such as stagnant flow, zero power or zero sub-cooling, test calculations for the verification and validation of the code etc.).

The existence of the resulting widely verified and validated module CCM represents an important basic element for the construction of a variety of other comprehensive thermal-hydraulic models and codes as well. Such models and modules can be needed for the simulation of the steady state and transient behaviour of different types of steam generators with special primary and secondary loops (vertical U-tube, vertical once-through or horizontal VVER-440 or -1000 assembles). One main field of application will be (and is already) the simulation of a 3D thermal-hydraulic situation by a number of parallel channels (reactor cores, VVER steam generators etc.), the (basic) channels distinguished by different key numbers N_{TYPES}. It shows special advantages in view of the determination of the mass flow distribution into different coolant channels after non-symmetric perturbations see (Hoeld, 2004a) or (Jewer et al., 2005), a problem which is far from being solved in many of the newest 3D studies. It allows also studying the validity of the 'open channel' method in a very detailed form.

The introduction of varying cross sections along the z axis allows to take care also of thermal non-equilibrium situations by simulating the two separate phases by two with each other interacting basic channels (for example if sub-cooled water rays are injected into a steam dome).

The resulting equations for different channels appearing in a complex physical system can be combined with other sets of algebraic equations and ODE-s coming from additional parts of such a complex model (heat transfer or nuclear kinetics considerations, top plenum, main steam system and downcomer of a steam generator etc.). The final overall set of ODE-s can then be solved by applying an appropriate time-integration routine. See for example (Hoeld, 2011).

The enormous efforts already made in the verification and validation of the codes UTSG-3, its application in a number of transient calculations at very extreme transient situations (fast opening of safety valves, dry out of the total channel with SC-s disappearing or created anew) brings the code and thus also CCM to a very mature and (what is important) easily applicable state. However, there is not yet enough experience to judge how the potential of the mixture-fluid models and especially of CCM can be expanded to other extreme cases (e.g., water and steam hammer). Is it justified to prefer separate-phase models versus the drift-flux based (and thus non-homogeneous) mixture fluid models? This depends, among other criteria, also on the quality of the special models and their exact derivation. Considering the arguments presented above it can, however, be stated that in general the here presented module can be judged as a very satisfactory approach.

7. Nomenclature

A_{Bk}	m²	BC cross sectional area (at BC node boundary k)

A_{Nn}, A_{Mn}	m^2	SC cross sectional area (at SC node boundary n, mean value)
C	-	Dimensionless constant
C_0	-	Phase distribution parameter
d_{HW}	m	Hydraulic diameter
f(z,t), f_{Nn}, f_{Mn}	-	General and nodal (boundary and mean) solution functions
f_{LIMCA}	-	Upper or lower limit of the approx. function f(z,t)
f_{ADD0}, f_{FMP0}	-	Additive and multiplicative friction coefficients
G, $G_F = G/A$	$\frac{kg}{s}$, $\frac{kg}{sm^2}$	Mass flow, mass flux
h, h^P, $c_P = h^T$	$\frac{J}{kg}$, $\frac{m^3}{kg}$, $\frac{J}{m^3 kg}$	Specific enthalpy and its partial derivatives with respect to pressure and temperature (= specific heat)
$h_{SW} = h'' - h'$, h'', h'	$\frac{J}{kg}$	Latent heat, saturation steam and water enthalpy
K_{EYBC}	-	Characteristic key number of channel BC
L_{FTYPE}= 0, 1 or 2	-	SC with saturated water/steam mixture, sub-cooled water or superheated steam
N_{BT}	-	Total number of BC nodes
$N_{BCA} = N_{CT}+N_{BCE}$, N_{BCE}	-	BC node numbers containing SC outlet or entrance
$N_{CT}=N_{BCA}-N_{BCE}$	-	Total number of SC nodes
P, $\Delta P_T = P_A - P_E$	$Pa= \frac{J}{m^3} = \frac{kg}{ms^2}$	Pressure and pressure difference (in flow direction)
Q_{BT}, Q_{Bk}	W	Total and nodal BC power into channel k
$q_{Bk} = U_{Bk}\, q_{LBk}/A_{Bk}$	$\frac{W}{m^3}$	Nodal BC power density into the fluid (= volumetric heat transfer rate)
$q_{FBk}=A_{Bk}\frac{q_{Bk}}{U_{Bk}}$	$\frac{W}{m^2}$	Heat flux from (heated) wall to fluid
$q_{LBk}=U_{TWBk}q_{FBk}=A_{Bk}q_{Bk}$	$\frac{W}{m}$	Linear power at BC node k
$q_{Mn} = \frac{Q_{Mn}}{V_{Mn}}$ $= \frac{1}{2A_{Mn}}(q_{LNn}+q_{LNn-1})$	$\frac{W}{m^3}$	Nodal SC power density into fluid (= volumetric heat transfer rate)
T, t	C, s	Temperature, time
U	m	(Heated) perimeter of a heated wall
$V_{Mn}= \frac{1}{2}(A_{Nn}+A_{Nn-1})\Delta z_{Nn}$	m^3	Mean nodal SC volume
v	$\frac{m}{s}$	Velocity

$X=\frac{G_S}{G}$ or $=\frac{h-h'}{h_{SW}}$	-	Steam quality (2-phase and expanded to 1-phase flow)
z, $\Delta z_{Nn}=z_{Nn}-z_{Nn-1}$	m	Local position, SC node length ($z_{Nn-1}=z_{CE}$ at n=0)
$z_{BA}-z_{BE}=z_{BT}$,$z_{CA}-z_{CE}=z_{CT}$	m	BC and SC outlet and entrance positions, total length
z_{BB}, z_{ML}	m	Boiling boundary and mixture level within a BC
α	-	Void fraction
α_{TWk}	$\frac{W}{m^2C}$	Heat transfer coefficient along a BC wall surface
Δ	-	Nodal differences
ε_{DPZ}	-	Coefficient controlling the additional friction part
ε_{QTW}	-	Correction factor with respect to $Q_{NOM,0}$
ε_{TW}	m	Abs. roughness of tube wall (ε_{TW}/d_{HW} = relative value)
Φ^2_{2PF}	-	Two-phase multiplier
Φ_{ZG}	-	Angle between upwards and flow direction
ρ, ρ^P, ρ^T	$\frac{kg}{m^3}$, $\frac{kg}{J}$, $\frac{kg}{m^3C}$	Density and their partial derivatives with respect to (system) pressure and temperature
Θ	s	Time constant
∂	-	Partial derivative

Subscripts

0, 0 (=E or BE)	Steady state or entrance to SC or BC (n or k =0)
A, E, T (=AE)	Outlet, entrance, total (i.e. from outlet to entrance)
B, S	Basic channel or sub-channel (=channel region)
A, S, F, D, X (P=A+S+F+D+X) and G	Acceleration, static head, direct and additional friction and external pressure differences (in connection with ΔP) and pressure differences due to changes in mass flux
Mn, BMk	Mean values over SC or BC nodes
Nn, Bk	SC or BC node boundaries (n = 0 or k = 0: SC or BC entrances)
D	Drift
S, W	Steam, water
P, T	Derivative at constant pressure or temperature
TW	Tube wall surface

Superscripts

/, //	Saturated water or steam
P, T	Partial derivatives with respect to P or T
(G_S), (α), z, s	Partial derivatives with respect to G_S, α or z (=gradient), slope

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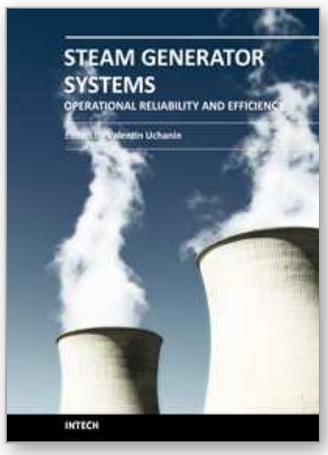

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