

## A THEORETICAL CONCEPT FOR A THERMAL-HYDRAULIC 3D PARALLEL CHANNEL CORE MODEL

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A generally applicable theoretical concept for an adequate description of the 3D thermal-hydraulic single- and two-phase flow phenomena is presented. It will be applied to a 3D core simulated by parallel channels, allowing both single- (with sub-cooled water or superheated steam) and/or two-phase flow situations within these channels. The concept is realized in the experimental code HERO-X3D, concentrating in a first step on an 'artificial' BWR or PWR core which may consist of a central channel, four quadrants and (eventually) a bypass channel. The validity of the 3D representation has to be proofed by demonstrating that also at non-symmetric perturbations of the core the mass flow distribution into the different channels is chosen automatically in such a way that the pressure decrease over each channel stays equal.

The heat generation within each 'fuel element' of such a core will be simulated by 'point kinetic representation' (This can for real situations then easily be replaced by already well developed 3D core kinetic codes). The heat transport out of a fuel element will be determined from the solution of the discretized Fourier heat conduction equation.

The theoretical concept is based on three important development lines:

- The existence of a very generally applicable and in itself complete thermal-hydraulic coolant channel module CCM (allowing the simulation of the steady state and transient behaviour of single- or two-phase flow within a general coolant channel),
- The separate treatment of the mass and energy from the momentum balance eqs. (avoiding thus the very time-consuming integration of 'stiff' eqs.) and
- The establishment of a procedure for the calculation of the mass flow distributions into different parallel channels based on the fact that the sum of pressure decrease terms over a closed loop must stay, despite of un-symmetric perturbations, zero.

A very detailed description of the theoretical concept is given, the development of the experimental code (HERO-X3D) is in progress. Test calculations for the case of the 'artificial' core will demonstrate the quality and validity of the entire concept.

**KEYWORDS:** *3D thermal-hydraulics, single- and two-phase flow,  
3-eq. mixture-fluid model, drift flux, heat transfer*

### 1. Introduction

Despite of more than 50 years research in the field of nuclear reactor theory the problem of a satisfactory description of a 3D thermal-hydraulic situation is still virulent. There has been and are still a number of theoretical attempts to solve this problem but they are far away to allow a practical application, for example for the calculation of the exact transient behaviour of characteristic parameters of a reactor core after a non-symmetric perturbation (e.g., movements of control rods at different parts of the core, loss of a single main circulation pump, perturbations caused by the influence of a single steam generator etc.).

There exist two main theoretical procedures to develop efficient thermal-hydraulic 3D codes:

- In the strictly **mathematical** concept (see e.g. [3,14,20]) the underlying basic conservation eqs. given in form of mostly hyperbolic partial differential eqs. (PDE-s) are solved (for all 3

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dimensions and as generally as possible) by applying exact mathematical rules. Since the models are usually restricted to only hydraulic phenomena thereby very often the possibilities of introducing physically justified and thus 'intelligent' simplifications to enhance the computational process are neglected, demanding boundary conditions which are not yet available and not considering the necessity to normalize different formulae with respect to available measurement data (as given, for example, for steady state conditions). The result is that these codes often afford an enormous amount of CPU-time, making them thus quite un-practicable.

- In the **parallel channel** concept a 3D volume is split into a cluster of parallel channels, solving for each channel the (now 1D) thermal-hydraulic problems on the basis of either a separate-phase or a mixture fluid approach with respect to the formulation of mass, energy and momentum balance conservation eqs. and establishing special methods to determine the mass flow distribution into the different channels after non-symmetric perturbations.

The here presented 3D concept belongs to the 2-nd class of approaches, i.e., to a parallel channel concept. It will be exercised on an 'experimental 3D code' (named HERO-X3D), concentrating in a first step on an 'artificial' core consisting of a central channel and four quadrants and (eventually) a bypass channel, allowing both single- (with sub-cooled water or superheated steam) or two-phase flow situations within these channels. At present no mass exchange in radial direction between these channels will be assumed (the mass flow will be distributed only at their entrances), later-on 'porous' channels will be foreseen too.

Having successfully developed such a 3D code its validity has to be proofed by demonstrating that despite of non-symmetric perturbations of the core the mass flow distribution into the different channels is chosen automatically in such a way that the pressure decrease terms over each channel stays equal. This is the consequence of the 'fifth' conservation law (besides the mass, energy, momentum and volume balance considerations), namely the fact that the sum of all pressure decreases over a closed loop must be zero.

The parallel channel thermal-hydraulic part of the 3D code is based on three important development lines:

- The existence of a very generally and universally applicable thermal-hydraulic coolant channel mixture-fluid module and code CCM needed for the simulation of the steady state and transient behaviour of single- or two-phase flow within these channels, based on a specially developed drift-flux correlation package MDS and a quadratic polygon approximation procedure PAX),
- the separate treatment of the mass and energy from the momentum balance eqs. (avoiding thus the very time-consuming integration of 'stiff' eqs. and having advantages for the 3D presentation as explained in chapter 4) and
- the derivation of a procedure (chapters 3.6 and 4) which controls the mass flow distribution into different parallel channels based on the fundamental law that (especially at non-symmetric perturbations) the sum of pressure decrease terms over a closed loop must be zero.

The establishment of an (1D) thermal-hydraulic coolant channel model and module CCM has been done with the objective to construct a generally applicable tool for the simulation of the steady state and transient behaviour of the most important parameters along any type of coolant channels. Thereby, different to other approaches, the derivation of the characteristic eqs. of the coolant channel module CCM is based on the assumption that the coolant channel in its general form can be looked at as a **basic channel** (BC) being characterized by a key-number KEYBC and consisting of a number of different flow regimes so that it can, accordingly, be subdivided into a number of sub-channels (SC-s) with variable BC and thus also SC-s cross flow areas. All of them belong, obviously, to only two types of SC-s, a SC with an only single-phase fluid (containing exclusively either sub-cooled water or superheated steam, characterized by  $L_{FTYPE}=1$  or 2) or a SC with a two-phase flow regime ( $L_{FTYPE}=0$ ).

After a nodalization of the BC (and thus the corresponding SC-s) and applying a 'modified finite volume method' for the spatial discretization of the partial differential eqs. (PDE-s) which describe the conservation equations of thermal-hydrodynamics and after taking into account corresponding initial and boundary conditions and additional constitutive equations, a set of non-linear ordinary differential equations (ODE-s) of 1-st order can be derived for each SC type (and being then transferred to the BC). By the formulation of this procedure special attention had to be given to the fact that during a transient the SC boundaries can and will cross the BC node boundaries, a SC can shrink to an only single node and even disappear or a new SC can be created. Hence for both SC types the possibility of variable entrance or outlet positions had to be foreseen. In the case of a SC with single-phase flow sub-cooled water can be heated-up (if  $L_{FTYPE} = 1$ ) or superheated steam cooled-down (if  $L_{FTYPE} = 2$ ) to saturation conditions, i.e., in both cases the coolant temperature can reach (within the BC) its limit value  $f_{LIMn} = T_{SATn}$ . Then the (time-varying) SC outlet boundary  $z_{CA}(t) < z_{BA}$  (if below the BC outlet position) represents a boiling boundary. In the case of a SC with two-phase fluid ( $L_{FTYPE} = 0$ ) the mixture can be heated-up to superheated steam, i.e. the void fraction will reach the value 1. The SC outlet position represents then the mixture level  $z_{ML}(t)$ . If the mixture is cooled-down to sub-cooled water the boiling boundary can be reached again.

A special quadratic **poly**gon **ap**proximation **pr**ocedure (PAX) had to be constructed to bind the mean nodal and nodal boundary function values of the functions appearing in the nodalized differential eqs. together, a procedure being, besides the drift flux correlation package, a central part of the theoretical model and module CCM.

The characteristic parameters of all SC-s within a BC will then be transferred to the corresponding BC positions, yielding thus the final set of constitutive eqs. and ODE-s of CCM.

The resulting set of eqs. for different channels as appearing in a complex physical system can then be combined with other ODE-s and algebraic eqs. from additional parts of such a complex model, e.g., from heat transfer or nuclear kinetics considerations, downcomer etc. The final overall set of ODE-s has then to be solved by applying an appropriate integration routine (See, for example, the implicit-explicit 'forward-euler, backward-euler' integration procedure FEBE [3,12]).

The module has been derived on the basis of the experiences of many years work with the development of an effective theoretical model and corresponding non-linear one-dimensional digital code UTSG-2 for vertical, natural-circulation U-tube steam generators as being used in PWR nuclear power plants [5]. After having successfully established the general module CCM the module has then been taken to replace, in a first step, the special coolant channel elements of the thoroughly tested U-tube steam generator code UTSG-2, constructing thus (among other improvements and additions) the advanced code version UTSG-3 [10]. Some of the most characteristic previous calculations with the UTSG-2 code which could be used both in a stand-alone manner but also as a part of the overall modular GRS system code ATHLET [2,7,10] could then be taken as benchmark cases. Post-calculating them with the advanced version (UTSG-3) and comparing the transients with the corresponding UTSG-2 results showed very satisfactory results and could be taken as a very convincing argument for the verification of the UTSG-3 code and thus also the underlying code package CCM.

This module can then be taken as a basic element for the simulation of the thermal-hydraulic steady state and transient behaviour of a 3D core, represented by  $N_{PCT}$  parallel channels. A short overview of the theoretical background of such an universally applicable thermal-hydraulic coolant channel module will be presented in chapter 3, taking into account the possibility of an up-, horizontal or downwards flowing fluid changing between sub-cooled, saturated and superheated conditions. One has, however, to be aware that CCM represents an in itself complete system which requests only BC-related and thus easily available input data (such as geometry data, initial and boundary conditions), the partitioning into SC-s is done automatically within the module, no any special actions of the user are demanded.

A special method how, e.g. after non-symmetric perturbations, the mass flow distribution into different parallel channels can be determined will be presented in chapters 3.6 and 4.

The heat generation (see chapter 5.1) within the fuel elements of each channel of such a 3D-core will, for reasons of simplicity, at present be simulated by a ‘point kinetic representation’ (This part can for real situations then easily be replaced by corresponding already well developed 3D core kinetic codes). The heat transport out of the fuel elements (as demonstrated in chapter 5.2) will be described by solving, in a well known manner, the Fourier heat conduction equation (subdividing the fuel rod into a number of radial layers, neglecting heat conduction into axial direction).

Besides the application of CCM for the simulation of 3D PWR-, BWR- or other nuclear reactor cores the existence of such a module represents an important basic element for the construction of a variety of other comprehensive thermal-hydraulic models too, such 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 assemblies).

Applying these considerations to the theoretical 3D concept will result in the experimental code (HERO-X3D). Test calculations will demonstrate the quality and validity of the entire concept.

## 2. Fundamental eqs. of thermal-hydraulics (Mixture-fluid approach)

Thermal-hydraulic coolant channel models are generally based on a number of conservation eqs. supported by adequate constitutive eqs.

### 2.1 Conservation eqs. for single- and two-phase flow:

#### 2.1.1 Mass balance :

$$\frac{\partial}{\partial t} \{A[(1-\alpha)\rho_w + \alpha\rho_s]\} + \frac{\partial}{\partial z} G = 0 \quad (1)$$

with the steam and water density terms  $\rho_w$  and  $\rho_s$  and a (along a coolant channel) variable cross flow area A, determining the total mass flow  $G = G_w + G_s$  in dependence of its value at node entrance.

#### 2.1.2 Energy balance :

$$\frac{\partial}{\partial t} \{A[(1-\alpha)\rho_w h_w + \alpha\rho_s h_s - P]\} + \frac{\partial}{\partial z} [G_w h_w + G_s h_s] = A q = U w \quad (2)$$

with a (positive or negative) local power density term q, (or heat flux w along a heated perimeter U), determining in case of a nodalization

- at single-phase flow conditions the mean nodal water or steam enthalpies ( $h_w$ ,  $h_s$ ) or, by applying water/ steam tables [6], corresponding coolant temperatures ( $T_w$ ,  $T_s$ ),
- at two-phase flow conditions the mean nodal void fraction  $\alpha_{Mn}$  over each node n.
- at the transition from single- to two-phase (and vice versa) the boiling boundary  $z_B$  (if  $\alpha=0$ ) or superheating boundary  $z_{SPH}$  (if  $\alpha=1$ ), taking advantage of the fact that at this position the coolant temperature becomes equal to the known saturation temperature ( $T_w$  or  $T_s = T_{SAT}$ ),

#### 2.1.3 Momentum balance:

$$\frac{\partial}{\partial t} (G/A) + \left(\frac{\partial P}{\partial z}\right)_A + \left(\frac{\partial P}{\partial z}\right) = \left(\frac{\partial P}{\partial z}\right)_S + \left(\frac{\partial P}{\partial z}\right)_F + \left(\frac{\partial P}{\partial z}\right)_X \quad (3)$$

determining (in the steady state case) the pressure differences or (in the transient case) the change in total mass flow.

The momentum balance eq. contains besides the general pressure gradient parameter ( $\frac{\partial p}{\partial z}$ ) and the term for the external perturbations ( $\frac{\partial p}{\partial z}$ )<sub>X</sub> (caused, for example, by a pump or the pressure adjustment due to mass exchange between parallel channels etc.) additional terms for the mass acceleration

$$\left(\frac{\partial p}{\partial z}\right)_A = \frac{\partial}{\partial z} [(G_w v_w + G_s v_s) / A] \text{ with } v_w \rightarrow G / (\rho_w A^2) \text{ or } v_s \rightarrow G / (\rho_s A^2) \text{ if } \alpha \rightarrow 0 \text{ or } 1 \quad (4)$$

the static head ( $\frac{\partial p}{\partial z}$ )<sub>S</sub>

$$\left(\frac{\partial p}{\partial z}\right)_S = - \cos(\Phi_{ZG}) g_c [\alpha \rho_s + (1-\alpha) \rho_w] \quad (5)$$

(with  $\Phi_{ZG}$  marking the angle between the upwards and flow direction, hence  $\cos(\Phi_{ZG}) = \pm |z_{EL}|/z_L$  represents the relative elevation height with a positive sign at upwards flow)

and the term for single- and two-phase friction

$$\left(\frac{\partial p}{\partial z}\right)_F = - 0.5 f_R |G| G / (d_{HW} \rho A^2) \text{ with } f_R = f_{DW} \text{ or } f_R = f_{DW} \Phi_{2PF}^2 \text{ at 1- or 2-phase flow} \quad (6)$$

with the constitutive eqs. for single- and two-phase friction factors  $f_{DW}$  and  $\Phi_{2PF}^2$  given below.

In order to compensate also pressure drop contributions from spacers, tube bends etc., terms which are analytically difficult to be represented, the pressure distribution along the channel has to be handled in a special way by introducing an adequate renormalization procedure (More details see chapter 3.6). The resulting pressure drop along the entire BC is the key for the application of the module within an assemble of 3D channels.

#### 2.1.4 Volume balance:

In a closed loop a fourth conservation eq. is demanded, namely the ‘volume balance eq.’. It is based on the fact that the sum of water and steam volume must be equal to the total available volume and is needed for the determination of an absolute (system) pressure parameter (e.g., the system pressure  $P_{SYS}$  in the top plenum of a steam generator as shown for example in [7,10]). In combination with the momentum balance eq. which yields the pressure differences over different parts of the loop the local pressure values can then be determined.

#### 2.1.5 Balance of pressure decrease terms over a closed loop:

In a network of loops (for example in case of a 3D representation) a fifth conservation eq. plays an important role. This is based on the physical law that the sum of all pressure decrease terms in a closed loop must be zero. It plays an important part in the establishment of a 3D thermal-hydraulic model, governing the mass flow distribution into different channels (see chapter 4).

#### 2.1.6 Treatment of mass and energy balance eqs. separately from momentum balance :

Solving the conservation eqs. in a direct way yields due to elements with fast pressure wave propagation (and thus very small time constants) a set of ‘stiff’ eqs. whose solution turns out to be enormously time-consuming. To avoid this costly procedure another method will be proposed, treating the energy and mass balance eqs. separately from momentum balance without loosing too much on exactness. Thereby the thermodynamic properties of water and steam in the mass and energy balance eqs. will be determined on the basis of an estimated pressure profile  $P(z,t) \cong P_{SYS}(t) + \Delta P_{bef}(z,t)$ , using, with respect to a system pressure  $P_{SYS}(t)$ , a pressure decrease term  $\Delta P_{bef}(z,t)$  which can be taken from a recursion or computational time step before. After having solved these two conservation eqs. (and not simultaneously with them) the nodal pressure gradient terms from eq.(4), (5) and (6) and thus, from the momentum balance, the actual nodal pressure decrease terms can be determined. The small, almost unnoticeable error can be outweighed by the enormous benefit in cutting-down the CPU time substantiated by two facts:

- The very time-consuming solution of stiff eqs. can be avoided and
- the mass flow distribution into different channels due to pressure balance considerations can be adapted already within each integration time step in a recursive way, i.e. the entire set of differential eqs. does not need to be solved for this purpose.

Due to the fast pressure wave propagation along a coolant channel the time-derivatives of local pressure terms along any position  $z$  will in most cases not differ essentially from corresponding terms at special channel positions (e.g., channel entrance or outlet). They can thus be assumed to be equal to a given external system pressure time derivative, i.e.  $\frac{d}{dt} P(z,t) \cong \frac{d}{dt} P_{SYS}$ .

## 2.2 Constitutive eqs.

For the exact description of the steady state and transient behaviour of single- or two-phase fluids there is, besides the conservation eqs., a number of mostly empirical constitutive eqs. demanded. Naturally, any other correlation package can be used for this purpose. However, the here presented correlations have been thoroughly tested at different opportunities, showing very satisfactory results.

### 2.2.1 Thermodynamic and transport properties of water and steam (Water/steam tables):

Saturation temperature  $T_{SAT}$ , densities ( $\rho'$ ,  $\rho''$ ), enthalpies ( $h'$ ,  $h''$ ) and their derivatives ( $T_{SAT}^P$ ,  $\rho'^P$ ,  $\rho''^P$ ,  $h'^P$ ,  $h''^P$ ) with respect to the system pressure ( $P$ ) for saturated water and steam and the corresponding values ( $\rho$ ,  $h$ ) for subcooled water or superheated steam (index W and S) together with their partial derivatives ( $\rho^T$ ,  $\rho^P$ ,  $h^T$ ,  $h^P$ ) with respect to their independent parameters  $T$  and  $P$  can be determined by using adequate water/steam tables, as realized in the code package MPP [6].

### 2.2.2 Single- and two-phase friction factors:

In the case of single-phase flow a friction factor  $f_R$  is applied, as recommended by Moody [17], being equal to the Darcy-Weisbach single-phase friction factor  $f_{DW}$ . It can be represented by

$$f_R = f_{DW} = 1 / \xi^2 \quad (\text{at single-phase flow}) \quad (7)$$

with the parameter  $\xi$  depending on the Reynolds number  $Re = Gd_H / (A\eta)$  and the relative roughness  $\varepsilon_{TW}/d_H$  of the wall surface. This factor can be approximated by the relation

$$\xi = 2 \log_{10}(d_H / \varepsilon_{TW}) + 1.14 \quad \text{if } Re > Re_{CTB} = 441.19 (\varepsilon_{TW} / d_H)^{-1.1772} \quad (8)$$

$$= -2 \log_{10}[2.51\xi/Re + \varepsilon_{TW} / (3.71d_H)] \quad \text{if } Re < Re_{CTB} \quad (9)$$

For two-phase flow conditions the factor  $f_R$  can be extended to

$$f_R = f_{DW} \Phi_{2PF}^2 \quad (\text{at two-phase flow}) \quad (10)$$

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 only on steam quality and pressure dependent two-phase multiplier  $\Phi_{2PF}^2$  is given by Martinelli-Nelson [16] as measured curves. A possible attempt to describe these curves analytically could be given by the approximation function

$$\Phi_{2PF}^2 = \exp [ f_1 X / (1+f_2 X+f_3 X^2)^{1/2} ] \rightarrow (\rho'/\rho'') (f_{DW})_S / (f_{DW})_W \quad \text{if } X \rightarrow 1 \quad (11)$$

as proposed by Hoeld [5,10] with the factors

$$f_1 = 44.216 + 0.7428 \cdot 10^{-6} P, \quad f_2 = 12.645 + 4.9841 \cdot 10^{-6} P \text{ and} \\ f_3 = 17.975 + 25.7440 \cdot 10^{-6} P \quad (P \text{ in Pa}) \quad (12)$$

thereby being aware that for the special case that the steam quality  $X$  approaches 1 the friction term is nearing the single-phase steam friction factor  $(f_{DW})_S$ , thus the two-phase multiplier has to be corrected (after a maximum at about 0.8) in an appropriate way.

### 2.2.3 Drift flux correlation:

In case of two-phase flow the three conservation eqs. have to be updated by an additional relation with the aim to get for the appearing fourth variable, namely the steam mass flow  $G_S$ , an adequate relation. This can be achieved by any two-phase correlation, for example a slip correlation. However, to take care also of stagnant or counter-current flows the here presented drift-flux correlation seems to be more adequate.

In connection with the development of the CCM module a very effective drift-flux package (named MDS) has been established [8,9] being based on special drift-flux correlations as derived by Sonnenburg [19], Ishii-Mishima [13] etc. For a vertical channel this correlation has the basic form

$$v_D = 1.5v_{WLIMIT}C_0C_{VD} [(1+C_{VD}^2)^{3/2} - (1.5+C_{VD}^2) C_{VD}] \text{ with } v_D \rightarrow v_{D0} = 9C_0v_{WLIMIT}/16 \text{ if } \alpha \rightarrow 0 \quad (13)$$

with the coefficient

$$C_{VD} = 2(1-C_0 \alpha) v_{SLIM} / (3C_0 \alpha v_{WLIMIT}) \quad (14)$$

The correlation yields (in combination with an adequate correlation for the phase distribution parameter  $C_0$ ) the drift velocity  $v_D$  in dependence of the void fraction  $\alpha$  and the limit velocities  $v_{SLIM}$  and  $v_{WLIMIT}$  (independent of the total mass flow  $G$ ). More details about the determination of the phase distribution parameter  $C_0$ , the limit velocities  $v_{SLIM}$  and  $v_{WLIMIT}$ , the entrainment fraction  $E_d$  and its onset can be found in the corresponding references (see e.g. Hoeld [8,9]). All of them are dependent on the given 'system pressure  $P$ ', the 'hydraulic diameter  $d_{HW}$ ' (with respect to a wetted surface  $A_{WSF}$ ), its inclination angle ( $z_{EL}/z$ ), specifications about the geometry type ( $L_{GTYPE}$ ) and (for low void fractions  $\alpha$ ) the knowledge if the channel is heated or not ( $L_{HEATD}=1$  if core or  $=0$  if riser)

Considering the definition eqs.

$$G_S = G - G_W = XG = A \alpha \rho'' v_S = G - A (1 - \alpha) \rho' v_W \quad (15)$$

$$v_D = (1 - \alpha C_0) v_S - (1 - \alpha) C_0 v_W \quad (16)$$

it follows (now also in dependence of the total mass flow  $G$ ) a relation for the steam mass flow

$$G_S = \alpha \rho'' (C_0 G / \rho' + A v_D) / C_{GC} \text{ with} \quad (17)$$

$$C_{GC} = 1 - (1 - \rho'' / \rho') \alpha C_0 \rightarrow 1 \text{ if } \alpha \rightarrow 0 \text{ and } \rightarrow \rho'' / \rho' \text{ if } \alpha \rightarrow 1 \quad (18)$$

Other characteristic local two-phase flow parameters (such as water mass flow  $G_W$ , water and steam velocities  $v_W$  and  $v_S$  and the steam quality  $X$  etc.) can be determined in a similar way. Special care had to be taken to the determination of the steam mass flow gradient (as demanded in chapter 3), especially for the situation that the upper or lower end of a SC is going to cross a BC node boundary (i.e., that  $\alpha \rightarrow 0$  or  $\rightarrow 1$ ) where the behaviour of this gradient plays an important part

$$\begin{aligned} G_S^{(\alpha)} \rightarrow G_{S0}^{(\alpha)} &= (\rho'' / \rho') (C_{00} G + A \rho' v_{D0}) = A \rho'' v_{S0} \text{ or } = 0 \text{ (if } L_{HEATD} = 0 \text{ or } 1) \text{ and } \alpha \rightarrow 0 \\ &\rightarrow G_{S1}^{(\alpha)} = A (\rho'' / \rho') (1 + C_{01}^{(\alpha)}) (G - \rho' v_{SLIM}) \text{ if } \alpha \rightarrow 1 \end{aligned} \quad (19)$$

In the steady state case or after an abrupt change in steam mass flux  $G_{SFX} = G_S / A$  (e.g., after a change in mass flow or cross section) it is obvious that the steam (and total) mass fluxes (and not the void fraction) will remain unchanged. Thus, taking the term  $G_S$  as an independent parameter, the other parameters ( $v_D$ ,  $C_0$  and the void fraction  $\alpha$ ) have to be determined from the inverse (INV) function

$$\alpha = f_{DRIFT}^{(INV)}(G_S \text{ or } v_D, G, P, z_{EL}/z, d_{HW}, \dots) \quad (20)$$

Besides vertical up- or downwards, co-, stagnant or even counter-current two-phase flow situations (along different types of channels 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.

#### 2.2.4 Heat transfer coefficients:

In connection with the thermal-fluid dynamics also correlations for heat transfer coefficients along different flow regimes (into and out of a tube wall) are needed, for example for the description of the heat transfer out of fuel rods as demonstrated in chapter 5.2. They can be calculated automatically if applying appropriate heat transfer coefficient packages such as HETRAC [4].

### 3. Drift-flux based thermal-hydraulic coolant channel model and module CCM

Starting from the fundamental eqs. of the classical 3-equation mixture fluid theory (as shown in chapter 2.1) and in combination with the (in chapter 2.2 presented) constitutive equations a thermal-hydraulic coolant channel model CCM had to be derived with the aim to simulate in a very general way the steady state and transient behaviour of characteristic time- and local-dependent parameters of a single- and two-phase fluid flowing up-, horizontal or downwards of a (basic) coolant channel.

In order to make the theoretical model applicable for a digital code (module CCM) the partial differential eqs. (PDE) have to be discretized by means of a finite element method, yielding thus (besides the constitutive eqs.) a set of non-linear ordinary differential eqs. (ODE-s) for each SC within a BC and thus also the entire BC. A special approximation procedure (PAX) had to be developed to relate the mean and boundary functions together, to take care of the possibilities that parameters can cross node boundaries etc.

#### 3.1 Initial and boundary conditions

As initial conditions (=starting values) for the transient calculations parameters resulting from steady state considerations have to be provided.

As boundary conditions the following input parameters are demanded:

- Power profile along the entire BC, i.e., the local power density term  $q_{BE}$  at BC entrance and either the power density terms  $q_{Bk}$  or the nodal power terms  $Q_{Bmk} = \frac{1}{2} V_{Bmk}(q_{Bk} + q_{Bk-1})$  for each BC node  $k$  (thereby assuming linear behaviour within a BC node),
- Channel inlet temperature  $T_{BEIN}$  (or enthalpy  $h_{BEIN}$ ).
- Total mass flow ( $G_{BEIN}$ ) and, in case of a two-phase flow mixture entering the BC, steam mass flow ( $G_{SBEIN}$ ) at BC entrance. For the later case (i.e., if  $0 < G_{SBEIN} < G_{BEIN}$ ) the corresponding void fraction  $\alpha_{BE}$  has then to be determined from the (inverse) drift-flux correlation (20).
- Pressures at BC in- and outlet ( $P_{BEIN}$ ,  $P_{BAIN} = P_{BEIN} - \Delta P_{BAEIN}$ ). For the steady state (= start) calculation these three input parameters are used to adjust the friction coefficients to the actual flow conditions (see chapter 3.6). In case of a closed loop  $P_{BAIN} = P_{BEIN}$ .
- System pressure time-derivative  $\frac{d}{dt} P_{SYS}$  (which will, as demanded in chapter 2.1.6, now represents its local derivative terms).

These boundary conditions allow then to simulate thermal-hydraulic situations of large channel assemblies (within nuclear power plants, test loops etc.) which can consist of a complex web of pipes and branches (represented by different BC-s distinguished by their key numbers KEYBC). If the ensemble consists of inner loops (e.g., in case of parallel channels) their boundary conditions have to obey to an additional conservation law, namely the fact that the sum of all pressure decrease terms along a closed loop must be zero. This means pressure differences between entrances and outlets of parallel channels must be equal, allowing thus to determine (as explained in the chapters 3.6 and 4) automatically the flow distribution of a total mass flow out of a branch into adjoining pipes.

In the first phase of the model development the boundary conditions are based on the assumption that the coolant channel represents a 'non-porous' channel with the coolant entering the BC only at its entrance. Other mass sources or sinks along the entire channel are not foreseen. This means that the entrance parameters of the other nodes along a BC (temperatures, total and/or steam mass flows and, if the flow areas stay unchanged, also void fractions etc.) can be considered to be equal to the outlet parameters of the node before. The presented theoretical model has, however, 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) can be exchanged also at nodal boundaries of neighbouring channels (and not only at BC entrance and outlet).

## 3.2 Spatial discretization of PDE-s of 1-st order

### 3.2.1 Coolant channel geometry and nodalization:

For discretization purposes the basic channel (with its  $N_{SCT}$  sub-channels and the total length  $z_{BT}=z_{BA}-z_{BE}$ ) has to be subdivided into a number,  $N_{BT}$ , of (not necessarily equidistant) nodes. Their positions  $z_{BE}$ ,  $z_{Bk}$  (with  $k=1, N_{BT}$ ), elevations  $z_{ELBE}$ ,  $z_{ELk}$ , nodal length  $\Delta z_{Bk}=z_{Bk}-z_{Bk-1}$ , nodal elevations  $\Delta z_{ELBk}=z_{ELBk}-z_{ELBk-1}$ , cross flow areas  $A_{Bk}$  (eventually different at different node boundaries) or averaged areas over these nodes,  $A_{BMk}=0.5(A_{Bk}+A_{Bk-1})$  and corresponding nodal volumes  $V_{BMk}=\Delta z_{Bk}A_{BMk}$  can then be assumed to be known by input.

Obviously, the corresponding sub-channels (SC-s) are then subdivided too, now into a number of  $N_{CT}$  SC nodes with geometry values being identical with the corresponding BC values, except, of course, at their entrance and outlet positions (The 1-st node of a SC is then identical with the BC node  $N_{BCE}$ ). The SC entrance position  $z_{CE}$  and their function value  $f_{CE}$  are either (if situated in the first of these SC-s) identical to 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 ( $z_{CA}$ ) or characterized by the fact that the corresponding outlet function value has reached an (upper or lower) limit ( $f_{LIMCA}$ ), representing then either a boiling boundary or a mixture level. Such a SC limit function ( $f_{LIMCA}$ ) follows from the given BC limit values and will be either, in the case of single-phase flow, the saturation temperature  $T_{SATCA}$ , or, in the case of two-phase flow mixture, a void fraction of the value  $\alpha = 1$  or  $= 0$ . The SC inlet and outlet positions can move during a transient from one BC node to another. Knowing their entrance and outlet positions ( $z_{CE}$  and  $z_{CA}$ ) lying not within the same BC node ( $z_{BNk-1} \leq z_{CE} < z_{BNk}$  at  $k = N_{BCE}$  and  $z_{Bk-1} \leq z_{CA} < z_{Bk}$  at  $k = N_{BCA}$ ) the total number of SC nodes ( $N_{CT}=N_{BCA}-N_{BCE}$ ) can be ascertained and thus also the corresponding positions ( $z_{Nn}$ ,  $z_{ELCE}$ ,  $z_{ELNn}$  at  $n=1, N_{CT}$ ), their lengths ( $\Delta z_{Nn}=z_{Nn}-z_{Nn-1}$ ), elevations ( $\Delta z_{ELNn} = z_{ELNn}-z_{ELNn-1}$ ), boundary and mean nodal cross sections ( $A_{Nn}$ ,  $A_{Mn} = 0.5(A_{Nn}+A_{Nn-1})$ ) and nodal volumes ( $V_{Mn} = z_{Nn}A_{Mn}$ ).

### 3.2.2 Discretization procedure (Finite volume element method):

For the discretization of the fundamental eqs.(1) to (3) a 'modified finite volume element method' is applied. Thereby, if integrating the partial differential eqs. (PDE-s) over the corresponding SC nodes, three types of discretization elements can be expected. Integrating a general function  $f(z,t) = f[T(z,t), P(z,t)]$  (e.g.,  $\rho$  or  $h$ ) within the PDE-s yields a nodal mean function value  $f_{Mn}(t)$ , integrating over a gradient a difference of functions values at the two node boundaries  $f_{Nn}(t)$ ,  $f_{Nn-1}(t)$ . For transient situations a third element has to be considered resulting from the speciality of the finite volume approach chosen for this problem. It is based on the fact that, different to other such procedures, the volume boundaries or (in the case of an 1-dimensional channel representation) the entrance and outlet boundaries of a SC must be assumed to be time-dependent. They can and will move from one BC node to another with the consequence that  $\Delta z_{Nn} \rightarrow 0$ . Hence, the integration over eventually time-varying nodal boundaries (e.g. SC entrance or outlet positions) yields the relation

$$\int_{z_{Nn-1}(t)}^{z_{Nn}(t)} \frac{\partial}{\partial t} f(z,t) dz = \Delta z_{Nn}(t) \frac{d}{dt} f_{Mn}(t) - [f_{Nn}(t) - f_{Mn}(t)] \frac{d}{dt} z_{Nn}(t) - [f_{Mn}(t) - f_{Nn-1}(t)] \frac{d}{dt} z_{Nn-1}(t) \quad (21)$$

$$\cong \Delta z_{Nn}(t) \left[ f_{Mn}^T \frac{d}{dt} T_{Mn}(t) + f_{Mn}^P \frac{d}{dt} P_{SYS}(t) \right] - [f_{Nn}(t) - f_{Mn}(t)] \frac{d}{dt} z_{Nn}(t) - [f_{Mn}(t) - f_{Nn-1}(t)] \frac{d}{dt} z_{Nn-1}(t) \quad (n=1, N_{CT})$$

i.e. time-derivatives of mean function values related to time-derivatives of SC entrance or outlet positions. It is thus obvious that appropriate methods had to be developed that could help to establish relations between mean nodal ( $f_{Mn}$ ) and node boundary ( $f_{Nn}$ ) function values.

Thereby it has to be distinguished between two cases:

- Steady state case: Setting within the conservation eqs.(1) to (3)  $\frac{\partial}{\partial t} = 0$  results in a set of  $N_{CT}$  non-linear algebraic eqs. Its solution yields the function values  $f_{Nn}$  positioned at the (known) node boundaries  $z_{Nn}$  ( $n=1, N_{CT}$ ) with the SC outlet position  $z_{CA} = z_{Nn}$  (at  $n=N_{CT}$ ) being either equal to the

BC outlet position  $z_{BA}$  or identical with the position  $z_{Nn}(n)$  at which the function  $f_{Nn}(n)$  has reached its limit function  $f_{CA}=f_{LIMCA}$  (then  $N_{CT}=n$ ). Together with the SC entrance function  $f_{CE}$  (at position  $z_{CE}$ ) and eventually a SC entrance gradient  $f_{CE}^{(z)} = f_{CEI}^{(z)}$  (know from input) the nodal mean function values  $f_{Mn}$  have to be determined which are then needed as starting values for the transient calculation.

- **Transient case:** The discretization of the PDE-s yields for each SC (within a BC) a set of  $N_{CT}$  ordinary differential eqs. (ODE-s) for either  $N_{CT}$ , if the SC outlet position is identical with BC outlet ( $z_{CA}=z_{BA}$ ), or, if this position lies within the BC ( $z_{CA}<z_{BA}$ , now with  $f_{CA}=f_{LIMCA}$ ), only for  $N_{CT}-1$  mean function values  $f_{Mn}$ . Instead of the ODE for the mean nodal function of the last SC node, an ODE for the SC outlet position  $z_{CA}$  (where the function reaches its known limit function  $f_{LIMCA}$ ) is then demanded. These sets will be combined to an overall set of ODE-s valid for the entire BC. By means of an appropriate integration procedure (see, e.g., FEBE [2]) corresponding BC function values  $f_{BMn}$  will result and thus also the mean function values  $f_{Mn}$  over the corresponding SC nodes and, if  $z_{CA}<z_{BA}$ , instead of the last  $f_{Mn}$  value (at  $n=N_{CT}$ ) the SC outlet position  $z_{CA}$ .

If the time-derivative of a function at SC (or BC) entrance is not explicitly known it can be estimated as

$$\frac{d}{dt} f_{CE} = [f_{CE}(t+\Delta t) - f_{CEB}]/\Delta t \quad \text{or} \quad = \frac{d}{dt} f_{CEB} \quad \text{if } f_{CEB}=f_{CE}(\text{at } t=t_B) \text{ and } \Delta t=t-t_B > 0 \quad \text{or if } \Delta t \rightarrow 0 \quad (22)$$

### 3.3 Quadratic polygon approximation procedure PAX

There exist different possibilities and concepts to connect the resulting mean nodal ( $f_{Mn}$ ) and the node boundary ( $f_{Nn}$ ) functions after the discretization of the PDE-s in an adequate way together in order to be able to determine besides the directly available parameters also other characteristic nodal parameters of a single- or a two-phase fluid. For this purpose a special 'quadratic **p**olygon **a**pproximation procedure has been developed within the scope of CCM, named 'PAX'.

Thereby it will be assumed that the solution function  $f(z)$  of such a PDE is split into a number of  $N_{CT}$  nodal functions  $f_n(z)$ . The 1-st ( $N_{CT}-1$ ) of them will then be approximated by a quadratic polygon, a polygon function which reaches not only over its node but (in order to take care of the tendency of the entire approximated curve) also over its adjoining one. It will additionally be assumed that, in order to smooth the approximation curves, the gradients at the node boundaries may obey the relations

$$\begin{aligned} f_{Nn}^{(z)} &= 2(f_{Mn+1} - f_{Mn})/(\Delta z_{Nn+1} + \Delta z_{Nn}) & (n = 1, N_{CT}-1, N_{CT} > 1) \\ &= (f_{CA} - f_{Nn-2})/(\Delta z_{CA} + \Delta z_{Nn-1}) & (n = N_{CT}, N_{CT} > 1 \text{ and } \Delta z_{CA} \rightarrow 0) \end{aligned} \quad (23)$$

The last nodal function (at  $n=N_{CT}$ ) (including thus also the special cases of creating a new SC or a SC having shrunk to a single node at  $n=N_{CT}=1$ ) has to be described by a straight line.

From the directly available function values one finally gets the approximation coefficients of these functions (as described in more detail in [7]) and thus for the steady state case the wanted mean nodal function values  $f_{Mn}$  in dependence of the nodal boundary values  $f_{Nn}$  and vice versa for the transient case together with their corresponding gradients and slopes and other important parameters being demanded by the thermal-hydraulic coolant channel model.

These are for **steady state** conditions (with  $f_{CA}=f_{LIMCA}$  if  $z_{CA}<z_{BA}$ )

$$\begin{aligned} f_{Mn} &= \frac{1}{2} (f_{CA} + f_{Nn-1}) & (n=N_{CT}) \\ &= [(\Delta z_{Nn+1} + \Delta z_{Nn})(2f_{Nn} + f_{Nn-1}) - \Delta z_{Nn} f_{Mn+1}]/(3\Delta z_{Nn+1} + 2\Delta z_{Nn}) & (n=1, N_{CT}-1, N_{CT} > 1) \end{aligned} \quad (24)$$

and for **transient situations** (with  $f_{CA}=f_{LIMCA}$  if  $z_{CA}<z_{BA}$ )

$$f_{Nn} = \frac{1}{2} [3f_{Mn} - f_{Nn-1} + (f_{Mn+1} - f_{Mn})\Delta z_{Nn}/(\Delta z_{Nn+1} + \Delta z_{Nn})] \quad (n=1, N_{CT}-2, N_{CT} > 2)$$

$$\begin{aligned}
&= [\Delta z_{CA}(f_{Mn}-f_{Nn-1}) + \frac{1}{2} \Delta z_{Nn} f_{CA}] / (2\Delta z_{CA} + \Delta z_{Nn}) & (n=N_{CT}-1, N_{CT}>1) \\
&= f_{CA} = 2 f_{Mn} - f_{Nn-1} & (n=N_{CT}) \quad (25)
\end{aligned}$$

The gradients are assumed to obey the relation (23).

Two types of slopes of a function along a node n are in use

$$\begin{aligned}
f_{Nn}^{(s)} &= (f_{Nn} - f_{Nn-1}) / \Delta z_{Nn} \quad \text{and} \quad \rightarrow f_{Nn}^{(z)} \sim f_{Nn-1}^{(z)} \quad (\text{if } \Delta z_{Nn} \rightarrow 0) & (n=1, N_{CT}) \quad (26) \\
f_{Mn}^{(s)} &= 2(f_{Mn} - f_{Nn-1}) / \Delta z_{Nn} \quad \text{and} \quad \rightarrow f_{Nn}^{(z)} \sim f_{Nn-1}^{(z)} \quad (\text{if } \Delta z_{Nn} \rightarrow 0) & (n=1, N_{CT}-1) \\
&= f_{CA}^{(s)} = f_{CA}^{(z)} = (f_{CA} - f_{Nn-1}) / \Delta z_{CA} & (n=N_{CT} \text{ and } \Delta z_{CA} > 0) \\
&= f_{CE}^{(s)} = f_{CE}^{(z)} = f_{CEI}^{(z)} \quad (\text{input to PAX}) & (n=N_{CT}=1 \text{ and } z_{CA}-z_{BE} \approx 0 \text{ or } z_{CE}-z_{BA} \approx 0) \quad (27)
\end{aligned}$$

For the special case that during a transient (at the entrance of a BC or its outlet) a SC starts to disappear or to be created anew (i.e.  $z_{CA} \rightarrow z_{BE}$  or  $z_{CE} \rightarrow z_{BA}$ ) a gradient of the solution function at SC entrance ( $f_{CEI}^{(z)}$ ) is demanded by the PAX procedure and has to be provided by input. This SC entrance gradient can be attained (as demonstrated in the chapters 3.5.2 and 3.5.3) by combining the mass and energy balance eqs.(1) and (2), yielding relations based on SC entrance terms such as the time-derivative of the SC entrance function (see eq.(22)).

In case of a SC outlet boundary varying within a BC (i.e., if  $z_{CA} < z_{BA}$ ) as a result of the integration procedure instead of the last  $f_{Mn}$  parameter the SC outlet boundary  $z_{CA}$  can be expected. The term  $f_{Mn}$  (at  $n=N_{CT}$ ) has thus to be determined from a special interrelation between the mean nodal function value  $f_{Mn}$  of the last SC node and its outlet position  $z_{CA}$ . Such an interrelation can be derived by inserting for the case  $n= N_{CT}$  from eq.(25) into eq.(24) yielding

$$\begin{aligned}
f_{Mn} &= \frac{1}{2} f_{CA} + \frac{1}{2} f_{CE} & (n= N_{CT} = 1) \\
&= \frac{1}{2} f_{CA} + \frac{1}{2} f_{Nn-1} = \frac{1}{2} f_{CA} + \frac{1}{2} [\Delta z_{CA}(f_{Mn-1}-f_{Nn-2}) + \frac{1}{2} \Delta z_{Nn-1} f_{CA}] / (2\Delta z_{CA} + \Delta z_{Nn-1}) & (n=N_{CT}>1) \quad (28)
\end{aligned}$$

Its differentiation gives then (for the case  $z_{CA} < z_{BA}$ ) the interrelation between the corresponding time-derivatives  $\frac{d}{dt} f_{Mn}$  of the last SC node and  $\frac{d}{dt} z_{CA}$

$$\frac{d}{dt} f_{Mn} = f_{FMCA}^t - f_{FZCA}^s \frac{d}{dt} z_{CA} \quad (\text{at } n=N_{CT} \text{ and } z_{CA} < z_{BA}) \quad (29)$$

with the coefficients

$$\begin{aligned}
f_{FMCA}^t &= \frac{1}{2} \frac{d}{dt} (f_{LIMCA} + f_{CE}) & (n= N_{CT} = 1 \text{ and } z_{CA} < z_{BA}) \\
&= \frac{1}{2} \frac{d}{dt} f_{LIMCA} + \frac{1}{2} [\Delta z_{CA} \frac{d}{dt} (f_{Mn-1} - f_{Nn-2}) + \frac{1}{2} \Delta z_{Nn-1} \frac{d}{dt} f_{LIMCA} \\
&\quad - \frac{1}{2} (f_{LIMCA} - f_{Nn-1}) \frac{d}{dt} z_{Nn-2}] / (2\Delta z_{CA} + \Delta z_{Nn-1}) & (n= N_{CT} > 1 \text{ and } z_{CA} < z_{BA}) \quad (30)
\end{aligned}$$

$$f_{FZCA}^s = 0 \text{ or } = \frac{1}{2} (2f_{Nn-1} - f_{Mn-1} + f_{Nn-2}) / (2\Delta z_{CA} + \Delta z_{Nn-1}) \quad (n= N_{CT} = 1 \text{ or } > 1 \text{ and } z_{CA} < z_{BA}) \quad (31)$$

It has to be noted that  $z_{Nn-2} = z_{CE}$ ,  $f_{Nn-2} = f_{CE}$ ,  $\frac{d}{dt} z_{Nn-2} = \frac{d}{dt} z_{CE}$ , and  $\frac{d}{dt} f_{Nn-2} = \frac{d}{dt} f_{CE}$  if  $N_{CT} = 2$ . Otherwise, if  $N_{CT} > 2$ ,  $\frac{d}{dt} z_{Nn-2} = 0$ . Since then the time-derivative  $\frac{d}{dt} f_{Nn-2}$  is not directly available it has to be estimated, e.g., by applying a similar procedure as proposed in eq.(22), or by assuming  $f_{Nn-2}$  to be an average value of  $f_{Mn-1}$  and  $f_{Mn-2}$ .

Based on these set of eqs. the subroutine PAX could be established. It plays an important role for the construction of an effective coolant channel module (CCM) by calculating automatically the nodal mean or nodal boundary values, their gradients and slopes at SC entrance and outlet and yields finally the needed input values characterising the entrance parameters of the subsequent SC. A driver code (PAXDRI) helps to check the validity of the code PAX.

### 3.4 Steady state single- and two-phase fluids

Setting within the basic PDE-s (valid for both single- or two-phase fluids) the time-derivatives equal to zero and applying the above presented discretization procedure yields (together with the above presented approximation procedure PAX) corresponding characteristic steady state nodal parameters which are needed as starting values for the transient case.

#### 3.4.1 Total nodal mass flow for both single- and two-phase flow conditions:

From eq.(1) it follows

$$G_{Nn,0} = G_{Nn-1,0} = G_{CE,0} = G_{CA,0} = G_{BE,0} = G_{BA,0} \quad (L_{FTYPE} = 0, 1 \text{ or } 2 \text{ and } n=1, N_{CT}) \quad (32)$$

#### 3.4.2 Additional characteristic nodal parameters of a SC with single-phase flow ( $L_{FTYPE} = 0$ ):

For this case the nodal coolant enthalpy values can be derived from the energy balance eq.(2)

$$h_{Nn,0} = h_{Nn-1,0} + Q_{Mn,0} / G_{Nn,0} \quad (\text{at } n=1, N_{CT}-1 \text{ and, if } h_{Nn,0} < h'_{Nn,0} \text{ or } h_{Nn,0} > h''_{Nn,0}, \text{ at } n=N_{CT}, \text{ i.e. } L_{FTYPE} = 1 \text{ or } 2) \\ = h'_{Nn,0} \text{ (water) or } h''_{Nn,0} \text{ (steam)} \quad (\text{if } L_{FTYPE} = 0) \quad (33)$$

The nodal temperature values  $T_{Nn,0}$  follow then from the thermodynamic water/steam tables [6], their mean values  $T_{Mn,0}$  from the given nodal boundary values  $T_{CE,0}$  and  $T_{Nn,0}$  (by applying the inverse PAX procedure) and, finally, the mean nodal enthalpy values,  $h_{Mn,0}$  and  $h_{Nn,0}$ , again from thermodynamic water/steam tables. Obviously for this type of channel it has to be stated that  $G_{SNn,0} = G_{Nn,0}$  or  $=0$  and  $\alpha_{Nn,0} = 0$  or  $1$  if  $L_{FTYPE} = 1$  or  $2$ .

#### 3.4.3 Additional characteristic nodal parameters of a SC with two-phase flow ( $L_{FTYPE} = 0$ ):

From the energy balance eq.(2) one gets the nodal steam mass flow terms

$$G_{SNn,0} = G_{SNn-1,0} + Q_{Mn,0} / h_{SWNn,0} \quad (\text{at } n = 1, N_{CT}-1 \text{ but also } n = N_{CT} = N_{BT} - N_{BCE} \text{ if } G_{SNn,0} < G_{Nn,0}) \\ = G_{N,0} \text{ or } 0 \quad (\text{if } n = N_{CT} \text{ and } G_{SNn,0} \geq \text{ or } \leq 0) \quad (34)$$

The nodal void fraction values  $\alpha_{Nn,0}$  follow then from the inverse drift flux correlation (eq.(21)), the mean nodal void fraction values ( $\alpha_{Mn,0}$ ), which are needed as starting parameters for the transient calculations, by applying the polygon approximation procedure PAX.

#### 3.4.4 SC outlet position and nodal power into the last SC node (for both single- and two-phase flow):

At fixed SC node boundaries (i.e., at  $n=1, N_{CT}-1$ ) but also at their entrance or outlet positions ( $n=0$  or  $=N_{CT}$ ) where the enthalpy values for sub-cooled water, superheated steam or the void fraction do not reach their limits, the SC positions  $z_{Nn}$  (and thus also the outlet positions  $z_{CA}$ ) are identical with the corresponding BC node boundaries  $z_{Bk}$  ( $k=N_{BCE}+n$ ) (and  $z_{CA}=z_{BA}$ ).

If (at the node  $n$ ) in the case of a SC with single-phase flow the coolant temperature reaches its limit value  $f_{LIMn}=T_{SATn}$  or, in the case of a SC with two-phase fluid, the steam mass flow  $G_{SNn,0}$  reaches its limits  $G_{N,0}$  or  $0$ , the number of SC nodes is given by  $N_{CT} = n$ . Thus the nodal heat power term  $Q_{Mn,0}$  into the last node (i.e., at  $n=N_{CT}$ ) can be determined by replacing in eq.(33) the term  $h_{Nn,0}$  by its saturation value  $h'_{Nn}$  or  $h''_{Nn}$  and, in case of two-phase flow, in eq.(34) the term  $G_{SNn,0}$  by its limit value  $G_{Nn,0}$  or  $0$ . Knowing now  $Q_{Mn,0}$  then, after having solved a quadratic or (in the case of a variable cross section) cubic algebraic eq., the steady state SC outlet boundary  $z_{CA,0}$  can be determined, representing one of the initial conditions of the system of ODE-s.

### 3.5 Transient behavior of single- and two-phase fluids

As a result of the (overall) integration the BC and thus also SC nodal mean values of the coolant temperatures ( $T_{Mn}$ ) and void fractions ( $\alpha_{Mn}$ ) and the SC outlet position  $z_{CA}$  can be expected.

Starting from the basic PDE-s (valid for both single- or two-phase fluids) and applying the above presented discretization procedure by taking into account the integration elements as established in eq.(21) yields finally a set of non-linear ordinary differential eqs. (ODE -s) of 1-st order, describing (together with their constitutive eqs.) the thermal-hydraulic behaviour of characteristic parameters of both single- (subcooled water or superheated steam) and two-phase fluids within a SC (and then combined into a BC). Since these relations should stay valid for stagnant or counter-current flow conditions too an adequate drift-flux correlation had to be incorporated (see chapter 2.2.3).

The quality of a mixture-fluid coolant channel model is very much dependent on the method how effective the problem of the varying SC entrance and outlet boundaries crossing BC node boundaries can be solved. In the here presented model the special procedure PAX takes care of it, providing the model with not only the absolute nodal boundary or mean values but also the slopes  $h_{Nn}^{(s)}$ ,  $h_{Mn}^{(s)}$  respectively  $\alpha_{Nn}^{(s)}$  at the corresponding SC node boundaries, replacing automatically slopes by gradients if  $\Delta z_{Nn} \rightarrow 0$  (see eqs.(26) and (27)).

### 3.5.1 SC mean nodal power and nodal power density values:

The SC mean nodal power and power density values ( $Q_{Mn}$ ,  $q_{CE}$  and  $q_{Nn}$ ) are usually identical with the corresponding (known) BC parameters ( $Q_{Bnk}$ ,  $q_{BE}$  and  $q_{BNk}$  with  $k=n+N_{BCE}$ ), except for the 1-st and last SC node. Knowing the SC outlet position  $z_{CA}$  (as a result of the integration procedure) and thus also  $N_{CT}$  one gets at this position

$$q_{CA} = q_{Nn} = q_{Nn-1} + (z_{CA} - z_{Nn-1}) (q_{BNk} - q_{BNk-1}) / (z_{BNk} - z_{BNk-1}) \quad (\text{at } n = N_{CT} \text{ with } k=n+N_{BCE}) \quad (35)$$

with the SC entrance power density values  $q_{CE}$  being either equal to  $q_{BE}$  or (or if  $N_{BCE} > 0$ ) equal to the outlet value of the SC before. Hence one gets as mean nodal power values then also for these nodes

$$Q_{Mn} = \frac{1}{2} A_{Mn} (z_{Nn} - z_{Nn-1}) (q_{Nn} + q_{Nn-1}) \quad (\text{at } n = 1 \text{ or } = N_{CT}) \quad (36)$$

### 3.5.2 SC with single-phase flow ( $L_{FTYPE} = 1$ or 2):

Considering the integration element as presented in eq.(21) then from the mass balance eq.(1) a relation for the total nodal mass flow at node boundaries can be derived

$$\begin{aligned} G_{Nn} &= G_{Nn-1} - V_{Mn} [\rho_{Mn}^T \frac{d}{dt} T_{Mn} + \rho_{Mn}^P \frac{d}{dt} P_{SYS}] + (\rho_{Nn} - \rho_{Mn}) A_{Nn} \frac{d}{dt} z_{Nn} + (\rho_{Mn} - \rho_{Nn-1}) A_{Nn-1} \frac{d}{dt} z_{Nn-1} \\ &= G_{Nn-1} - G_{1Tn} - G_{1Pn} + G_{1Zn} + G_{1Zn-1} \end{aligned} \quad (n=1, N_{CT}) \quad (37)$$

with  $\frac{d}{dt} z_{Nn} = \frac{d}{dt} z_{CE}$  or  $= \frac{d}{dt} z_{CA}$  if  $n=0$  or  $= N_{CT}$ , otherwise  $=0$ .

Similarly it follows from the energy balance eq.(2) the time-derivative for the mean nodal coolant temperature (thereby having eliminated  $G_{Nn}$  by inserting from the eq. above)

$$\begin{aligned} \frac{d}{dt} T_{Mn} &= (q_{DMn} - G_{Nn-1} h_{Nn}^{(s)} / A_{Mn} + q_{Pn} + q_{Zn}) / (\rho_{Mn} h_{Mn}^T C_{TMn}) \\ &= T_{TMn}^t + T_{TZCA}^s \frac{d}{dt} z_{Nn} + T_{TZCE}^s \frac{d}{dt} z_{Nn-1} \end{aligned} \quad (n=1, N_{CT}) \quad (38)$$

with the coefficients

$$C_{TMn}^t = 1 - \rho_{Mn}^T (h_{Nn} - h_{Mn}) / \rho_{Mn} h_{Mn}^T = 1 - (T_{Nn} - T_{Mn}) \rho_{Mn}^T / \rho_{Mn} \quad (39)$$

$$q_{Pn} = [1 - \rho_{Mn} h_{Mn}^P + \rho_{Mn}^P (h_{Nn} - h_{Mn})] \frac{d}{dt} P_{SYS} \quad (40)$$

$$q_{Zn} = \frac{1}{2} \rho_{Mn} h_{Nn}^{(s)} (A_{Nn} / A_{Mn}) \frac{d}{dt} z_{Nn} + [\frac{1}{2} \rho_{Mn} h_{Mn}^{(s)} - (\rho_{Mn} - \rho_{Nn-1}) h_{Nn}^{(s)}] (A_{Nn-1} / A_{Mn}) \frac{d}{dt} z_{Nn-1} \quad (41)$$

and the abbreviations

$$T_{TMn}^t = (q_{DMn} - G_{Nn-1} h_{Nn}^{(s)} / A_{Mn} + q_{Pn}) / (\rho_{Mn} h_{Mn}^T C_{TMn}) = T_{Qn}^t - T_{Gn}^t + T_{Pn}^t \quad (42)$$

$$T_{TZCA}^s = \frac{1}{2} T_{Nn}^{(s)} A_{Nn} / (A_{Mn} C_{TMn}) \quad (\text{at } n = N_{CT}, \text{ otherwise } =0) \quad (43)$$

$$T_{TZCE}^s = \frac{1}{2} [T_{Mn}^{(s)} - 2(1 - \rho_{Nn-1} / \rho_{Mn}) T_{Nn}^{(s)}] A_{Nn-1} / (A_{Mn} C_{TMn}) \quad (\text{at } n = 1, \text{ otherwise } =0) \quad (44)$$

Knowing  $T_{Mn}$  from the integration procedure then also  $T_{Nn}$ ,  $T_{Nn}^{(s)}$  and  $T_{Mn}^{(s)}$  (and the gradients), as defined by the eqs.(26) and (27), follow from the PAX procedure and thus, by applying the water / steam tables [6], also the corresponding enthalpy values. For the special case that during a transient (at either BC entrance or outlet) a SC (with single-phase flow) starts to disappear or to be created anew from to the PAX procedure (see eq.(27)) the temperature gradient at SC entrance is demanded as input. This term can be derived if inserting from the mass into the energy balance eq., yielding

$$T_{CE}^{(z)} = (A_{CE}/G_{CE})[(q_{DCE} + q_{PCE})/h_{CE}^T - \rho_{CE} \frac{d}{dt} T_{CE}] \quad (\text{if } N_{CT} = 1) \quad (45)$$

Comparing the eqs.(29) and (38) a relation for the boiling boundary time-derivative (as long as  $z_{CA} < z_{BA}$ ) can be established

$$\frac{d}{dt} z_{CA} = (T_{FMCA}^t - T_{TMCA}^t) / (T_{FZCA}^s + T_{TZCA}^s) \quad (n = N_{CT} \text{ and } z_{CA} < z_{BA}) \quad (46)$$

Hence, if inserting into eq.(38), also  $\frac{d}{dt} T_{Mn}$  ( $n=1, N_{CT}$ ) is given. For the nodal mean void fraction values and their time-derivatives and the nodal steam mass flow values it follow the trivial relations

$$\frac{d}{dt} \alpha_{Mn} = 0 \text{ and either } \alpha_{Nn} = \alpha_{Mn} = 0 \text{ and } G_{SNn} = 0 \text{ or } \alpha_{Nn} = \alpha_{Mn} = 1 \text{ and } G_{SNn} = G_{Nn} \quad (L_{GTYPE} > 0, n=1, N_{CT}) \quad (47)$$

### 3.5.3 SC with two-phase flow ( $L_{FTYPE} = 0$ ):

From the mass balance eq.(1) it follows a relation for the total nodal mass flow

$$\begin{aligned} G_{Nn} &= G_{Nn-1} + V_{Mn} (\rho' - \rho'')_{Mn} \left( \frac{d}{dt} \alpha_{Mn} - \alpha_{GPn}^t - \alpha_{AZCA}^s \frac{d}{dt} z_{Nn} - \alpha_{AZCE}^s \frac{d}{dt} z_{Nn-1} \right) \\ &= G_{Nn-1} + G_{2An} - G_{2Pn} - G_{2ZCA} - G_{2ZCE} \end{aligned} \quad (n=1, N_{CT}) \quad (48)$$

with the coefficients

$$\alpha_{GPn}^t = \frac{d}{dt} (P_{SYS}) [(1-\alpha)\rho'^P + \alpha\rho''^P]_{Mn} / (\rho' - \rho'')_{Mn} \quad (49)$$

$$\alpha_{AZCA}^s = \frac{1}{2} \alpha_{CA}^{(s)} A_{CA} / A_{Mn} \quad (\text{at } n = N_{CT}, \text{ otherwise } = 0) \quad (50)$$

$$\alpha_{AZCE}^s = \frac{1}{2} \alpha_{Mn}^{(s)} A_{CE} / A_{Mn} \quad (\text{at } n = 1, \text{ otherwise } = 0) \quad (51)$$

and from the energy balance eq.(2) a relation for the mean nodal void fraction time-derivatives

$$\begin{aligned} \frac{d}{dt} \alpha_{Mn} &= (q_{DMn} / h_{SWNn} - G_{SNn}^{(s)} / A_{Mn}) / \rho''_{Mn} - \alpha_{Pn}^t + \alpha_{AZCA}^s \frac{d}{dt} z_{Nn} + \alpha_{AZCE}^s \frac{d}{dt} z_{Nn-1} \\ &= \alpha_{AMn}^t + \alpha_{AZCA}^s \frac{d}{dt} z_{Nn} + \alpha_{AZCE}^s \frac{d}{dt} z_{Nn-1} \end{aligned} \quad (n=1, N_{CT}) \quad (52)$$

with the coefficients

$$\alpha_{AMn}^t = (q_{DMn} / h_{SWNn} - G_{SNn}^{(s)} / A_{Mn}) / \rho''_{Mn} - \alpha_{Pn}^t = \alpha_{Qn}^t - \alpha_{Gn}^t - \alpha_{Pn}^t \quad (53)$$

$$\alpha_{Pn}^t = \frac{d}{dt} P_{SYS} [(1-\alpha)\rho'^h + \alpha(\rho''^h + \rho''^P h_{SW}) - 1]_{Mn} / (\rho''^h h_{SW})_{Mn} \quad (54)$$

$$G_{SNn}^{(s)} = \Delta G_{SNn} / \Delta z_{Nn} \rightarrow G_{SNn}^{(s)} = G_{SNn}^{(\alpha)} \alpha_{Nn}^{(z)} \quad \text{if } \Delta z_{Nn} \rightarrow 0 \quad (55)$$

From the integration procedure one gets  $\alpha_{Mn}$ , from the PAX procedure (eqs.(26) and (27)) then also  $\alpha_{Nn}$ , the slopes  $\alpha_{Nn}^{(s)}$  and  $\alpha_{Mn}^{(s)}$  and the corresponding gradients. The eqs.(17), (48) and (52) represent then 3 eqs. for the 3 variables  $G_{SNn}$ ,  $G_{Nn}$  and  $\frac{d}{dt} \alpha_{Mn}$ . Eliminating in the eqs.(48) and (52) the mean nodal void fraction time-derivative  $\frac{d}{dt} \alpha_{Mn}$  yields a direct relation between the terms  $G_{SNn}$  and  $G_{Nn}$

$$G_{Nn} + (\rho' / \rho'' - 1)_{Mn} G_{SNn} = G_{Xn} \quad (n = 1, N_{CT}) \quad (56)$$

introducing thereby the auxiliary mass flow term  $G_{Xn}$  which refers only to values from node entrance

$$G_{Xn} = G_{Nn-1} + (\rho' / \rho'' - 1)_{Mn} (G_{SNn-1} + Q_{Mn} / h_{SWNn}) - V_{Mn} (\rho' - \rho'')_{Mn} (\alpha_{Pn}^t + \alpha_{GPn}^t) \quad (57)$$

An other relation for  $G_{Nn}$  can be established if starting from the drift flux correlation (13) taking advantage from the fact that the drift velocity  $v_{DNn}$  and the phase distribution parameter  $C_{0Nn}$  can be

determined, only as a function of the void fraction  $\alpha_{Nn}$  and geometry parameters, independently from the total mass flow  $G_{Nn}$ . Hence, combining the resulting eq.(17) with eq.(56) yields

$$G_{Nn} = [G_{Xn} - (\rho'/\rho''-1)_{Mn} \rho''_{Nn} A_{Nn} \alpha_{Nn} v_{DNn} / C_{GCNn}] / [1 + (\rho'/\rho''-1)_{Mn} (\rho''/\rho')_{Nn} \alpha_{Nn} C_{0Nn} / C_{GCNn}] \quad (58)$$

The nodal steam mass flow  $G_{SNn}$  and its slope  $G_{SNn}^{(s)}$  follow from the eqs.(56) and (55), the mean nodal void fraction time-derivative  $\frac{d}{dt} \alpha_{Mn}$  finally from eq.(52).

For the special case that a (mixture flow) SC starts to disappear or to be created anew the void fraction gradient at SC entrance being demanded as input to the PAX procedure (see eq.(26)) can be derived, if rearranging eq.(53)

$$G_{SCE}^{(s)} = G_{SCE}^{(z)} = G_{SCE}^{(a)} \alpha_{CE}^{(z)} = A_{CE} q_{DCE} / h_{SWCE} - A_{CE} \rho''_{CE} \left( \frac{d}{dt} \alpha_{CE} + \alpha_{Pn}^t \right) \quad (N_{CT}=1) \quad (59)$$

taking into account that  $G_{SCE}^{(a)}$  follows from the drift flux correlation and  $\frac{d}{dt} \alpha_{CE}$  to be determined as proposed by eq.(22) (Note:  $\frac{d}{dt} \alpha_{LIMCA}=0$ ).

Finally, by comparing the eqs.(29) and (52) for the case that  $z_{CA} < z_{BA}$  a relation for the mixture level time-derivative can be established

$$\frac{d}{dt} z_{CA} = (\alpha_{FMCA}^t - \alpha_{AMCA}^t) / (\alpha_{FZCA}^s + \alpha_{AZCA}^s) \quad (n = N_{CT} \text{ and } z_{CA} < z_{BA}) \quad (60)$$

and thus, if inserting into eq.(52), for the terms  $\frac{d}{dt} \alpha_{Mn}$  ( $n = 1, N_{CT}$ ). The mean nodal coolant temperature and enthalpy terms are only dependent on the local pressure

$$T_{Mn} = T_{SAT}(P_{Mn}) \quad \text{resp.} \quad h_{Mn} = h'(P_{Mn}) \quad \text{or} \quad h''(P_{Mn}) \quad (n = 1, N_{CT}) \quad (61)$$

In case of a transition from one BC into another obviously only the mass flow terms remain unchanged, not the void fractions. This term has then to be calculated from the corresponding total and steam mass flow parameters  $G_{BE}$  and  $G_{SBE}$  by applying the inverse drift flux correlation (see eq.(21)).

### 3.6 Pressure drop along SC-s and BC

After having solved the mass and energy balance eqs. the exact pressure difference terms  $\Delta P_{Nn}$  and  $\Delta P_{BNn}$  along each of the SC and BC nodes can be determined if discretizing the momentum balance eq.(3). With respect to the system pressure  $P_{SYS}$  (given as boundary condition) then also the absolute nodal pressure values  $P_{BNn}$  over a BC can be determined.

Integrating the momentum balance eq.(3) (in flow direction) over the SC nodes yields (for both single- or two-phase flow situations) a relation for the pressure increase  $\Delta P_{Nn}$  along each SC node  $n$  (= pressure drop if provided with a negative sign)

$$\Delta P_{Nn} = P_{Nn} - P_{Nn-1} \cong \Delta z_{Nn} \Delta P_{BAEIN} / (z_{BA} - z_{BE}) = -\Delta P_{GNn} - \Delta P_{Ann} + \Delta P_{SNn} + \Delta P_{XNn} + [1 + (f_{FMP0} - 1) \varepsilon_{DP}] \Delta P_{FNn} + \Delta P_{FADD} \Delta z_{Nn} / (z_{BA} - z_{BE}) \quad (n=1, N_{CT}) \quad (62)$$

consisting of contributions from the static head ( $\Delta P_{SNn}$ ), mass acceleration ( $\Delta P_{Ann}$ ), wall friction ( $\Delta P_{FNn}$ ) and external pressure acceleration (pump or other outside perturbations with  $\Delta P_{XNn} > 0$  or  $< 0$ ). In the transient case an additional pressure difference term ( $\Delta P_{GNn}$ ) is appearing resulting from time-dependent changes in total mass flow.

The total pressure difference  $\Delta P_{BAE} = P_{BAI} - P_{BEI}$  between BC outlet and entrance follows then from summing up the corresponding contributions of all SC nodes of all SC-s within a BC

$$\Delta P_{BAE} = -\Delta P_{GBAE} - \Delta P_{ABAE} + \Delta P_{SBAE} + \Delta P_{XBAE} + \Delta P_{FBAE} + \Delta P_{ZBAE} \quad (63)$$

with the term  $\Delta P_{GBAE}$  over the entire BC being defined as

$$\Delta P_{GBAE} = \int_{z_{BE}}^{z_{BA}} \frac{d}{dt} [G(z,t)/A(z)] dz \cong \frac{1}{2} \sum_{n=1}^{N_{BT}} \Delta Z_{Nn} \frac{d}{dt} (G_{BNn}/A_{BNn} + G_{BNn-1}/A_{BNn-1}) \quad (64)$$

To the overall pressure balance in the eqs.(63) an additional friction term

$$\Delta P_{ZBAE} = (f_{FMP0}-1) \varepsilon_{DPZ} \Delta P_{FBAE} + \Delta P_{FADD} \quad (65)$$

has been added in order to take into account the fact that the actual total friction part along a BC ( $\Delta P_{FBAE}$ ) can not be described in a satisfactory manner by sole analytical expressions. There will always be uncertainties in the exact determination of the friction coefficients, the correct consideration of all contributions from spacers, tube bends, abrupt changes in cross section etc.

This means that either an additive friction term (index FADD) is added to the formula above or the friction part is provided with a multiplicative friction factor  $f_{FMP0}$ . Which of them should prevail can be governed from outside by an input parameter  $\varepsilon_{DPZ} = \varepsilon_{DPZI}$ . Thereby the additive part will be assumed to be proportional to the square of the total coolant mass flow (e.g., at BC entrance)

$$\Delta P_{FADD} = -f_{ADD0}(z_{BA}-z_{BE})G_{BE} |G_{BE}| / (2\rho_{BE} d_{HWBE} A_{BE}^2) \quad (66)$$

The steady state terms  $\Delta P_{ZBAE,0}$  (and thus also  $f_{FMP0}$  and  $\Delta P_{FADD0}$  with  $f_{ADD0}$ ) can now be determined from the fact that at steady state conditions the pressure difference term over the entire BC is given by input ( $\Delta P_{BAE,0} = \Delta P_{BAEIN}$ ) and that  $\Delta P_{GBAE,0} = 0$ . Hence, if defining the additive steady state pressure difference term  $\Delta P_{FADD,0}$  as the  $(1-\varepsilon_{DPZ})$ -th part of the total additional friction term

$$\Delta P_{FADD,0} = (1-\varepsilon_{DPZ})\Delta P_{ZBAE,0} \quad (67)$$

the friction factor  $f_{ADD0}$  for the additive part follows directly from eq.(66), the multiplicative friction factor  $f_{FMP0}$  from eq.(65)

$$f_{FMP0} = 1 + \Delta P_{ZBAE,0} / \Delta P_{FBAE,0} \quad (\text{if } \varepsilon_{DPZ} = 0 \text{ or } > 0) \quad (68)$$

It is obvious that the input data must obey certain restrictions. Since the total (steady state) friction part has to stay always negative ( $\Delta P_{FBAE,0} + \Delta P_{ZBAE,0} < 0$ ) it has to be demanded that the input term  $\Delta P_{BAEIN,0}$  is chosen in such a way that  $\Delta P_{BAEIN,0} < \Delta P_{BULM}$  ( $= \Delta P_{SBAE,0} - \Delta P_{ABAE,0} + \Delta P_{XBAE,0}$ ). Additionally, if only  $\Delta P_{ZBAE,0} > 0$ ,  $\varepsilon_{DPZ}$  has to be set automatically = 1, i.e.  $\Delta P_{FADD,0} = f_{ADD0} = 0$ , determined from eq.(67) if  $f_{FMP0} (< 1)$ .

The validity of the multiplicative and additive coefficients  $f_{FMP0}$  and  $f_{ADD0}$  has then to be expanded to transient situations too, by assuming that these coefficients should remain time-independent.

In order to express (in the transient case) the term  $\Delta P_{GBAE}$  in dependence of  $\frac{d}{dt}(G_{BE})$  the following rearrangement is proposed

$$\Delta P_{GBAE} \cong \frac{1}{2} \sum_{n=1}^{N_{BT}} \Delta Z_{Nn} \frac{d}{dt} (G_{BNn}/A_{BNn} + G_{BNn-1}/A_{BNn-1}) \cong \left[ \frac{d}{dt} (G_{BE}) + G_{BDIF}^t \right] / d_{G_{BE}} \quad (69)$$

with the coefficients

$$d_{G_{BE}} = \left[ \sum_{n=1}^{N_{BT}} (\Delta Z_{Nn} / A_{BMn}) \right]^{-1} \quad (70)$$

$$G_{BDIF}^t = \frac{1}{2} d_{G_{BE}} \sum_{n=1}^{N_{BT}} \Delta Z_{Nn} \left[ \frac{d}{dt} (G_{BNn} - G_{BE}) / A_{BNn} + \frac{d}{dt} (G_{BNn-1} - G_{BE}) / A_{BNn-1} \right] \quad (\text{general case})$$

$$= \frac{1}{2} \frac{1}{N_{BT}} \sum_{n=1}^{N_{BT}} \left[ \frac{d}{dt} (G_{BNn} - G_{BE}) + \frac{d}{dt} (G_{BNn-1} - G_{BE}) \right] \quad (\text{if equidistant nodes and } A_{BNn} = A_{BE}) \quad (71)$$

The time-derivatives in  $G_{BDIF}^t$  can be established in a similar way as proposed in eq.(22). However, since a change in the inlet mass flow will usually be transported very fast to the mass flow terms at the higher BC positions it can be expected that the differences in the time derivatives will be small and thus also the coefficient  $G_{BDIF}^t$  (compared with  $\frac{d}{dt}(G_{BE})$ ). It has to be noted that this small correction term, needed for the next time-step, is based on the present time-derivative differences.

### 3.7 Code package CCM

Based on the theory derived above a number of corresponding routines have been developed being comprised in the package CCM, a **c**oolant **h**annel **m**odule for single- and two-phase fluids. These routines are needed to describe in a very compact way the steady-state and transient thermal-hydraulic behaviour of the most characteristic parameters of a fluid within a BC.

Thereby CCM combines automatically different SC types to a unique system so that, according to the given input data set, no special actions from outside are required. The different SC-s within a BC change automatically from one SC type to another, i.e. two-phase flow follows single-phase flow and vice versa. The new SC boundary conditions are either identical to the entrance conditions of the BC or outlet conditions of the SC before. At the junction of two adjacent SC nodes usually the inlet parameters to a node are identical to the corresponding outlet parameters of the node below. Water or steam mass terms being exchanged at node boundaries between two parallel ‘porous’ coolant channels (with pressure differences as driving forces) are not yet taken into account.

Within CCM the SC parameters will automatically be converted into their corresponding BC values. The resulting set of ODE-s will then be solved by applying an appropriate integration procedure (e.g., the integration routine FEBE [12]).

## 4. Mass flow distribution into parallel channel assemblies

Knowing the main pressure drop parameters for each of the (eventually non-symmetrically perturbed)  $N_{PCT}$  parallel channels (distinguished by their key numbers  $k = KEYBC$ ) as provided by CCM (see chapter 3.6), among them also the terms  $d_{GBE}$  and  $G_{BDIF}^t$ , the total mass flow time-derivatives  $\frac{d}{dt}G_{BE}$  at each channel entrance has to be determined. This can be done, for example, at the end of the integration step but before (!! ) the integration (outside of CCM) by determining the input parameters  $\Delta P_{BAEIN}$  for each channel  $k$  (as described in chapter 3.1) by taking into account that the input terms  $\Delta P_{BAEIN}$  of all parallel channels have to be the same and the sum with the outer part of the loop be equal to 0. Then it follows from the combination of the eqs.(63) and (69)

$$\frac{d}{dt}(G_{BE}) = d_{GBE} (\Delta P_{SBAE} + \Delta P_{XBAE} + \Delta P_{FBAE} + \Delta P_{ZBAE} - \Delta P_{ABAE} - \Delta P_{BAEIN}) - G_{BDIF}^t \quad (72)$$

After the integration then the wanted mass flow distribution ( $G_{BEk}$ ) into all these channels is given. Thereby it has to be noted that these considerations need to be restricted to only the section of parallel channels (not the entire outlet loop), an enormous advantage with regard to the CPU-times and a consequence of the separate treatment of the mass and energy balance from momentum balance eqs.

## 5. Heat generation within and conduction out of a fuel rod

### 5.1 Nuclear point kinetics representation

For reasons of simplicity in a first attempt as a power source for each position  $z$  of a fuel rod of a channel  $k$  a weighted nuclear point kinetic representation will be chosen containing power terms from the prompt power fission and the decay of short lived fission products (combined in 6 groups of delayed neutrons) in form of the differential eqs.

$$\delta_r \dot{Q} = (\beta/\Lambda_p) [(1+\delta_r Q) \delta\rho - \delta_r Q + \sum_{i=1}^6 (\beta_i / \beta) \delta_r C_i] \quad (73)$$

$$\delta_r \dot{C}_i = \lambda_i (\delta_r Q - \delta_r C_i) \quad (i=1,6) \quad (74)$$

The fact that the time constant  $\Lambda_p/\beta$  is very small has the consequence that in case of an explicit integration of this set of ODE-s very small time steps are demanded and thus very time-consuming computation takes place. It is thus sometimes very useful to avoid such a time-consuming integration of this 'stiff eq.' system by neglecting this term and setting the time-derivatives equal to zero, i.e., to apply the 'prompt-jump' approximation procedure, substituting the ODE-s by the algebraic relation

$$\delta_r Q = [\delta\rho + \sum_{i=1}^6 (\beta_i / \beta) \delta_r C_i] / (1-\delta\rho) \quad (75)$$

The total (according to the nuclear kinetics) generated power density profile  $q_{NK}(z,t)$  along such a core channel is then given by the relation

$$q_{NK}(z,t) = q_{NK0}(z) [1 + \delta_r Q(z,t)] \quad (76)$$

with  $q_{NK0}(z)$  denoting the steady state power density profile (resulting from the given initial reactivity distribution within each channel  $k$  and known from input). The parameter has to be normalized in such a way that the sum of the entire total nodal power terms of all the channels  $k$  must agree with the given nominal (steady state) power term  $Q_{NOM}$ .

The total reactivity  $\delta\rho$  is the sum of the local reactivity terms due to movement of control rods and the corresponding reactivity feedback terms with respect to changes in fuel rod temperature (= Doppler) and coolant density (void fraction and/or coolant temperatures)

$$\delta\rho = \delta\rho_{CR} + \delta\rho_D + \delta\rho_\gamma \quad (77)$$

The (local) external reactivity worth of the control rod movement ( $\delta\rho_{CR}$  in \$) will be given directly as input. Thereby  $\delta\rho_{CR}$  is usually = 0, except for the case that the control rod tip has moved during the transient into the node (then  $\delta\rho_{CR} = -\delta\rho_{CRIN}$ ) or out of it (then  $\delta\rho_{CR} = \delta\rho_{CRIN}$ ). Possible reactivity contributions  $\delta\rho_{BOR}$  from the usually very slow changes in boron acid concentration is only for long-term transients of interest.

The change in the (local) Doppler reactivity feedback term can be approximated by the function

$$\delta\rho_D = \rho_D - \rho_{D0} \cong b_{\rho 2} \{ \exp( b_{\rho 1} [(T_{FM} + 273.15)^{1/2} - (T_{FM0} + 273.15)^{1/2}] ) - 1 \} \exp(b_{\rho 3} \alpha) \quad (78)$$

( $\rho_D$  in \$,  $T_{FM}$  averaged fuel rod temperature at position  $z$  in C,  $\alpha$  void fraction at position  $z$  of coolant channel,  $b_{\rho 1}$ ,  $b_{\rho 2}$ ,  $b_{\rho 3}$  for each reactor specific approximation coefficients given by input.).

In a similar way the dependency of the void reactivity feedback term from the local void fraction  $\alpha$  can be expressed by an approximation function of the form

$$\rho_\gamma \cong \alpha_{\gamma 1} \alpha + \alpha_{\gamma 2} \alpha^2 \quad (79)$$

with the (again for each reactor specific) given approximation coefficients  $\alpha_{\gamma 1}$ ,  $\alpha_{\gamma 2}$  in \$, i.e.,

$$\delta\rho_\gamma = \rho_\gamma - \rho_{\gamma 0} \cong (\alpha_{\gamma 1} + 2\alpha_{\gamma 2} \alpha_{H0}) \delta\alpha + \alpha_{\gamma 2} (\delta\alpha)^2 \quad (80)$$

in dependence of the relative change in local void fraction  $\delta\alpha$  (in rel. units).

A small part ( $\varepsilon_\gamma$ ) of the produced nuclear kinetic power is transported directly into the coolant (e.g., by means of  $\gamma$ - rays) so that only the part  $1-\varepsilon_\gamma$  stays (equally distributed) within the fuel pellet.

After a reactor shut-down (at  $t = t_{SCR}$ ) only the decay heat (with its density value  $q_{DCH}$ ) will contribute to the overall heat source. Hence, the entire (in radial direction equally distributed) heat power density term  $q_F$  acting (at any position  $z$ ) within the fuel is given by the relation

$$q_F(z,t) = (1 - \varepsilon_\gamma) q_{NK}(z,t) + q_{DCH}(t) \quad (81)$$

## 5.2 Heat conduction out of a fuel rod

### 5.2.1 Fundamental equations:

The (radial) heat conduction out of a fuel rod into a single- or two-phase fluid flowing along a coolant channel (and no conduction in axial direction) is governed by the 'Fourier heat conduction eq.'

$$\rho_F c_F r \frac{\partial}{\partial t} T_F(r,t) = \frac{\partial}{\partial r} [r \lambda_F(r) \frac{\partial}{\partial r} T_F(r,t)] + r q_F(r,t) \quad (82)$$

with its radial power density part  $q_F(r,t)$  being given (at any axial position  $z$ ) by eq.(81).

Thereby a (single) fuel rod (index F) is assumed to consist of a fuel pellet (with its radius  $r_{FA}$ ), a gap and a canning (or clad). With respect to the application of a finite element method for the discretization of the partial differential eq. of 2-nd order (and hyperbolic type) the pellet (=fuel rod) itself has to be subdivided into  $N_{FLT}$  equidistant radial fuel layers (with a layer thickness of  $\Delta r_F = (r_{FA} - r_{Fi})/N_{FLT}$  and radial positions of the layer boundaries  $r_{Fj} = j \Delta r_F$ ).

Since the thermal resistance of the thin canning wall can usually be neglected and specifications about the gap thickness are due to the unknown creeping of the canning much too uncertain it seems to be reasonable to replace the heat transfer coefficient  $\alpha_{FA}$  between fuel pellet and coolant by an overall heat transfer coefficient ( $\alpha_{OVF}$ ). This coefficient can be a combination of heat resistance on behalf of its heat transfer coefficient ( $\alpha_{FA}$ ) at the surfaces between canning outer surface/coolant and the overall thermal resistance  $R_{GCAN}$  of gap and canning. The main contribution to it, namely the heat transfer coefficient  $\alpha_{FA}$  at fuel rod surface can be determined from an adequate heat transfer coefficients package (e.g. HETRAC [4], chapter 2.2.4) taking as basis the fuel and coolant temperatures from a recursion or a time step before.

As initial condition to the heat conduction eq. the radial steady state fuel rod (=pellet) temperature profile is demanded  $T_F(r, t=0) = T_{F0}(r)$  resulting from the solution of the steady state part of this eq.

Its boundary conditions are given (for each time step  $t$  and position  $z$ ) by the heat transfer conditions at the centre ( $j=0$ ) and surface ( $j=N_{FLT}$ ) of a fuel rod (= pellet)

$$w_{Fj} = -\lambda_{Fj} T_{Fj}^{(r)} = 0 \text{ i.e. } T_{Fj}^{(r)} = 0 \text{ and } T_{Fj} = T_{FMX} (= \text{maximum fuel rod temperature}) \text{ (at } j=0) \quad (83)$$

$$w_{FA} = -\lambda_{FA} T_{FA}^{(r)} = \alpha_{OVF}(T_{FA} - T_C) \text{ i.e., } \Delta r_F T_{FA}^{(r)} = -2 (T_{FA} - T_C) / C_{FA} \quad (\text{at } j=N_{FLT}) \quad (84)$$

with  $T_C$  denoting the given coolant temperature, the radial heat flux terms  $w_{Fj}$  (at any layer position  $j$ ) being defined as

$$w_{Fj} = -\lambda_{Fj} T_{Fj}^{(r)} \quad \text{with } w_{FA} = w_{Fj} \text{ (at } j=N_{FLT}) \quad (j=1, N_{FLT}) \quad (85)$$

and the (dimensionless) coefficient

$$C_{FA} = 2\lambda_{FA}/(\Delta r_F \alpha_{OVF}) \quad (86)$$

which value lays usually within the range of 0.01 to 0.02.

The dependency of the fuel rod heat conduction coefficient  $\lambda_F$  from its temperature  $T_F$  (and partially also from its burn-up situation) can be given by a table or by a approximation function

$$\lambda_F \cong 2 \frac{\lambda_{FLIM}}{1 + T_F / T_{FLIM}} \text{ (if } T_F < T_{FLIM}) \text{ or } \lambda_F \cong \lambda_{FLIM} = \lambda_F \text{ (at } T_F = T_{FLIM}) \text{ (if } T_F \geq T_{FLIM} = 1300 \text{ C)} \quad (87)$$

The density ( $\rho_F$ ) and specific heat ( $c_F$ ) of the fuel pellet are independent from the rod temperatures.

The Fourier heat conduction eq. can now be discretized and split into in a set of  $N_{FLT}$  non-linear ordinary differential eqs. (ODE-s) of 1-st order by integrating the eq. along these layers. Hence, from the definition eq. for the mean fuel rod layer temperature

$$\frac{1}{2} (r_{Fj}^2 - r_{Fj-1}^2) T_{FMj} = (j - \frac{1}{2}) (\Delta r_F)^2 T_{FMj}(t) = \int_{r_{Fj-1}}^{r_{Fj}} r T_F(r,t) dr \quad (j=1, N_{FLT}) \quad (88)$$

it follows, in dependence of the given radial power density terms  $q_{Fj}$ , a set of ODE-s of the form

$$\frac{d}{dt} T_{FMj} = [(j - \frac{1}{2}) q_{Fj} - j w_{Fj} + (j-1) w_{Fj-1}] / [(j - \frac{1}{2}) \Delta r_F \rho_F c_F] \quad (j=1, N_{FLT}) \quad (89)$$

To calculate with regard to the directly available parameters also other characteristic fuel rod parameters a special approximation procedure had to be applied. Thereby it has to be distinguished, due to the different parameters which can be expected from the solution of the discretized heat conduction eq.(89), between a steady state ( $L_{STS}=1$ ) and transient case ( $L_{STS}=0$ ), yielding as a direct solution either heat flux values  $w_{Fj}$  ( $L_{STS}=1$ ) or, as a result of the integration procedure, mean layer temperature values  $T_{FMj}$  ( $L_{STS}=0$ ),.

### 5.2.2 Approximation procedure:

One such possible procedure is to assume that, for example, the temperature profile within a layer can be represented by adequate quadratic polygon functions. From the boundary conditions at fuel rod surface and fuel rod centre (as described in the eqs.(83) and (84)) and due to the trivial fact that the temperatures and heat flux values (and thus temperature gradients) at layer entrance have to be equal to the corresponding values at the outlet of the layer before it follows that the approximation coefficients can be replaced by corresponding layer parameters. Hence one gets two characteristic eqs. which are either based on the layer boundary temperature gradients

$$T_{Fj} = T_{Fj-1} + \frac{1}{2} \Delta r_F (T_{Fj}^{(r)} + T_{Fj-1}^{(r)}) \quad (j=1, N_{FLT}) \quad (90)$$

or on the mean layer temperature values (starting thereby from the definition eq.(88))

$$T_{Fj} = m_j T_{FMj} + (1 - m_j) T_{Fj-1} + n_j \Delta r_F T_{Fj-1}^{(r)} \quad (j=1, N_{FLT}) \quad (91)$$

with the coefficients

$$m_j = j(j-1) + \frac{1}{2} \quad (= \frac{1}{2}; \frac{5}{2}; \frac{13}{2} \text{ etc. if } j = 1; 2; 3 \text{ etc.}) \quad (92)$$

$$n_j = 2[2(j^2 + j + \frac{1}{3}) / (2j-1) - m_j] \quad (= \frac{11}{3}; \frac{31}{9} = \frac{7}{2} - \frac{1}{18}; -\frac{47}{15} \text{ etc. if } j = 1; 2; 3 \text{ etc.}) \quad (93)$$

If combining both relations by eliminating the term  $T_{Fj-1}$  it follows

$$T_{Fj} = T_{FMj} + (1-1/m_j) \frac{1}{2} \Delta r_F T_{Fj}^{(r)} + (1-1/m_j + 2n_j/m_j) \frac{1}{2} \Delta r_F T_{Fj-1}^{(r)} \quad (j=1, N_{FLT}) \quad (94)$$

and, together with the boundary condition (3), a relation for the 1-st layer temperature

$$T_{F1} = T_{FM1} + \frac{1}{2} \Delta r_F T_{F1}^{(r)} = 2 T_{FM1} - T_{FMX} = T_{FM1} + \frac{1}{4} \Delta r_F T_{F1}^{(r)} \quad (j=1) \quad (95)$$

A general relation for the fuel rod surface temperature  $T_{FA}$  can (in dependence of  $T_{FMX}$ ) be established if beginning with  $j = N_{FLT}$  in eq.(91), replacing there successively the parameters  $T_{Fj-1}$ ,  $T_{Fj-2}$  etc. by their next lower terms and taking advantage of the fuel rod boundary conditions (83) and (84)

$$T_{FA} = [T_C + C_{FA} T_{FMX} + C_{FA} \Delta r_F \sum_{n=1}^{N_{FLT}-1} T_{Fn}^{(r)}] / (1 + C_{FA}) \quad (j=N_{FLT}) \quad (96)$$

A second (general) relation for the fuel rod surface temperature follows from eq.(91) if setting there  $j=N_{FLT}$  and combining it again with the boundary conditions (83) and (84)

$$T_{FA} = [(m_j-1)T_C - C_{FA} T_{FMj} + (m_j+n_j-1)C_{FA} \frac{1}{2} \Delta r_F T_{Fj-1}^{(r)}] / (m_j-1 - C_{FA}) \quad (j=N_{FLT}) \quad (97)$$

### 5.2.3 Steady state ( $L_{STS}=1$ ):

The steady state solution (which represents the initial conditions for the transient case) can be derived if setting the time derivatives within the discretized heat conduction eq.(89) equal to zero, yielding thus a set of  $N_{FLT}$  non-linear algebraic eqs. of the form

$$j w_{Fj} = (j-1)w_{Fj-1} + (j-\frac{1}{2})\Delta r_F q_{Fj} \quad (j=1, N_{FLT}, L_{STS}=1) \quad (98)$$

If starting at  $j=1$  (with  $w_{Fj-1}=0$  and thus  $w_{Fj}=\frac{1}{2}\Delta r_F q_{Fj}$  at  $j=1$ ) and replacing repeatedly the heat flux by its next higher parameter one finally gets a relation for the outlet heat flux

$$w_{FA} = \Delta r_F \frac{1}{N_{FLT}} \sum_{j=1}^{N_{FLT}} (j-\frac{1}{2}) q_{Fj} \text{ or } \cong \frac{1}{2} r_{FA} q_{FM} \text{ if assuming } q_{Fj} \cong q_{FM} \quad (L_{STS}=1) \quad (99)$$

and thus also the heat flux values of all the layers below in dependence of the mean (=total) power density  $q_{FM}$  averaged over all known  $q_{Fj}$  terms. The fuel rod surface temperature  $T_{FA}$  follows then from the boundary condition (83)

$$T_{FA} = T_C + w_{FA} / \alpha_{OVF} \cong T_C + \frac{1}{2} r_{FA} q_{FM} / \alpha_{OVF} \quad (L_{STS}=1) \quad (100)$$

in dependence of the (given) mean (=total) power density  $q_{FM}$ . From eq.(87) then the heat conduction coefficient  $\lambda_{FA}$  and from eq.(84) the outlet temperature gradient can be determined.

One then gets from the eqs.(90), (87) and (84) (if beginning with the layer below  $N_{FLT}$ ) a relation for the (steady state) radial fuel rod temperatures of the layers below

$$T_{Fj-1} = [T_{Fj} - \frac{1}{2} \Delta r_F T_{Fj}^{(r)} + \frac{1}{4} \Delta r_F w_{Fj-1} / \lambda_{FLIM}] / [1 - \frac{1}{4} \Delta r_F w_{Fj-1} / (T_{FLIM} \lambda_{FLIM})] \quad (j=1, N_{FLT}) \quad (101)$$

ending finally with the central (= maximum) fuel rod temperature  $T_{FMX} (= T_{Fj-1})$ . Hence, from eq.(91), the steady state mean layer temperatures  $T_{FMj}$  for each layer  $j$  can be determined, being the basis for the transient considerations.

### 5.2.4 Transient situation ( $L_{STS}=0$ ):

As already pointed out the mean layer temperature values  $T_{FMj}$  are (for each time step and each axial position  $z$ ) in this case already known from the integration procedure. The other characteristic fuel rod parameters will then be determined by applying the above presented approximation procedure, distinguishing thereby between the cases  $N_{FLT} = 1$  or  $N_{FLT} > 1$ .

To derive then from the basic eqs.(90) and (91) relations for additional characteristic fuel rod parameters in dependence of the given mean fuel rod temperature values  $T_{FMj}$  it has to be distinguished between the cases  $N_{FLT} = 1$  or  $> 1$ .

If the fuel rod is assumed to be represented by only a single layer ( $N_{FLT}=1$ ), a case to which most of the very comprehensive and well known modular thermal-hydraulic codes confine themselves, it follows from the eqs.(96) and (95) relations for the fuel rod outlet temperature, its gradient and the maximum fuel rod temperature

$$T_{FA} = (T_C + 2C_{FA} T_{FM1}) / (1 + 2C_{FA}) = 2 T_{FM1} - T_{FMX} = T_{FM1} + \frac{1}{4} \Delta r_F T_{FA}^{(r)} \quad (N_{FLT}=1) \quad (102)$$

The corresponding correlations for the heat conduction coefficient  $\lambda_{FA}$  and thus heat flux value  $q_{XFA}$  at fuel rod surface are given by the eqs.(87) and (84).

Because of the wide range in radial temperature decrease along the fuel rod it can thus also large temperature variations during a transient be expected. Hence, it seems sometimes advisable and necessary to subdivide a fuel rod into more than one radial layer. This can be done, for example, by combining the eqs.(94) and (95) in order to eliminate the term  $T_{FA}$ , allowing thus to determine  $T_{FMX}$  and then, if following the eqs.(91) and (90), the terms  $T_{Fj}$  (and thus also  $T_{FA}$ ) and their gradients. This means for the case  $N_{FLT} = 2$

$$T_{FMX} = T_{FM1} + \left[ \frac{1}{5} (1 + C_{FA}) (T_{FM1} - T_{FM2}) - 2C_{FA} (T_{FM1} - T_C) \right] / \left[ 1 + \frac{5}{2} C_{FA} + \frac{7}{90} (1 + C_{FA}) \right] \quad (N_{FLT} = 2) \quad (103)$$

For both cases ( $N_{FLT} = 1$  or  $> 1$ ) corresponding correlations for the heat conduction coefficient  $\lambda_{FA}$  and thus heat flux value  $w_{FA}$  at fuel rod surface result then from the eqs.(87) and (84) yielding thus finally the right-hand side of eq.(89) needed for the next integration step.

### 5.3 Total and nodal heat transfer into each coolant channel

The characteristic fuel rod parameters are derived above in dependence of the input terms

$q_{NOM}$ ,  $T_C$ , geometry ( $r_{FA}$ ,  $N_{FLT}$ ,  $N_{FRC}$ ,  $U_{Bk}$ ,  $A_{Bk}$ ) and material values ( $\alpha_{OVF}$ ,  $\rho_F$ ,  $c_F$ ,  $\lambda_{FLIM}$  at  $T_{FLIM}$ ,  $\varepsilon_\gamma$ )

Based on it, two additional output parameters have to be established needed for the connection to other parts of the combination fuel rod/coolant channel. These are the

- ‘overall mean fuel rod temperature  $T_{FM}$ ’ resulting from the mean layer temperature values  $T_{FMj}$ , needed for the determination of the Doppler feedback term in nuclear kinetics considerations and
- since knowing the outlet heat flux term  $q_{XFA}$  the ‘total coolant power density  $q_{Bk}$ ’

$$q_{Bk} = (1 - \varepsilon_\gamma) w_{FA} U_{Bk} / A_{Bk} + \varepsilon_\gamma q_{NOM} \quad (\text{with } U_{Bk} = N_{FRC} U_F) \quad (104)$$

leaving (at each axial BC position  $k$ ) the  $N_{FRC}$  fuel rods of a channel and demanded as input for the theoretical description of the thermal-hydraulics of a single- or two-phase flow represented by the coolant channel module CCM (with  $q = q_{Bk}$  as input for each basic channel  $k$ )

## 6. Experimental thermal-hydraulic 3D core code HERO-X3D

The resulting theoretical model and code (named HERO-X3D) will be checked on an ‘experimental’ 3D code configuration concentrating in a first step on an ‘artificial’ core consisting of a central channel and four quadrants and (eventually) a bypass channel allowing both single- (with sub-cooled water or superheated steam) or two-phase flow situations within these channels.

Each channel will consist of a number of  $N_{FRC}$  (equally valid) fuel rods and a corresponding control rod. The power generation within these fuel rods can be influenced by the movement of a control rod or by influences coming from the thermal-hydraulics as simulated by the generally and thus also for PWR or SWR cores applicable coolant channel module CCM. Non-symmetric perturbations of such a core can be simulated by perturbing the different channels in an adequate way.

Having successfully developed such a code and proofed the validity of the 3D representation by demonstrating that also at non-symmetric perturbations of the core the mass flow distribution into the different channels is chosen automatically in such a way that the pressure decrease terms over each channel stay equal.

The development of the code HERO-X3D is in progress. Test calculations will demonstrate the quality and validity of the entire concept.

## 7. Nomenclature

$A_F = r_{FA}^2 \pi$	$m^2$	Area of a single fuel rod
$A_{Bk}, A_{Nn}, A_{Mn}$	$m^2$	Cross flow area (at BC or SC node boundary), mean value over SC node n
C	–	Dimensionless constant
$C_0$	–	Phase distribution parameter (within drift-flux correl.)
$\delta_i C_i (i=1,6)$	–	Relative amount of the 6 group of precursors (=input)
$C_{FA} = \Delta T_F \alpha_{OVF} / \lambda_{FA}$	–	Coefficient
$c_F$	Ws/(kgC)	Spec. heat capacity of fuel pellet (independent of $T_F$ )
$G = G_S + G_W$	kg/s	Total, steam and water mass flow
$h, h^P, c_P = h^T$	Ws/kg, $m^3/kg$ , Ws/(kgC)	Specific enthalpy and their partial derivatives with respect to pressure and temperature (= specific heat)
$k = K_{EYBC}, k=1, N_{PBC}$	–	Characteristic key number of each (basic) channel, total number of basic (=parallel) channels
$L_{FTYPE} = 0, 1 \text{ or } 2$	–	SC with saturated water/steam mixture, sub-cooled water or superheated steam
$N_{BT}, N_{CT}$	–	Total number of BC or SC nodes
$N_{BCE}, N_{BCA} = N_{BCE} + N_{CT}$	–	BC node containing entrance or outlet of SC
$N_{FLT}, N_{FRC}, N_{PCT}$	–	Total number of radial layers along a fuel rod, fuel rods within a BC and of BC-s (=parallel channels)
$P, \Delta P = P_A - P_E$	Pa= $Ws/m^3$	Pressure and pressure difference (in flow direction)
$Q, Q_{NOM}, Q_{Mn}$	$W = m^3/kg$	Total, nominal and mean nodal power into (!) channel
$q_F, q_{FA}$	$W/m^3 = 1/kg$	Radial fuel power density profile, at outlet=ch.entrance
$q_{BE}, q_{Bk}, q_{CE}, q_{Nn}$	$W/m^3 = 1/kg$	Nodal power density at (axial) BC or SC nodes
$r, r_{FA} = \Delta r N_{RT}$	m	Fuel rod radius and outlet (pellet) radius
$T, t$	C, s	Temperature, time
$U_k$	m	(Heated or cooled) perimeter of channel k
$V_{Mn} = \frac{1}{2} (A_{Nn} + A_{Nn-1}) \Delta z_{Nn}$	$m^3$	Volume of SC node n
v	m/s	Velocity
$W_{Fj}, W_{FA}$	$W/m^2 = m/kg$	Radial heat flux of layer j, out of a single fuel rod
$X = G_S / G$	–	Steam quality
$z, \Delta z_{Nn} = z_{Nn} - z_{Nn-1}$	m	Local variable, SC node length ( $z_{Nn-1} = z_{CE}$ at $n=0$ )
$z_{BA}, z_{BE}, z_{CA}, z_{CE}$	m	BC and SC outlet and entrance positions
$\alpha$	–	Local void fraction
$\alpha_{OVk}$	$W/(m^2C)$	(Overall) heat transfer coefficient at fuel rod surface
$\beta, \beta_i, \Lambda_p, \Lambda_i (i=1,6)$	– or s	Coefficients of ‘nuclear point kinetics’ representation
$\epsilon_{CN}$	m	Absolute roughness along canning ( $\epsilon_{TW}/d_{HW}$ =rel.value)
$\epsilon_{DPZ} (0 - 1)$	–	Rate of additional friction
$\epsilon_Q$	–	Correction factor with respect to $Q_{NOM,0}$
$\epsilon_\gamma$	–	Rate of direct heating of coolant (mainly due to $\gamma$ -rays)
$\lambda_{FR}, \lambda_{CN}$	$W/(mC)$	Heat conductivity along fuel rod and canning
$\rho, \rho^P, \rho^T$	$kg/m^3, kg/(Ws)$ $kg/(m^3C)$	Density and their partial derivatives with respect to pressure and temperature
$\delta\rho, \delta\rho_{CR}$	\$	Change of total reactivity and of reactivity due to movement of control rods
$\delta\rho_\gamma, \delta\rho_D$	\$	Reactivity feedbacks due to change in coolant density (=mainly void) or fuel rod temperature (=Doppler)
$\partial$	–	Partial derivative

### Subscripts

A, E	BC or SC outlet or entrance
B, S	Basic channel or sub-channel
A,F,Z,S,X	Acceleration, direct and additional friction, static head or external pressure difference (if in connection with $\Delta P$ )
D	Drift
F, FA	Fuel rod, fuel rod surface
k	Coolant channel k
Mn, BMk	Mean values over SC or BC nodes
Nn, BNk	SC or BC node boundaries
P, T	Derivative at constant pressure or constant temperature
R (or $\delta_r$ )	Relative
S, W	Steam, water

### Superscripts

/, //	Saturated water or steam
P, T	Partial derivatives with respect to pressure or temperature
(G <sub>s</sub> ), ( $\alpha$ ), (r)	Partial derivatives with respect to G <sub>s</sub> , $\alpha$ or r

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