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Evaluation of the hydrodynamic model in PARET/ANL

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SSM perspective

Background

The fuel rod analysis program SCANAIR has been developed by IRSN (Institut de Radioprotection et de Sûreté Nucléaire) for analysis of reactivity initiated accidents (RIA) in light water reactors. The Swedish Radiation Safety Authority (SSM) has access to SCANAIR in exchange for annual contributions for its further development. This ensures a possibility for SSM to do own analysis of fuel rods in reactivity initiated accidents. The development and administration of the program is done by Quantum Technologies AB on assignment from SSM.

SSM's development of SCANAIR is primarily focused on the thermohydraulic models, with the aim of improving the analytical capabilities for fuel in boiling water reactors. In a previous work, a two-phase flow model was developed, which was incorporated by IRSN in SCANAIR V_7_5. The present work is the 2017 contribution to SCANAIR development and contains an evaluation of alternative models and concepts that will improve the aforementioned two-phase thermohydraulic model in SCANAIR. The model is based on the two-phase hydrodynamic model used in the PARET/ANL computer program developed by Idaho National Laboratory (INL) and Argonne National Laboratory (ANL) in the 1960s.

Results

This current project has identified and assessed hydrodynamic models that would facilitate a better description of the effects of water density, the difference in velocity between water and steam and the friction in the water channel, if implemented in SCANAIR. Improvements like these lead to a better understanding of the phenomena that are acting during an event and will in the future result in better analytical models for the safety analysis of nuclear power plants.

Objective

Knowledge of phenomena occurring in a fuel rod during an event and how these phenomena are implemented in analytical tools is essential to SSM for the supervision of nuclear power plants. The current project also enables SSM to actively be a part of the large efforts that are made internationally with testing, understanding and improving the tools for analysis of reactivity initiated accidents

Need for further research

Continued work on developing SCANAIR's analysis capabilities is planned in cooperation with IRSN. A next step for the development of the thermohydraulic model in SCANAIR would be to implement the suggested improvement and validate it against existing tests. On the longer time scale there will be new tests in the CABRI reactor with thermohydraulic conditions closer to those of current nuclear power plants. Following these tests development of analytical models will be continued

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This report concerns a study which has been conducted for the Swedish Radiation Safety Authority, SSM. The conclusions and viewpoints presented in the report are those of the author/authors and do not necessarily coincide with those of the SSM.

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Evaluation of the hydrodynamic model in PARET/ANL

December 3, 2018.

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Contents

Summary

This report provides a critical evaluation of the hydrodynamic model in version 5.0 of the PARET/ANL computer program. The objective is to assess if the model, or concepts therof, can be used for replacing or improving the simpler model in QT-COOL, which is an optional coolant channel module in the SCANAIR fuel rod analysis program. In earlier work, we found that the hydrodynamic model for two-phase (water and steam) flow in QT-COOL is simplistic and in need of improvements. Moreover, we identified the model in PARET/ANL as a suitable alternative, having a reasonable balance between modelling adequacy and computational complexity.

Following a brief general introduction to PARET/ANL, the hydrodynamic model in the program is reviewed in detail. Particular attention is given to the simplifications and approximations that are made to cast the governing equations into a numerically tractable system of four equations for the space-time variation of the four fundamental variables: coolant specific enthalpy, axial mass flux, pressure and void (steam) fraction. Secondly, the methods used for solving these equations are reviewed, and thirdly, the availability and status of program documentation and source code are assessed.

Based on our evaluation, it is recommended that the following modelling concepts from PARET/ANL should be implemented in QT-COOL: Firstly, a void fraction correlation and effective coolant densities that consider the velocity difference (slip) between steam and liquid can be easily introduced in the existing conservation equations for mass and energy in QT-COOL. This would provide a more realistic description of the two-phase coolant than in the current homogeneous equilibrium model, where velocity slip between the two phases is neglected. The well known void fraction correlation by Rouhani and Axelsson, with some modifications, seems to be a better alternative than the correlation used in PARET/ANL. Secondly, the momentum equation can be added to the set of conservation equations considered in the hydrodynamic model of QT-COOL. This requires changes to the overall solution algorithm, and also the introduction of correlations for coolant channel friction loss.

The recommended improvements of the hydrodynamic model in QT-COOL will provide a more adequate description of two-phase coolant conditions, without excessively increasing modelling complexity, computational effort and execution time.

Sammanfattning

Föreliggande rapport utgör en kritisk utvärdering av den hydrodynamiska modellen i version 5.0 av beräkningsprogrammet PARET/ANL. Utvärderingen syftar till att avgöra huruvida modellen, eller dess ideér, kan användas för att ersätta eller förbättra den enklare modell som används i QT-COOL, vilket är en alternativ kylkanalsmodul i bränslestavanalysprogrammet SCANAIR. I ett tidigare arbete har vi funnit att den hydrodynamiska modellen för tvåfasströmning (vatten och ånga) i QT-COOL är överförenklad och i behov av förbättring. Samtidigt identifierade vi modellen i PARET/ANL som ett lämpligt alternativ, med en rimlig balans mellan funktionalitet och beräkningsmässig komplexitet.

Efter en kortfattad allmän introduktion till PARET/ANL, presenteras en detaljerad genomgång av programmets hydrodynamiska modell. Särskild uppmärksamhet ges till de förenklingar som görs för att omvandla de styrande ekvationerna till ett numeriskt hanterbart system av fyra ekvationer för variationen i tid och rum av de fyra grundläggande variablerna: kylmediets specifika entalpi, axiella massflöde, tryck och ångandel. Därefter granskas metoderna som används för att lösa dessa ekvationer, och programmets dokumentation och källkod utvärderas med avseende på tillgång och status.

På grundval av vår utvärdering rekommenderas att följande modelleringskoncept från PARET/ANL införs i QT-COOL: Först och främst kan en korrelation för ånghalten samt effektiva densiteter, i vilka hastighetsskillnaden (slip) mellan vatten- och ångfas beaktas, enkelt införas i de befintliga konserveringslagarna för massa och energi i QT-COOL. Detta torde ge en mer realistisk beskrivning av tvåfaskylmediet än i dagens homogena jämviktsmodell, där hastighetsskillnaden mellan de två faserna försummas. Den välkända ånghaltskorrelationen av Rouhani och Axelsson, med vissa modifieringar, framstår som ett bättre alternativ än korrelationen som används i PARET/ANL. I ett andra steg kan röresemängdsekvationen fogas till de konserveringslagar som beaktas av den hydrodynamiska modellen i QT-COOL. Detta tarvar förändringar i den övergripande lösningsalgoritmen, och att korrelationer för kylkanalens friktionsförluster införs.

De rekommenderade förbättringarna av den hydrodynamiska modellen i QT-COOL kommer att ge en mer passande beskrivning av kylmediets tvåfastillstånd, utan alltför stora ökningar av komplexitet i modellen, beräkningsbörda och exekveringstid.

1 Introduction

1.1 Coolant thermal-hydraulics in RIA conditions

A reactivity initiated accident (RIA) is a nuclear reactor accident that involves an unwanted increase in fission rate and reactor power. The immediate consequence of an RIA is a fast rise in fuel power and temperature [1]. In light water reactors (LWRs), heat transfer from the fuel rod cladding tubes to the water coolant is essential for limiting the fuel rod temperature excursion during the accident. This heat transfer may be hindered by the occurrence of a boiling crisis, i.e. a transition to a regime with film boiling and low heat transfer across the cladding-to-coolant interface due to the formation of an insulating continuous vapour film at the surface. If film boiling occurs during a reactivity initiated accident, the cladding surface temperature may increase to well above 1000 K. If the high cladding temperature is maintained for a sufficient period of time, the fuel rod may fail through cladding high-temperature ballooning and burst, or through cladding disruption by thermal shock upon quenching [1].

In-reactor and ex-reactor experiments suggest that cladding-to-coolant heat transfer is much different during RIAs than under steady-state reactor operating conditions or slow overpower transients, due to the rapid heating of the cladding [2-4]. Heating rates up to several thousands kelvin per second are expected in some RIA scenarios that involve inadvertent ejection of control rods from the core [1]. A widespread hypothetical explanation to the differences is that the temperature gradient in the fluid close to the cladding surface may be much steeper under fast heating than under stationary conditions, since the time is insufficient for conduction and convection to transfer heat away from the surface even on the local scale [5, 6]. The liquid close to the surface may also be significantly superheated under fast heating conditions, since the fluid is not in thermodynamic equilibrium. This would affect the nucleation and growth kinetics of bubbles that subsequently form a continuous vapour film at the cladding surface.

1.2 General modelling approaches

Computational models for cladding-to-coolant heat transfer and coolant thermal-hydraulics in RIA conditions are needed in two different categories of computer programs: codes used for core-wide neutron kinetics analyses of the accidents and codes used for detailed studies of the thermal-mechanical response of individual fuel rods to the accidents [1]. Today, there are about a dozen computer programs in the latter category, which are used worldwide for thermal-mechanical fuel rod analyses of postulated RIAs in LWRs and for interpretation of RIA simulation experiments performed in pulse reactors.

Thermal-mechanical fuel rod analysis programs applied to RIAs typically contain two kinds of sub-models for calculating cladding-to-coolant heat transfer: a hydrodynamic model for the coolant and a library of correlations for the cladding-to-coolant heat transfer coefficient in the different heat transfer regimes expected during the accident [7].

The hydrodynamic models currently applied for the coolant in the aforementioned type of programs are one-dimensional, meaning that they consider only axial flow and axial gradients in fluid properties: the physical properties of the fluid are assumed to be constant all over the flow channel cross-section for a given axial elevation. This is somewhat surprising, in light of the steep radial gradients in fluid properties that arise close to the cladding surface during the accident. These gradients call for two-dimensional (axial-radial) models for the coolant that surrounds the fuel rod. Early versions of the SCANAIR computer program contained a link to such a two-dimensional coolant channel module, developed at the Kurchatov Institute (KI), Russia [8], but this link has been removed in later versions of the program. We also note that researchers at the Moscow Power Engineering Institute (MPEI) have proposed two-dimensional coolant channel models for analyses of reactivity initiated accidents [9, 10], but it seems that neither the KI nor the MPEI model is in use today. The reason is unclear, but it may be due either to the complexity and computational cost involved with multi-dimensional, multi-phase flow models, or to the difficulties in calibrating and validating these elaborate models against the limited amount of data at hand from transient heat transfer experiments.

There is a considerable variation in complexity among the coolant hydrodynamic models currently applied in computer codes for fuel rod thermal-mechanical analyses in RIA conditions. The simplest approaches consider the one-dimensional energy and mass balance equations for single-phase (liquid) water, whereas the most complex models consider two-phase (liquid and steam) one-dimensional flow with mass, momentum and energy balance equations for each phase.

The libraries of correlations applied for the cladding-to-coolant heat transfer coefficient also vary among the fuel rod analysis codes. Most of the correlations in use today originate from non-RIA applications, although there are a few codes that make use of empirical correlations that have been fitted directly to data from RIA simulation tests [5, 11, 12]. The non-RIA correlations generally underestimate the critical heat flux and the cladding-to-coolant heat transfer coefficient in the film boiling regime, and empirical scaling factors must be introduced for the correlations to reproduce cladding temperatures observed in RIA simulation tests. These scaling factors are introduced in an ad-hoc manner for a particular set of tests, and it is unclear to what extent the same scaling factors apply to other coolant conditions.

A benchmark of computer programs used for thermal-mechanical fuel rod analyses in RIA conditions, organized by the Working Group on Fuel Safety (WGFS) of the OECD Nuclear Energy Agency (NEA) Committee on the Safety of Nuclear

Installations (CSNI), has revealed that large differences and uncertainties exist among the applied cladding-to-coolant heat transfer models, especially when a boiling crisis takes place [7, 13-15].

1.3 Models in the SCANAIR computer program

The SCANAIR computer program is developed and maintained by Institut de Radioprotection et de Sûreté Nucléaire (IRSN), France. The program, which is intended specifically for analyses of the thermal-mechanical behaviour of LWR fuel rods under reactivity initiated accidents [16, 17], is used by French organizations, but also by the Swedish Radiation Safety Authority (SSM), the VTT Technical Research Centre of Finland, and Centro de Investigaciones Energéticas, Medio-ambientales y Tecnológicas (CIEMAT), Spain. The latter organizations provide annual in-kind contributions to the development of the program.

The default coolant channel module in SCANAIR contains cladding-to-coolant heat transfer models that cover coolant conditions of pressurized water reactors (PWRs) [5] as well as the specific coolant conditions of the room temperature test capsule in the Japanese Nuclear Safety Research Reactor (NSRR) [11]. The latter conditions are of particular interest, since fuel rod experiments under simulated RIA conditions in this test capsule, with stagnant water at room temperature and atmospheric pressure as coolant, answer to the major part of the current experimental database on LWR fuel rod behaviour in RIA conditions [1].

The hydrodynamic model in the default coolant channel module in SCANAIR is restricted to single-phase fluids and treats either liquid sodium or liquid water. The conservation equations for mass and energy of the liquid are solved in one dimension, using the liquid temperature and mass flow rate at the lower end of the vertical coolant channel as time-dependent input to the calculations. The coolant pressure is also given as time-dependent input to the calculations: it is assumed to be uniform, since the conservation equation for momentum is not solved by the model.

Since it is restricted to single-phase flow, the deafault coolant channel module in SCANAIR is not applicable to hot operating conditions in boiling water reactors (BWRs). Organizations interested in applying SCANAIR for analyses of RIAs in BWRs are therefore extending the program with suitable models. For example, the VTT Technical Research Centre of Finland has developed an interface between SCANAIR and their in-house thermal-hydraulic code GENFLO [18]. GENFLO is a general software that contains a five-equation hydrodynamic model for the two-phase (liquid and steam) water coolant. Hence, in contrast to the default single-phase model in SCANAIR, the GENFLO model lends itself to analyses of BWR cooling conditions and VTT intends to model the coolant properties and the cladding-to-coolant heat transfer by use of the models available in GENFLO [19].

A somewhat different approach has been taken by Quantum Technologies in Sweden, who has implemented an optional coolant channel module in SCANAIR as

an in-kind contribution to SCANAIR development under contract with SSM [20, 21]. This module, named QT-COOL, contains a simple two-equation homogeneous equilibrium model (HEM) for the two-phase water coolant. More precisely, the liquid-steam mixture is treated as a homogeneous pseudo fluid that obeys the usual equations of a single-phase fluid. The conservation equations for energy and mass are solved in one dimension, but not the momentum equation. This means that the coolant pressure must be given as input to the program. The QT-COOL module also contains a fairly large set of cladding-to-coolant heat transfer correlations for a wide range of cooling conditions [20]. QT-COOL is available as an optional coolant channel module in SCANAIR from version V_7_5 and later.

The QT-COOL module was originally developed for general thermal-mechanical analyses of LWR fuel rods under steady-state conditions and slow transients, and not specifically for modelling conditions under reactivity initiated accidents. For this reason, the module has been validated against RIA simulation tests in the NSRR [21, 22] and also applied in the aforementioned RIA fuel code benchmark [7, 13-15]. In summary, these projects have revealed that QT-COOL underestimates the cladding-to-coolant heat transfer under transient film boiling conditions and overestimates the steam (void) fraction growth rate, when passing from single-phase liquid to mixed-phase conditions during the RIA. In fact, the first finding is not restricted to QT-COOL. Similar results have been obtained by others when simulating RIA experiments with fuel rod codes that use steady-state models for the cladding-to-coolant heat transfer: the transient film boiling heat transfer is generally under-estimated by steady-state models.

The aforementioned shortcomings in QT-COOL were further studied in [3], and it was concluded that the QT-COOL coolant channel module is inadequate for modelling axial coolant flow in situations that involve rapid vapour generation anywhere along the fuel rod. The main reason is that QT-COOL does not account for coolant inertia effects on axial flow, since conservation of momentum is not considered in the fundamental equations solved by the module. In addition, QT-COOL treats the two-phase coolant as a homogeneous mixture of water and steam, where the two phases are assumed to have the same velocity. This simplification inherently leads to overestimation of the coolant void fraction.

1.4 Objective, scope and organization of the work

Based on the assessment in [3], it was proposed that the hydrodynamic model in the QT-COOL module should be improved with regard to its simplistic modelling of two-phase axial flow. However, it was also recognized that the hydrodynamic model should be kept as simple as possible in order to retain reasonable execution times and also to match the fairly simple models that are used in the module for cladding-to-coolant heat transfer. To this end, the two-phase hydrodynamic model used in the PARET/ANL computer program [23] was identified as a suitable candidate with regard to balance between modelling adequacy and computational complexity. The hydrodynamic model in PARET/ANL solves the conservation equations for mass,

momentum and energy in one dimension, accounting for inertia effects, frictional loss and the velocity difference (slip) between steam and liquid.

The work presented in this report is a feasibility study, with the aim to assess if the PARET/ANL hydrodynamic model, or concepts thereof, can be used for replacing or improving the simpler model in QT-COOL. The report is organized as follows:

Section 2 starts with a bief general presentation of the PARET/ANL computer program. The phenomena treated by the program and the methods and models used are described. The availability of source code and documentation is addressed, and the status of the program with regard to verification, validation and testing is discussed.

Section 3 of the report deals specifically with the hydrodynamic model in PARET/ANL. The fundamental equations behind the model and the approximations and assumptions made in solving the equations are presented, together with the numerical solution methods. Particular attention is paid to the models used for representing the two-phase coolant.

The main conclusions of the work are summarized in section 4, and recommendations are given on how the QT-COOL coolant channel module can be improved. Some of these improvements can be made by introducing selected models, concepts and methods from the PARET/ANL hydrodynamic model, but we also identify alternative models that are deemed to be more suitable for the purpose.

2 Summary of the PARET/ANL program

2.1 Purpose, methods and models

In the 1960s, a computer program was developed for analysing the course and consequences of reactivity accident tests that were conducted in the Special Power Excursion Reactor Test (SPERT) facility at what is now the Idaho National Laboratory (INL) in Idaho Falls, USA. The computer program was called PARET – Program for the Analysis of Reactor Transients, and the first official version appeared in 1969 [24]. Since the 1980s, PARET has been maintained and improved by researchers at the Argonne National Laboratory (ANL), and later versions of the program are therefore called PARET/ANL [23]. Much of the work in the 1980s and 1990s was related to the worldwide effort to reduce fuel enrichment in research and test reactors, the so-called RERTR program. As part of this program, version 5.0 of PARET/ANL was in 2002 made available to the international community through the OECD Nuclear Energy Agency (NEA) Data Bank Computer Program Services and the US Radiation Safety Information Computational Center (RSICC) [25]. Later versions of the program exist, but are not publicly available [26].

PARET/ANL is used for analysing reactivity excursions in small reactor cores, cooled with light or heavy water, and the program solves the coupled thermal, hydrodynamic and nuclear kinetic equations. In version 5.0 of the program, the core can be represented by a maximum of four regions over its lateral/radial cross section and twenty axial segments; see Figure 1.

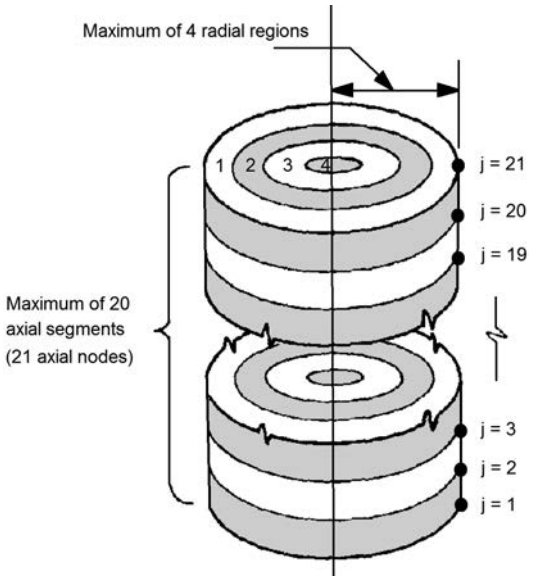

Figure 1: Maximum number of core lateral/radial regions and axial segments in PARET/ANL version 5.0. Later versions allow significantly finer discretization of the core, both axially and laterally.

In the thermal and hydrodynamic calculations, each lateral region is treated as a separate coolant channel and can be given its own power generation, coolant mass flow rate and hydraulic parameters. Each region or coolant channel is associated with a single (lumped) fuel element, which can be either an axisymmetric fuel rod or a rectangular plate. The fuel rod or plate may be discretized laterally into up to 43 layers, comprising fuel material, fuel-to-cladding gap, cladding and oxide layer.

Lateral heat transfer in the aforementioned fuel elements is considered by solving the one-dimensional heat conduction equation. This equation is solved in each axial segment of each coolant channel (core region), with boundary conditions at the fuel-coolant interface calculated from the local coolant conditions through a set of heat transfer correlations for different coolant conditions and heat transfer regimes.

The space-time variation of the coolant conditions is calculated for each coolant channel separately by solving the one-dimensional (axial) conservation equations for mass, energy and momentum along the channel. Either the total pressure drop or the coolant inlet mass flux must be specified with respect to time for each coolant channel or core region. Hence, both buoyancy-driven flow in pool-type reactors and forced flow conditions in loop-type reactors can be modelled. The hydrodynamic model is described in detail in section 3 of this report.

The reactor power, and hence, the heat generation in fuel and coolant, is either specified as a function of time or determined by solving the point reactor kinetics equations, based on a specified inserted reactivity versus time. In the latter case, reactivity feedback from changes in fuel temperature and dimensions, as well as water temperature and density, are considered in the solutions. As shown in Figure 2, the feedback effects are calculated point-wise throughout each laterial and axial region of the core. The point-wise contributions are then weighted volumetrically and summed to yield the total reactivity feedback.

Input to PARET/ANL includes physical dimensions and geometry of the reactor system; fluid flow parameters; initial system pressure; thermal properties of the fuel element materials and thermal expansion coefficient of the cladding as a function of temperature; channel pressure drop or inlet mass flow rate of the coolant to the channels as a function of time; inlet enthalpy of the coolant; certain boiling parameters; delayed neutron information; point-to-average neutron flux ratios; reactivity coefficients; initial power level; externally inserted reactivity or core power level as a function of time.

Output from the program includes the current time step increment and current values of global parameters; core power and total energy generated during the transient; current reactivity and reactivity feedback, with breakdown to individual contributions. Also, at each axial node point, the output includes coolant temperature, mass flux, void fraction, and regime (e.g liquid, nucleate boiling, etc); fuel center, fuel surface, and clad surface temperatures; fuel surface heat flux; local pressure; total pressure drop along each coolant channel, including its individual parts

(frictional, elevation, etc). Input and output can be either in SI or British units, at the user's choice. The program uses British units internally.

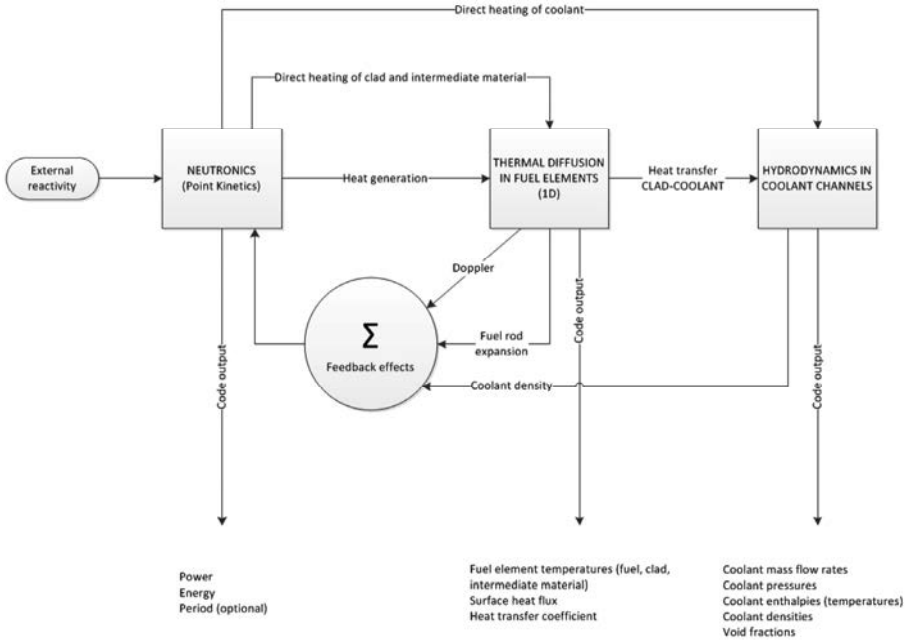

Figure 2: Structure of the PARET/ANL program [24].

2.2 Availability of source code and documentation

The source code to version 5.0 of PARET/ANL is publicly available through the OECD NEA and the US RSICC. The source code is delivered together with a user's guide, compiling instructions, and input-output files for a few test cases. The user's guide [27] provides a detailed description of the input format for PARET/ANL, but otherwise, it contains very little information. There is also a user's guide to version 7.6 of the program [26], which additionally contains some general guidelines for using the code in different kinds of analyses. These guidelines are based on experience gained from applications of PARET/ANL to different experiments in SPERT and elsewhere.

For a description of the theoretical and modelling basis of the program, the user is referred to the original report from 1969 [24]. This report also describes the finite difference methods used for discretizing the governing equations with respect to space and the applied time stepping scheme. However, there is no documentation of the numerical implementation of these solution methods, nor is there any documentation of the source code or program structure. Hence, there is a significant gap in the documentation, which, in combination with the poorly commented source code, renders model development and modification difficult. This is further discussed in section 3.4.2.

2.3 Verification, validation and testing

The original PARET program was validated against experiments in the SPERT-III facility, in which cores with highly enriched plate type fuel as well as low-enriched uranium dioxide fuel rods with stainless steel cladding were used. The coolant conditions in these experiments covered operating conditions expected in unborated pressurized water reactors of that time. The reader is referred to [24] and references therein for further details and conclusions from this validation.

The PARET/ANL program has additionally been validated against experiments in the SPERT-I, SPERT-II and SPERT-IV facilities [28-30], TRIGA reactors, and also by comparisons with other computer programs, such as RELAP [31, 32]. The most important results from this work are summarized in appendix VIII of [26]. With regard to the coolant channel thermal-hydraulic modelling in PARET/ANL, the main conclusions were:

- Cases with significant void (steam) generation in the coolant lead to numerical problems in the form of unphysical oscillations for the calculated mass flux. These oscillations could, to some extent, be prevented by reducing the time step size. However, the coolant channel module was deemed unfit for cases with large void fractions.
- The model used for calculating the void fraction in subcooled boiling (see section 3.3.1) was found to be sensitive to the model parameters. These parameters had to be fitted to the operating conditions of a particular core, i.e. to the coolant pressure, mass flux and temperature.
- The correlations used for calculating fuel-to-coolant heat transfer in PARET/ANL are derived and validated for steady-state conditions. Hence, they have the same limitations as the cladding-to-coolant heat transfer correlations used in the QT-COOL module.

3 Hydrodynamic model in PARET/ANL

3.1 General description

As mentioned in section 2.1, version 5.0 of PARET/ANL models the reactor core by use of up to four radial/lateral regions, which constitute parallell and vertical flow channels for the coolant. The channels can have either rectangular or annular cross section, representing reactor cores with plate or rod type fuel. A single fuel element is modelled in each coolant channel, meaning that the fuel element represents the lumped properties of all plates or rods in that particular region of the core.

The coolant may be either light or heavy water. It may exist as single-phase liquid or vapour (steam), or in any mixture of the two phases. In the default model, it is assumed that the two-phase mixture is in thermodynamic equilibrium, meaning that the liquid and vapour phases are saturated. An optional model is also available, by which vapour formation in subcooled conditions can be treated; see section 3.3.1.

The flow channels are modelled independently, using different instances of the same one-dimensional hydrodynamic model for each channel. The time-dependent input to this model consists of the coolant inlet pressure and enthalpy, the power generated within the fuel and coolant, and either the inlet coolant mass flux or the total pressure drop along the channel. The power generated in the fuel and coolant of each channel can be either prescribed versus time, or calculated from a prescribed reactivity insertion through the point kinetics model in PARET/ANL; see Figure 2. The cladding-to-coolant heat transfer in each channel is modelled through a library of correlations, covering various flow- and heat transfer regimes. These correlations are of general nature and intended for steady-state conditions or slow transients.

3.2 Thermal-hydraulic conservation equations

The hydrodynamic model in PARET/ANL solves the conservation equations for mass, energy and momentum in one dimension, employing a four-equation model for the water-steam coolant. The velocity difference (slip) between the vapour and liquid phase is considered by use of an empirical model, which is said to be based on the data by Martinelli and Nelson [33]. This model is further discussed in section 3.3.1.

The one-dimensional conservation equations for mass, momentum and energy solved along each vertical flow channel in PARET/ANL are [24]:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial G}{\partial z} = 0 , \tag{1}$$

$$\frac{\partial G}{\partial t} + \frac{\partial}{\partial z}\left(\frac{G^2}{\rho'}\right) = -\frac{\partial p}{\partial z} - \frac{f|G|G}{2\bar{\rho}D_h} - \bar{\rho}g , \tag{2}$$

$$\rho''\frac{\partial H}{\partial t} + G\frac{\partial H}{\partial z} = q''' . \tag{3}$$

Here, t and z are the time and axial position, respectively, G is the mass flux, p the pressure, H the flow weighted (mixing cup) specific enthalpy, g is the acceleration of gravity, D_h is the hydraulic diameter of the coolant channel, f is a friction factor and q''' is the volumetric heat source. The latter stems from direct gamma heating of the coolant as well as heating from the surface of the fuel element within the coolant channel. Moreover, $\bar{\rho}$ is the average density of the two-phase coolant at the considered cross section, evaluated through

$$\bar{\rho} = \alpha\rho_g + (1-\alpha)\rho_l , \tag{4}$$

where ρ_g and ρ_l is the density of the gas (steam) and liquid, respectively, and α is the cross sectional fraction of steam (void fraction).

The conservation equations for momentum and energy comprise effective slip-flow densities, denoted by ρ' and ρ''. These properties are related to the steam quality and void fraction of the two-phase fluid and depend on the velocity difference (slip) between the vapour and liquid phases. They are defined in section 3.3.2.

With regard to the fundamental equations solved, the main differences between the hydrodynamic models in PARET/ANL and the QT-COOL module are:

- The momentum equation is considered in PARET/ANL, but not in QT-COOL. Hence, the coolant pressure is calculated with respect to space and time, considering the friction between the fluid and the walls of the coolant channel. The correlations used for calculating the friction factor f under different flow conditions are described in section 3.3.3.
- A velocity difference (slip) between the vapour and liquid phases is considered in PARET/ANL, but not in QT-COOL. The slip enters the conservation equations through the effective densities $\bar{\rho}$, ρ' and ρ''.

It should be remarked that a simplifying assumption regarding the energy equation is done in both PARET/ANL and QT-COOL: energy dissipation by friction and energy contributions from pressure changes in space and time are neglected in both hydrodynamic models.

The three conservation equations (1)-(3) have to be solved simultaneously in order to calculate the space-time variation of the primary variables G, p and H. The axial velocities of the steam and liquid phases can then be calculated from the mass flux G and the fluid phase composition through

$$u_g = \frac{xG}{\alpha\rho_g}, \tag{5}$$

$$u_l = \frac{(1-x)G}{(1-\alpha)\rho_l}, \tag{6}$$

where $0 \le x \le 1$ is the flow quality (mass flow fraction of steam). For situations with saturated boiling, x is calculated from the flow weighted specific enthalpy of the two-phase coolant through

$$x = \frac{H - H_l}{H_g - H_l}, \tag{7}$$

where H_l and H_g are the specific enthalpies of saturated liquid and saturated steam. Equation (7) implies that thermodynamic equilibrium exists between steam and liquid, and that both phases are saturated. In PARET/ANL, there is also an optional model for calculating the void fraction and steam quality in subcooled conditions, i.e. when $H < H_l$. This model is presented and assessed in section 3.3.1.

From eqs. (5) and (6), we find the velocity slip between the steam and liquid phases

$$S = \frac{u_g}{u_l} = \frac{x}{(1-x)}\frac{(1-\alpha)}{\alpha}\frac{\rho_l}{\rho_g}. \tag{8}$$

When the coolant consists of a mixture of steam and liquid, i.e. when x and α are in the open interval from zero to unity, an additional relation has to be added to close the system of conservation equations and to obtain a solution for the space-time variation of G, p, H and α. This is usually done by introducing a correlation that relates the void fraction α to the properties of the two-phase fluid and the characteristics of the two-phase flow. An extensive review and validation of such correlations is given in [34, 35], and the correlation used in PARET/ANL is evaluated in section 3.3.1.

A widely used approach for calculating α is to introduce a correlation for the velocity slip between the phases. By re-arranging eq. (8), we find the relation

$$\alpha = \left(1 + \frac{1-x}{x}\frac{\rho_g}{\rho_l} S \right)^{-1}, \tag{9}$$

by which α can be calculated from the two-phase fluid properties and S, which is usually correlated to fluid properties as well as flow conditions. For the special case of $S \equiv 1$, i.e. when the gas and liquid phases are assumed to have the same velocity, we arrive at a homogeneous equilibrium model, as the one used in QT-COOL. For this particular case, it can be shown that the effective densities of the two-phase fluid degenerates to the volumetric average density, i.e. $\rho' = \rho'' = \bar{\rho}$.

In PARET/ANL, time dependent boundary conditions must be provided by the user in the form of prescribed time histories for the primary variables G, p and H at the coolant channel inlet. Alternatively, the mass flux boundary condition at the inlet

may be replaced by prescribing the inlet pressure plus the total pressure drop along the flow channel versus time. In this case, the program calculates the mass flux from the prescribed pressure drop, using eq. (2) with appropriate models for the friction factor *f*.

3.3 Models for two-phase coolant

3.3.1 Void fraction

In the case of saturated boiling, i.e. when $H_l < H < H_g$, the mass flow fraction of steam, x, is calculated from the flow weighted specific enthalpy of the fluid, H, through eq. (7). The void fraction, α, is then calculated from a correlation, which is said to be based on data from experiments by Martinelli and Nelson [33]. The same data are used for supporting the correlation for the friction factor under two-phase flow conditions; see section 3.3.3.

The correlation for α versus x used in PARET/ANL is not documented. A reference is made to an internal Westinghouse report from 1956, which is unavailable through public libraries. However, inspection of the source code reveals that the following simple slip correlation is implemented

$$S = \mathrm{Min}\left(S_o + 30x,\ 7 \right), \tag{10}$$

where S_o is in the range from 3.4 to 4.4, depending on pressure. The void fraction is then calculated from S, x and the steam/liquid density ratio through eq. (9).

Equation (10) implies that S increases from S_o to 7 as x goes from 0 to about 0.1, and then remains constant for higher values for x. This behaviour is unphysical. More realistic slip models usually acknowledge that S turns to unity as $x \rightarrow 0$ and $x \rightarrow 1$, i.e. when a few steam bubbles are entrained in flowing liquid or a few liquid droplets are entrained in flowing steam [34].

The void fraction versus x, calculated through eqs. (9) and (10), is plotted in Figure 3 for three different pressures. Included in the figure is also data by Martinelli and Nelson [33, 36] and void fractions calculated with a homogeneous equilibrium model (HEM, with S=1) and a drift-flux correlation by Rouhani and Axelsson [37]. The latter has been found to be among the best in an extensive validation of different void fraction models [34, 35], and it is described in Appendix A. It is obvious from Figure 3 that it reproduces the Martinelli-Nelson data with fair accuracy. The correlation in PARET/ANL, on the other hand, fits the data only for the lowest pressure.

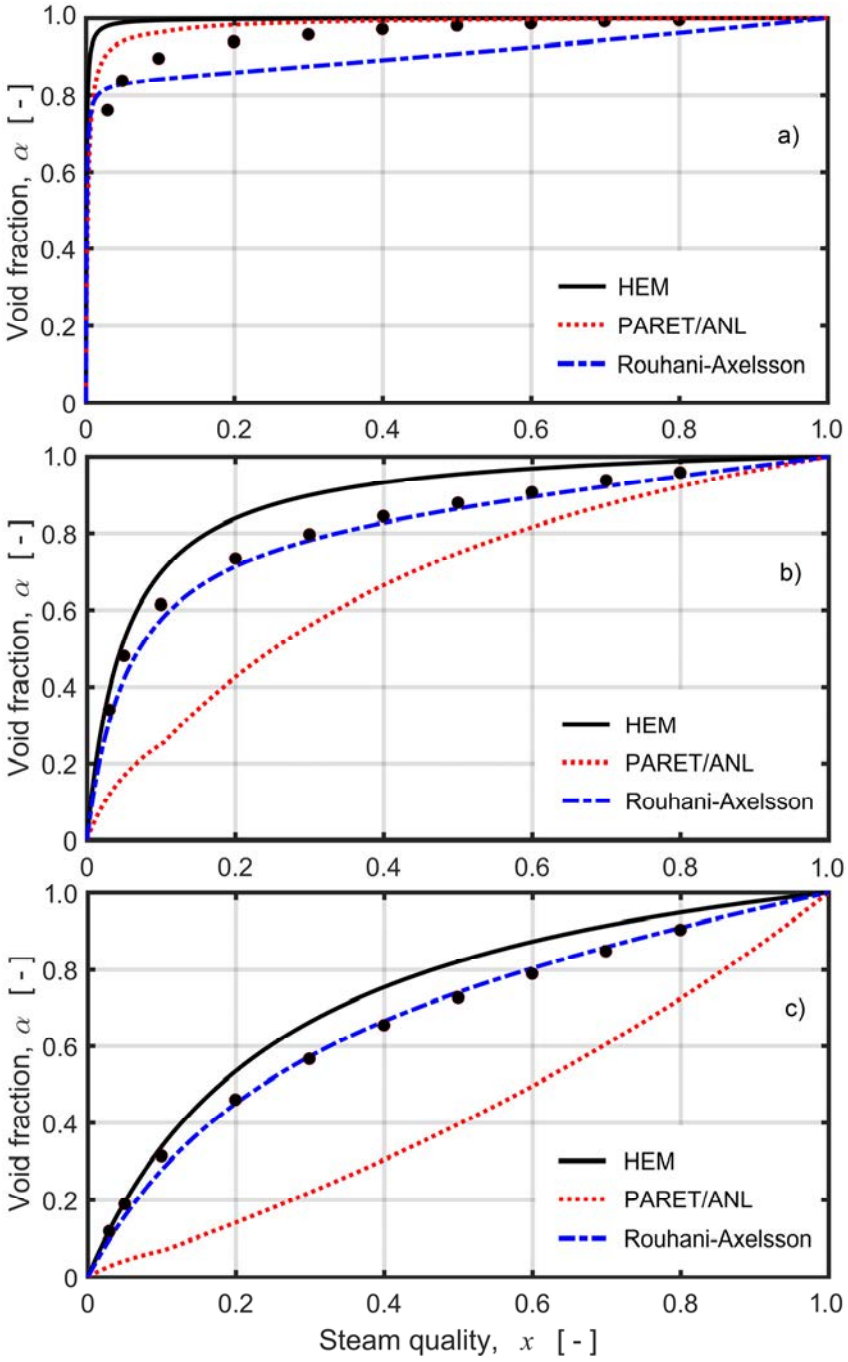

Figure 3: Void fraction versus steam quality. Data for water-steam at a) 0.1 MPa, b) 6.89 MPa and c) 17.2 MPa by Martinelli and Nelson [33] in comparison with calculated results from different models. A mass flux of 1000 kg$(m^2s)^{-1}$ was used in the Rouhani-Axelsson model; see Appendix A.

As already mentioned, the void fraction correlation in PARET/ANL is not documented, but some edits in the source code[1] suggest that the correlation is originally intended for a maximum pressure of 50 psi (0.34 MPa), but that this limit has been removed at a later stage. This is also implicitly indicated on page 12 of [27]. Based on the results in Figure 3, it is reasonable to believe that this widening of the pressure range was done without validating the correlation against the high pressure data by Martinelli and Nelson [33]. It should be remarked that a closed-form expression for α versus x, which reproduces the Martinelli-Nelson data over a wide range of pressures, has been presented recently [36]. Finally, it is obvious from Figure 3 that the homogeneous equilibrium model overestimates the void fraction for all pressures.

There is an optional model in PARET/ANL, by which the transient void fraction in subcooled condition ($H<H_l$) can be estimated. In the model, which is based on the work of Zuber [38], the evolution of the void fraction with respect to space and time is calculated through

$$\frac{\partial \alpha}{\partial t} + C_2 u_l \frac{\partial \alpha}{\partial z} + \frac{\alpha}{\tau} = \frac{\lambda v_g q'''}{(H_g - H_l)}, \tag{11}$$

where $v_g = 1/\rho_g$ is the specific volume of saturated steam. Equation (11) comprises three model parameters: λ is the fraction of the volumetric heat source assumed to contribute to direct vapour production, τ is the steam bubble collapse time and C_2 is a non-dimensional model parameter. The user's guide [26, 27] for PARET/ANL provides the following recommended values for these parameters: $\lambda = 0.05$, $\tau = 10^{-3}$ s, $C_2 = 0.8$. These recommended values are based on inverse modelling of a very limited number of SPERT experiments with PARET/ANL, and it is stated that large uncertainties exist for λ and τ, which are expected to depend on the flow rate and subcooling of the water coolant [26].

For illustration, we apply eq. (11) to the RIA simulation test FK-1, which was carried out in the standard room temperature test capsule in the Nuclear Safety Research Reactor, Japan. The coolant is stagnant water at room temperature and atmospheric pressure, and it is contained in a cylindrical capsule with an inner diameter of 120 mm. We have earlier analysed the FK-1 test with the SCANAIR V_7_5 program [22], and here, we make use of the calculated time history for the cladding-to-coolant heat flux from these analyses. The heat flux is shown in Figure 4, together with the evolution of α for the coolant in the test capsule, calculated through eq. (11). In the calculations, the second left-hand-side term of eq. (11) has been neglected, the recommended values for the model parameters have been used, and the volumetric heat source is calculated from $q''' = q'' P_{he} / A_{cs}$, where q'' is the cladding-to-coolant heat flux, P_{he} is the heated perimeter of the test rod, and A_{cs} is the cross-sectional area of the coolant flow channel within the test capsule. Hence, any direct heating of the water by gamma attenuation is neglected.

[1] Source code to the supporting programs proph2og and propd2og, which are used in a pre-processing stage for generating look-up tables for light and heavy water properties versus pressure and temperature.

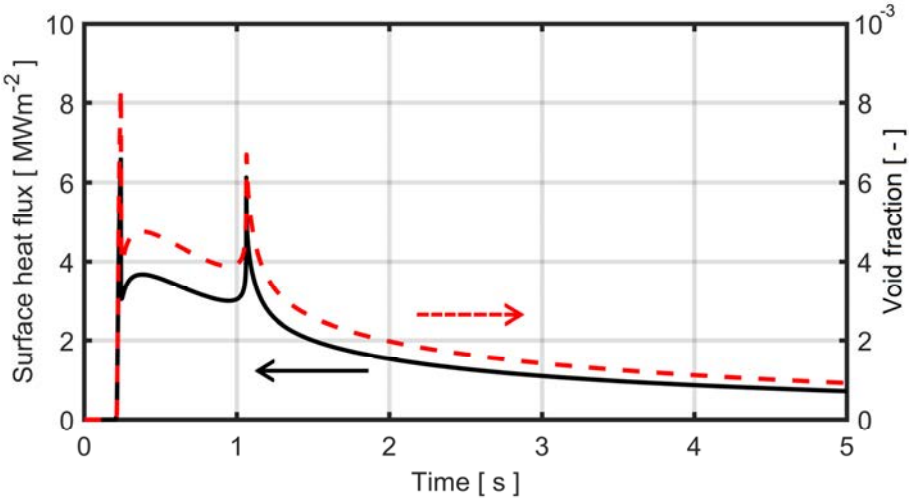

Figure 4: Void fraction (red dashed line) calculated through eq. (11) for the NSRR FK-1 RIA simulation test. The cladding-to-coolant surface heat flux (solid black line) is calculated with SCANAIR V_7_5 [22].

It is clear from Figure 4 that the calculated void fraction is strongly correlated to the cladding-to-coolant heat flux. There is very little delay in the response to changes in the heat flux, since the bubble collapse time τ is merely one millisecond in the calculations. The calculated void fraction is surprisingly low, with a maximum value of about 8×10^{-4}, notwithstanding a peak surface heat flux well above 6 MWm^{-2}. We recall that significant void generation has been observed in similar tests in the NSRR, where sensors have been used to detect transient movements of the free water surface in the test capsule. The results indicate that the model parameters λ and/or τ should be increased, to better capture the conditions in the NSRR room temperature test capsule. Finally, it should be remarked that the model defined by eq. (11) is more than fifty years old, and that progress has been made in modelling void generation in subcooled boiling [39].

3.3.2 Effective two-phase densities

As mentioned in section 3.2, three different effective densities for the two-phase water coolant are used in combination with the conservation equations for mass, momentum and energy. The derivation of these effective properties in a general case is given in [40]. Here, we present the expressions used in PARET/ANL.

Firstly, the average coolant density across an arbitrary cross section of the coolant channel with flow area A is

$$\bar{\rho} \;=\; \frac{1}{A}\int_A \rho \, dA \;=\; \rho_l(1-\alpha) \;+\; \rho_g\alpha \,. \tag{12}$$

Secondly, the effective density that appears in the momentum conservation equation is defined by

$$\frac{1}{\rho'} \;=\; \frac{1}{G^2 A}\int_A \rho u^2 \, dA \;=\; \frac{(1-x)^2}{\rho_l(1-\alpha)} \;+\; \frac{x^2}{\rho_g \alpha}\,. \tag{13}$$

Thirdly, the effective slip-flow density that enters the energy equation is defined by

$$\rho'' \;=\; \left[\; \rho_l x \;+\; \rho_g(1-x) \;\right] \frac{\partial \alpha}{\partial x}\,. \tag{14}$$

Equation (14) is a simplified expression, which is valid only in case the vapour and liquid phases are saturated [24, 40]. This is a fundamental assumption and approximation in the PARET/ANL hydrodynamic model.

The effective two-phase densities $\bar{\rho}$ and ρ' approach the densities of pure liquid and pure steam, as $x = \alpha \rightarrow 0$ and $x = \alpha \rightarrow 1$, respectively. However, this is not always the case for ρ''. This can be easily seen by using eq. (9) for evaluating $\partial\alpha / \partial x$, which combined with eq. (14) results in

$$\rho'' \;=\; \frac{\rho_l \rho_g S \left[\; \rho_l x \;+\; \rho_g(1-x) \;\right]}{\left[\; \rho_l x \;+\; \rho_g S(1-x) \;\right]^2}\,. \tag{15}$$

Obviously, ρ'' turns to ρ_l / S as $x \rightarrow 0$ and to $\rho_g S$ as $x \rightarrow 1$. In other words, ρ'' approaches the single-phase densities only for the special case of no slip, $S \equiv 1$. We also note that for the special case of no slip, $\bar{\rho} = \rho' = \rho''$.

Figure 5 shows the three effective densities, calculated as a function x at three different coolant pressures. In the calculations, we have used the PARET/ANL correlation for α versus x, as presented in section 3.3.1 and Figure 3. The calculated results depend strongly on the applied void fraction correlation, and there is reason to suspect that the results for higher pressures suffer from the poor modelling of α versus x in PARET/ANL. We also note that the unphysical slip model in PARET/ANL makes the effective density ρ'' depart by a factor 7 from the single-phase steam density, while it departs by a factor 3.4–4.4 from the single-phase liquid density. These undesired discontinuities will most certainly cause numerical problems when passing from two-phase to single-phase flow conditions.

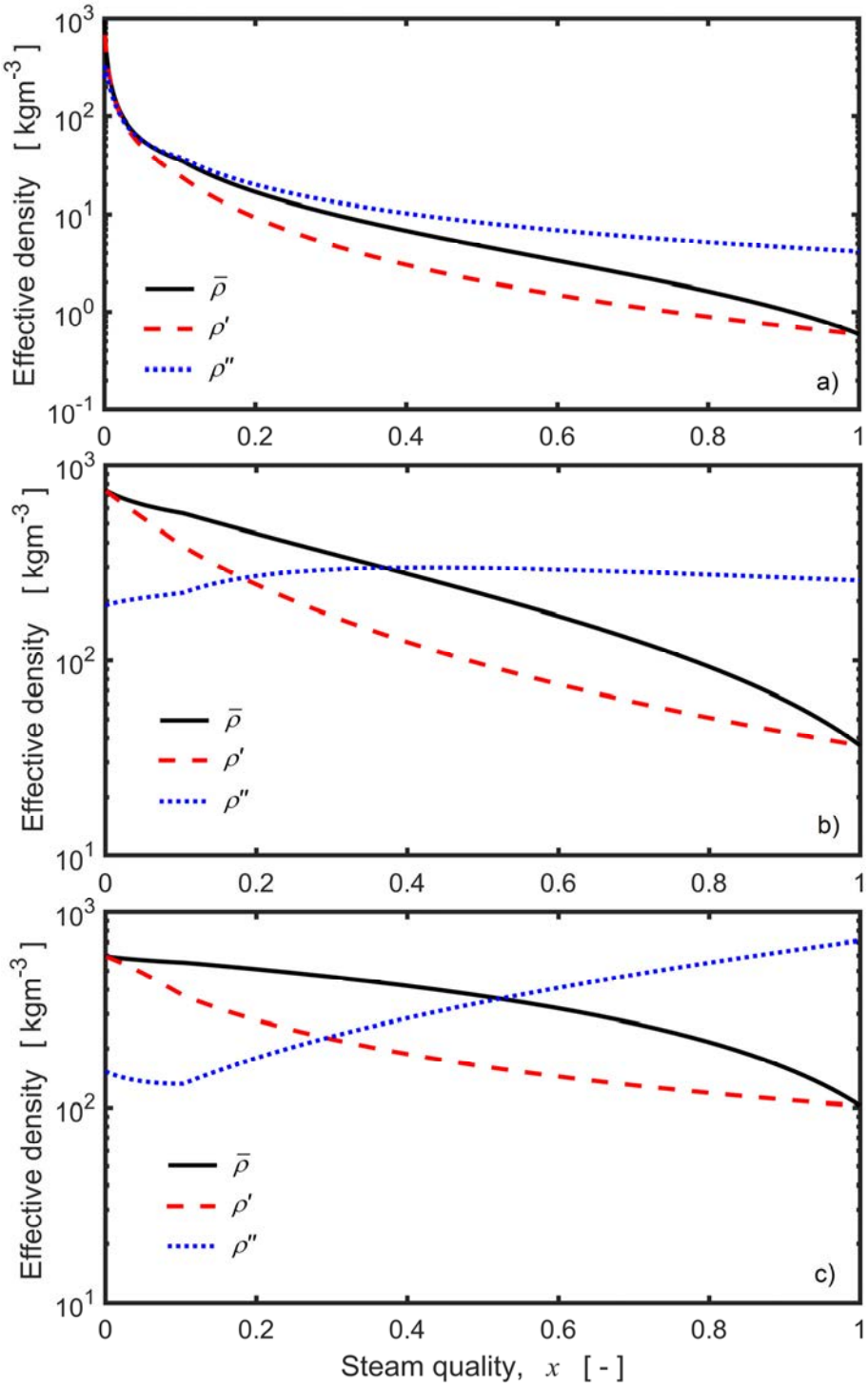

Figure 5: Effective coolant densities versus steam quality, calculated for a) 0.1 MPa, b) 7.0 MPa and c) 15.5 MPa by use of the PARET/ANL void fraction model.

3.3.3 Friction loss coefficient

The momentum equation contains a friction loss coefficient, or friction factor, which depends on the flow channel geometry, the flow regime and the coolant properties. For single-phase flow without boiling, i.e. in pure liquid or vapour phase, the friction factor is calculated from the Reynolds number, $Re = GD_h / \mu$, through an empirical relationship developed at Westinghouse. A Westinghouse report from 1959 is referenced in [24] and said to cointain the supporting data, but this report seems to be unavailable in open literature. The relationship, which has been slightly modified in later versions of the program [27], is plotted in Figure 6 for pin-type fuel designs. Here, f_1 is used to mark that the friction factor pertains to single-phase conditions, and the dynamic viscosity μ entering the Reynolds number is for pure liquid or steam. We note from Figure 6 that there is a discontinuity in the calculated f_1 for Re = 2000.

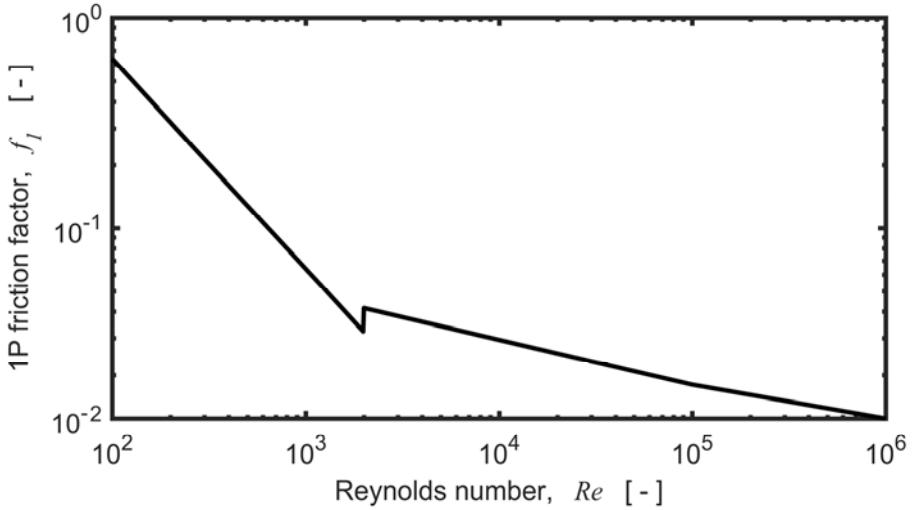

Figure 6: Single-phase friction factor applied in PARET/ANL for pin-type fuel designs [24, 27].

When boliling occurs in the subcooled liquid, whether in the form of nucleate-, transition- or film boiling, the friction factor f_1 is slightly reduced. The reason is that the boling introduces turbulence, which lowers the wall friction. PARET/ANL uses empirical relationships, developed at Westinghouse, to account for this effect. The relationships, which are fairly complex and contain heat transfer correlations for different boiling regimes, are presented in [24], but the material in support of the relationships is unavailable.

For two-phase flow, i.e. for saturated boiling conditions, the friction factor is calculated through $f = f_1 \phi_2$, where ϕ_2 is a two-phase multiplier. This multiplier is in PARET/ANL evaluated from the data by Martinelli and Nelson [33] through a look-up table, using coolant pressure and steam quality as interpolation parameters. Part of the Martinelli-Nelson data for ϕ_2 is shown in Figure 7. It is clear that the

friction factor may change by several orders of magnitude, as the steam quality increases.

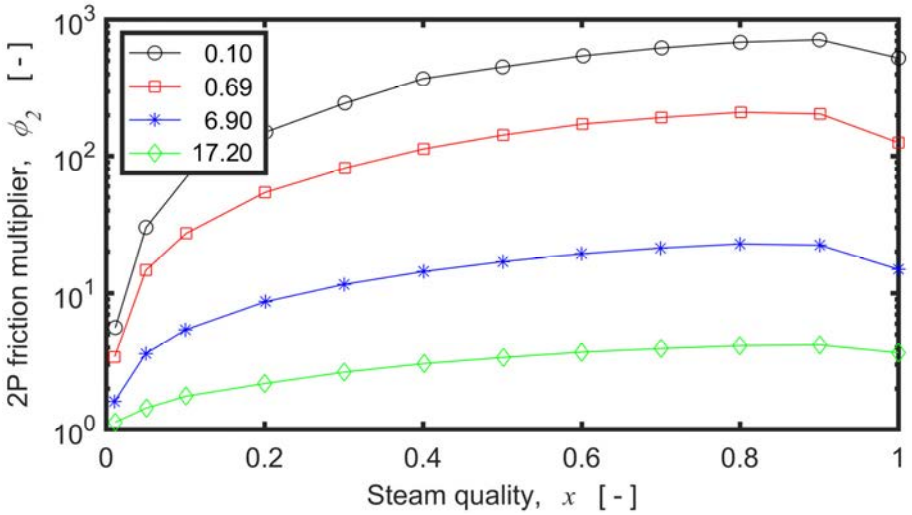

Figure 7: Part of the Martinelli-Nelson data base for two-phase friction multiplier ϕ_2, used in PARET/ANL. Numbers in the legend pertain to pressure in MPa. The data are reproduced from [36].

3.4 Numerical implementation

As already mentioned in section 2.2, there is a significant gap in the documentation of PARET/ANL regarding the numerical methods used for solving the conservation equations for mass, momentum and energy in the hydrodynamic model. The model description [24] ends with the space-time discretized conservation equations. No further descriptions of the solution methods or numerical implementation are provided, except for the actual source code.

3.4.1 Solution method

The solution method for the one-dimensional hydrodynamic equations in PARET/ANL is described as a modified momentum integral method [24]. The momentum integral method in its original form involves the solution of the three conservation equations by evaluating all water/steam properties at a reference pressure, which is considered as being known input to the solution [41]. In PARET/ANL, however, the momentum integral method has been modified to consider the dependence of fluid density upon local fluid pressure. More precisely, the coolant channel inlet pressure is a prescribed function of time, but the change in axial pressure distribution along the coolant channel is calculated as a function of time by an incremental algorithm. In any particular time step, Lagrangian extrapolation is used to estimate the local pressures at end of the time step. The extrapolated pressures are used as a basis for evaluating current fluid densities. The scheme includes an iteration on local fluid pressures, until extrapolated values are in agreement with the calculated values. Only density is considered to be a function of

both local temperature and local pressure; the other fluid properties are evaluated as functions of local temperature at the specified inlet pressure.
The governing conservation equations for mass, momentum and energy are solved for each coolant channel separately, using a finite difference method in space; see the axial discretization in Figure 1. The spatially discretrized equations are integrated with respect to time by incrementally advancing the solution. For each time step, local increments in each axial segment are calculated for the fundamental unknowns, *H, G, p* and α. According to the model description [24], the increments are calculated in a three-step procedure, where iterations are performed over the last two steps:

Step A:
Local increments of *H* over the current time step are first calculated from the discretized energy equation. The calculation is fully explicit, meaning that ΔH is calculated on the basis of known results for *H, G, p* and α from the preceding time step. The local power and the coolant channel boundary conditions during the current time step are input to the calculations. Since the time integration is explicit, there is an upper limit for the time step length if the solution is to remain stable. More precisely, the Courant-Friedrichs-Lewy (CFL) condition for stability is

$$\Delta t \quad < \quad \underset{j}{\mathrm{Min}} \left| \frac{\rho'' \Delta z_j}{G_j} \right|, \tag{16}$$

where Δz_j is the length of any axial segment along the coolant channel and ρ_j'' and G_j are the coolant local effective density and mass flux in that segment.

Step B:
Local increments of *G* over the current time step are calculated from the combined mass and energy equations, making use of ΔH from Step A. End-of-time-step values for local void fractions and effective coolant densities are estimated based on extrapolated local pressures. In case of saturated boiling, the local void fraction is calculated from the steam quality, *x*. In sub-cooled boiling, it may be set zero or calculated through the simplified Zuber model in eq. (11); see section 3.3.1.

Step C:
The axial pressure distribution at end of the current time step is evaluated through the discretized momentum equation by use of the friction factor correlations and the calculated end-of-time-step axial distributions for *H, G* and α. If needed, Steps B and C are repeated, until local pressures converge.

The time step length used in the solution scheme is based on user-supplied input for target time step length versus time during the modelled transient. This target step length is adaptively reduced, if required to maintain numerical stability and accuracy. In addition to the CFL condition in eq. (16), there are limits on allowable step length from the neutronics model in PARET/ANL [24]. In boiling conditions, the step length is also reduced such that the change in coolant local density over a single time step is limited.

3.4.2 Source code status

The source code to PARET/ANL version 5.0 is written in FORTRAN 77. Except for a few calls to system dependent FORTRAN procedures for retrieving current date and time, the source code does not depend on any external libraries or supporting software. The main body of the program comprises 66 FORTRAN 77 files that should be compiled and linked to build an executable. There are also two additional source code files that contain supporting programs for generating light or heavy water coolant properties in the form of look-up tables that are used in PARET/ANL. Either of these supporting programs is run in a pre-processing step, in which a binary file with tabulated coolant properties for a user-defined pressure range is created. This table look-up file typically contains data for 27 pressures, and for each pressure, liquid properties evaluated at 49 temperatures and vapour properties for 61 temperatures are tabulated.

The PARET program dates back to the early 1960s, and the original source code was written in non-standard FORTRAN and assembly language. Most of the source code to version 5.0 is said to originate from 1973, when the US National Energy Software Center (NESC) performed a major revision and update of the code [27]. Subsequent extensions and modifications to the program, resulting in PARET/ANL version 5.0, have been done on the basis of the 1973 source code.

Consequently, the source code to PARET/ANL version 5.0 is old-fashioned and contains features that are no longer supported in FORTRAN 95 and later standards of the language. Typical for its time, the code is written in a very compact style, with no empty lines and hardly no comments. Implicit type declarations are used for most variables, and the meaning (content and unit) of variables and data structures is not stated. Moreover, the input and output of subroutines and functions are not identified by declarations, lists or comments. This is a major defficiency, since much of the data is transferred between high-level subroutines via common blocks, and thus, not identifiable through parameter lists. In conclusion, the state of the source code, in combination with the complete lack of documentation of source code organization and involved data structures, makes it very difficult to navigate, understand and modify the code.

4 Conclusions and recommendations

The hydrodynamic model in the PARET/ANL computer program was critically evaluated, with the aim to identify possible ways of improving the optional QT-COOL coolant channel module in SCANAIR. The work in this report can be seen as a feasibility study to assess if the PARET/ANL hydrodynamic model, or concepts thereof, can be used for replacing or improving the simpler model in QT-COOL. The assessment pertains to version 5.0 of PARET/ANL, which since 2002 is available to the public through the OECD NEA Data Bank Computer Program Services and the US Radiation Safety Information Computational Center.

4.1 Summary of the PARET/ANL hydrodynamic model

The PARET/ANL program is used for analysing reactivity excursions in small reactor cores, cooled with light or heavy water, and is solves the coupled thermal, hydrodynamic and nuclear kinetic equations. The hydrodynamic model is one-dimensional and considers single-phase (water or steam) or two-phase (water and steam) flow in a heated vertical channel. The hydrodynamic model is applied to up to four parallel coolant channels, which are treated separately. Hence, cross-flow between the channels is precluded, and coolant lateral mixing is assumed only at the core lower and upper plena.

The two-phase coolant is described with a four-equation model: in addition to the conservation equations for mass, momentum and energy along the channel, an empirical correlation for the velocity difference (slip) between the steam and liquid is used for calculating the space-time variation of coolant specific enthalpy, mass flux, pressure and liquid/steam fractions. The aforementioned conservation equations have the same form, irrespective of the coolant being single-phase liquid, single-phase steam, or a two-phase mixture of liquid and steam. In the latter case, the two-phase coolant is represented by a pseudo-fluid through the use of effective slip-flow densities. These densities depend on the coolant pressure, specific enthalpy and void (steam) fraction. The void fraction, in turn, is affected by the assumed velocity slip between the steam and liquid. An empirically based slip model is used in PARET/ANL, which correlates the slip to steam quality and pressure.

Empirical models are also used for calculating the coolant channel wall friction and for estimating the void fraction under conditions of subcooled boiling. The governing equations are in PARET/ANL solved by use of a finite difference method in space, combined with adaptive time stepping in a scheme that involves both explicit and implicit methods.

In summary, there are three fundamental differences between the hydrodynamic models in PARET/ANL and QT-COOL:

- Local coolant pressures are calculated in PARET/ANL, but not in QT-COOL. The reason is that the latter model does not include the conservation equation for momentum.
- Velocity slip is considered between liquid and steam in PARET/ANL, whereas QT-COOL uses a homogeneous equilibrium model, in which the steam and liquid are assumed to flow with the same velocity.
- Steam generation (voiding) in subcooled boiling condition can be modelled in PARET/ANL. In QT-COOL, voiding is possible only in saturated boiling conditions.

4.2 Documentation, validation and testing of the model

The solution methods in the PARET/ANL hydrodynamic model, including the simplifications made to cast the governing equations into tractable form, are fairly well described in a series of publications from the 1960s [24, 40, 41]. On the other hand, empirical correlations used in PARET/ANL for calculating velocity slip and friction loss are based on data from early investigations in the USA, for which some documentation is practically unavailable. The information could possibly be retrievable from local archives or libraries in the USA, but it is unavailable from major public domain databases.

Most of the source code to version 5.0 of PARET/ANL originates from a major revision of the code that was made in 1973. The code is written in FORTRAN 77, and it contains hardly no comments, variable declarations or definitions of input and output to subroutines and functions. This, in combination with a complete lack of documentation regarding the source code organization and its data structures, makes the source code appear as a black box.

The PARET/ANL program has been validated against experiments in the SPERT facilities, TRIGA reactors, and also by comparisons with other computer programs, such as RELAP [26]. With regard to the hydrodynamic model, one of the most important conclusions of this validation was that cases with significant void (steam) generation in the coolant lead to numerical problems in the form of unphysical oscillations for the calculated mass flux. For this reason, the model was deemed unfit for cases with large void fractions.

Moreover, the optional model used for calculating the void fraction in subcooled boiling (see section 3.3.1) was reported to be sensitive to the model parameters. These parameters has to be fitted to the operating conditions of a particular core, i.e. to the coolant pressure, mass flux and temperature. In section 3.3.1, we tested this model by applying it to conditions that are typical for the room temperature test capsule in the NSRR. The model gave unrealistically low void fractions for these conditions, when using the recommended set of model parameters.

In section 3.3.1, we also validated the correlation applied for velocity slip in the PARET/ANL hydrodynamic model. This empirical correlation is essential, since it influences the coolant void fraction and the effective slip-flow densities that enter the governing equations in conditions of two-phase flow. The correlation was found to be applicable only to a narrow (0.1–0.34 MPa) pressure range. Moreover, since the calculated velocity slip does not tend to unity as single-phase conditions are approached, unphysical results are obtained for one of the effective slip-flow densities; see ρ'' in Figure 5.

4.3 Recommended improvements to QT-COOL

Our evaluation of the hydrodynamic model in version 5.0 of PARET/ANL suggests that concepts from the model can be fairly easily introduced in the QT-COOL module. Hence, the modelling capacity of QT-COOL can be improved with moderate efforts.

For example, a slip-based void fraction correlation, see eq. (9), and effective slip flow densities can be easily introduced in the existing conservation equations for mass and energy in QT-COOL. This would provide a more realistic description of the two-phase coolant, resulting in lower void fraction, than in the current homogeneous equilibrium model. With slightly more effort, the momentum equation can be added to the set of conservation equations considered in the hydrodynamic model of QT-COOL. This requires changes to the overall solution algorithm, and also the introduction of correlations for coolant channel friction factors. The correlations applied in PARET/ANL can be used as a starting point, but since they are poorly documented, they have to be validated against experimental data or other well-known correlations.

The above improvements of the hydrodynamic model in QT-COOL are recommended. They will provide a more adequate description of two-phase coolant conditions, without excessively increasing modelling complexity, computational effort and execution time. The necessary changes and extensions of the QT-COOL source code have to be made from scratch. It is not worthwhile to use any part of the PARET/ANL source code, since the code is poorly documented and therefore difficult to re-use.

We also note that the slip-based void fraction correlation used in PARET/ANL is unfit for implementation in QT-COOL. As mentioned in section 4.2, the correlation is applicable only to low pressures, and it also yields unphysical results for one of the effective slip-flow densities. A suitable alternative can be the void fraction correlation by Rouhani and Axelsson; see Appendix A. It is based on the drift-flux approach and has been found to be among the best in an extensive validation of different void fraction models [34, 35]. In section 3.3.1, we found that the Rouhani-Axelsson void fraction correlation reproduces the experimental data by Martinelli and Nelson [33] over a wide pressure range that covers all conceivable operating conditions in boiling and pressurized water reactors. However, the correlation is not

perfect. For example, the velocity slip calculated through the correlation does not tend to unity as conditions of single-phase steam flow are approached, meaning that it gives unphysical results for the effective slip-flow density ρ''; see section 3.3.2. This shortcoming should be fixed. In this context, we also note that it would be possible to empirically introduce a time dependence (time lag) for the void fraction in the originally time-independent Rouhani-Axelsson model. However, it is unclear whether suitable experimental data exist for validation of such a time-dependent model. Some studies that can possibly be useful for validation of a time-dependent model are available in the open literature [42, 43].

The available database of ex-reactor and in-reactor tests that can be used for validation and calibration of the improved QT-COOL coolant channel module has been assessed in previous work [3]. Some of these tests have already been used for validating the current version of QT-COOL [21, 22], but there are other tests that have not yet been used. The early in-reactor tests in the Power Burst Facility (PBF), USA, belong to the second category and seem to be of particular interest. The reason is that the testing conditions were very close to those expected in boiling water reactors at hot zero power operating conditions.

Finally, it is concluded that a model for the void (steam) fraction in subcooled boiling conditions is currently not needed in QT-COOL. The main reason is that such a model would provide information that would anyhow not be useful for the fairly simple cladding-to-coolant heat transfer correlations that are today used in QT-COOL. Calculation of transient steam generation that occurs in subcooled conditions under a reactor power excursion is relevant mostly for assessing the moderator feedback in core kinetics calculations [39]. This phenomenon is not relevant in SCANAIR.

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Appendix A:
Rouhani-Axelsson void fraction correlation

The void fraction correlation by Rouhani and Axelsson [37] is based on the drift flux approach and calibrated to experimental data that cover a wide range of pressures, heat fluxes, mass fluxes and levels of subcooling. The correlation is given by

$$\alpha = \frac{x}{\rho_g}\left[C_o\left(\frac{x}{\rho_g}+\frac{1-x}{\rho_l}\right) + \frac{U_{GM}}{G}\right]^{-1}, \tag{A.1}$$

where C_o is a non-dimensional distribution factor

$$C_o = 1.0 + 0.2(1-x), \tag{A.2}$$

and U_{GM} is the drift velocity

$$U_{GM} = \frac{1.18(1-x)}{\sqrt{\rho_l}}\left[g\sigma(\rho_l-\rho_g)\right]^{1/4}. \tag{A.3}$$

In eq. (A.3), g is the acceleration of gravity and σ the water-steam surface tension. Other quantities in eqs. (A.1) to (A.3) are defined in the body of the report.

It should be remarked that the factor (1-x) in the expression for U_{GM} was not included in the oiginal formulation of the correlation by Rouhani and Axelsson. It was added by Steiner [44], in order to force α turn to 1 as $x \rightarrow 1$. The Rouhani-Axelsson void fraction correlation has been identified as one of the best performing models of its kind [34, 35, 45].

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