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# Simulation of Thermal Hydraulic at Supercritical Pressures with APROS

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## ABSTRACT

The proposed concepts for the fourth generation of nuclear reactors include a reactor operating with water at thermodynamically supercritical state, the *Supercritical Water Reactor* (SCWR). For the design and safety demonstrations of such a reactor, the possibility to accurately simulate the thermal hydraulics of the supercritical coolant is an absolute prerequisite.

For this purpose, the one-dimensional two-phase thermal hydraulics solution of APROS process simulation software was developed to function at the supercritical pressure region. Software modifications included the redefinition of some parameters that have physical significance only at the sub-critical pressures, improvement of the steam tables, and addition of heat transfer and friction correlations suitable for the supercritical pressure region.

## 1 INTRODUCTION

During the recent years, there has been an increased interest in the possibility to simulate the thermal hydraulics of water at supercritical pressures, on one hand due to the research on the Generation IV concept of a supercritical water cooled nuclear reactor, and on the other due the constantly increasing number of fossil-fueled supercritical power plants in operation.

Operating any kind of a power plant with supercritical coolant is efficient, because when boiling of the coolant is prevented by the supercritical pressure, the coolant can be heated to a much higher temperature, which in turn increases the plant's thermal efficiency from about 33 % to about 40—50 %. Supercritical fossil-fueled power plants have been in power production for decades, but building a supercritical water-cooled nuclear reactor has proven to be much more demanding task due to the much stricter safety and durability criteria for all the system components. It is just these criteria that call for the need for the possibility to accurately simulate the thermal hydraulics of the supercritical coolant.

While the numeric models developed for simulation of thermal hydraulics in power plants during the past few decades have proven reliable and efficient, they cannot be directly applied to simulation at supercritical pressures, where the distinction between vapor and liquid disappears.

### 1.1 APROS

APROS (Advanced Process Simulator) is a general-purpose process simulation software suitable for simulation of industrial processes, such as combustion and nuclear power plants, personnel training simulators, and pulp and power mills. It has been developed in cooperation by VTT Technical Research Centre of Finland and Fortum Nuclear Services Ltd. since the late 1980's.

The principal features of APROS include one-dimensional two-phase solution of thermal hydraulics, one- or three-dimensional core neutronics solution and simulation of automation and electric systems. In addition, an extensive nuclear reactor containment model is included for safety analysis purposes.

### 1.2 Peculiarities at supercritical pressures

At supercritical pressures the distinction between liquid and gas disappears, and any fluid stays forcibly in a single phase. Even though boiling is physically impossible, heating (or decreasing the pressure) causes the thick, liquid-like fluid to change smoothly to a thin and vapor-like fluid.

Usually a temperature called the *pseudo-critical temperature*, $T_{pc,}$ is associated with this *pseudo-phase transition*. The pseudo-critical temperature is defined as the temperature at which the specific isobaric heat capacity $c_p$ is maximized for the given supercritical pressure $p$:

$$T_{pc}(p) \equiv \arg\max_{T} c_p(p,T), \quad p > p_{crit} \tag{1}$$

The line formed by these pseudo-critical temperatures, the *pseudo-critical line*, can be thought to approximately divide the region of supercritical pressures to subregions of pseudo-liquid and pseudo-gas. It should also be noted that each pseudo-critical temperature is naturally associated with a unambiguous enthalpy value which can be called the pseudo-critical enthalpy $h_{pc}$.

While the pseudo-phase transition is smooth by nature, the thermophysical properties of the fluid change very rapidly in the vicinity of the pseudo-critical line, which is one of the main concerns for the numeric simulation. Some of these changes are illustrated in figure 1.

## 2 NUMERIC SIMULATION OF THERMAL HYDRAULICS

### 2.1 Conservation laws

The numeric simulation of thermal hydraulics in APROS is based on the fundamental physical principles of conservation of mass, momentum and energy. These principles are formulated as general conservation laws, which are then discretized with respect to space and time, so that their time-behavior can be solved with a digital computer.

In APROS the spatial discretization is carried out in one dimension using the *staggered grid scheme* and the *finite differences* method. This leads to the division of the simulated system into control volumes referred to as *nodes* and *branches* (the mass and energy equations are solved in the former and the momentum equation in the latter).

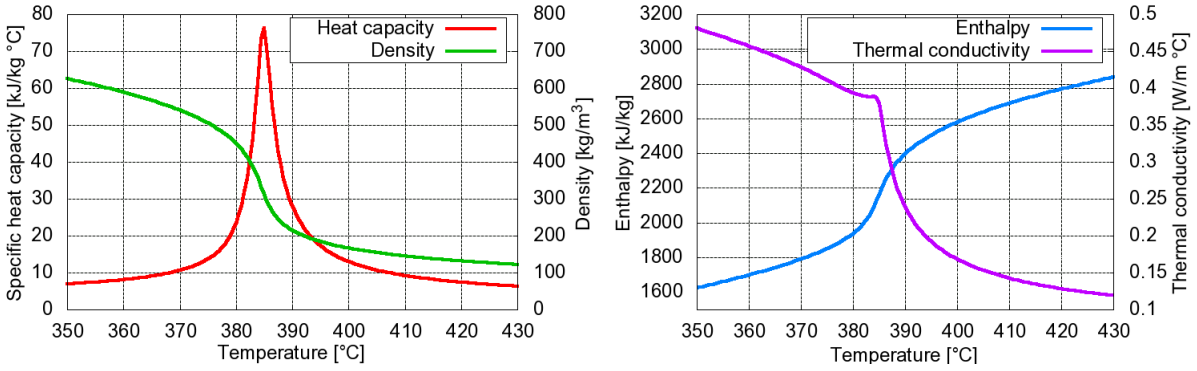


*Figure 1: Some thermophysical properties of water at 25.0 MPa, near the pseudo-critical line. On left: specific isobaric heat capacity and density. On right: specific enthalpy and them of water at 25.0 MPa, near the pseudo-critical point.*

The distinction between the different phases (liquid and vapor) can be modeled in a variety of ways. In APROS the two most relevant thermal hydraulics models for the current discussion are the *homogeneous model*, which assumes that both the phases share a common temperature and velocity, and the *6-equation model* (*the two-fluid model*), which treats the phases as separate fluids. The 6-equation model is based on the method presented in article [2].

While the homogeneous model would be ideal for supercritical pressures, where the fluid stays always in one phase, it gives bad results on transient simulations in which the pressure is allowed to

drop suddenly to subcritical conditions. This is why the 6-equation model is generally preferred even at supercritical pressures, when high accuracy is needed.

For the 6-equation model, the one-dimensional conservation laws can be written as follows:

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \frac{\partial(\alpha_k \rho_k u_k)}{\partial z} = \Gamma_k \tag{2}$$

$$\frac{\partial(\alpha_k \rho_k u_k)}{\partial t} + \frac{\partial(\alpha_k \rho_k u_k^2)}{\partial z} = \Gamma_k u_{ik} + \alpha_k \rho_k \mathbf{r} g + F_{wk} + F_{ik} \tag{3}$$

$$\frac{\partial(\alpha_k \rho_k h_k)}{\partial t} + \frac{\partial(\alpha_k \rho_k u_k h_k)}{\partial z} = \alpha_k \frac{\partial p}{\partial t} + \Gamma_k h_{ik} + q_{ik} + q_{wk} + F_{wk} u_k + F_{ik} u_{ik} \tag{4}$$

Here $k$ stands for the phase (liquid or gas), $i$ for interface, $\alpha$ volume fraction, $\rho$ density, $t$ simulation time, $u$ flow velocity, $z$ for the one-dimensional coordinate, $h$ total solved enthalpy (enthalpy plus the kinetic term $u^2/2$), $p$ pressure and $\Gamma_k$ the mass change rate from phase $k$ to the other phase (i.e. the total mass per unit time undergoing a change of phase). $F$ is a friction force and $q$ a heat flow.

To solve this partial differential equation system for the variables $h_l$, $h_g$, $u_l$, $u_g$, $\alpha$ and $p$, it is first discretized with respect to space and time and non-linear terms are linearized using 1st degree Taylor polynomials with respect to pressure $p$ and void fraction $\alpha$. This discretization then leads to an algebraic equation system, which is solved using an iterative pressure-correction algorithm.

## 2.2 Constitutive equations

Important details on the flow conditions are lost when the spatial discretization of equations (2)-(4) is carried out. These details have to be compensated by so-called *constitutive equations*, which are typically empirically-derived formulations that correlate given parameters (such as $u$, $p$ and diameter of the flow channel) to measured effects (e.g. heat flow between the channel wall and the fluid, friction pressure loss).

Constitutive equations are needed for heat transfer between the wall of the flow channel and the fluid phases, and between the interface and the two phases. For friction, constitutive equations are needed between the wall and the fluid phases as well as between the phases, thus making a total of 7 correlations for the 6-equation model in the general case. For the supercritical pressure region only 4 correlations are needed, as only one wall heat transfer and one wall friction correlation are needed for the wall-to-fluid case. Constitutive equations for the interfacial terms are still needed for numerical reasons, even though they have no physical significance at supercritical pressures.

The correlations are very strongly dependent on the flow regime, so different correlations are needed for each flow regime. Because normally the actual flow mode consist of more than one flow regime, the net effect of heat transfer or channel wall skin friction is calculated by evaluating the heat transfer- or skin friction coefficients using the correlations of each flow regime involved in the flow, and then summing these coefficients weighted by the importance of the corresponding flow regime.

This same methodology was applied to make the simulation work at supercritical pressures: in addition to the typical flow regimes treated in APROS (*bubbly*, *slug*, *churn*, *annular*, *droplet* and *stratified* flows), also *supercritical* is considered a separate flow regime. The friction and heat transfer correlations for the regime are described in the following.

### 2.2.1 Channel wall skin friction

The friction between supercritical fluids and heated walls was extensively studied in the former Soviet Union. The skin friction factor ($\xi$) correlation of Kirillov *et al.* [3]:

$$\xi = \frac{1}{\left(1.82 \log_{10}(\mathrm{Re_b}) - 1.64\right)^2} \left(\frac{\rho_w}{\rho_b}\right)^{0.4} \tag{5}$$

has been previously used in preliminary SCWR system analysis [10], and seems to be the only widely used wall friction correlation for supercritical pressure region. Thus it was chosen as the skin friction correlation for supercritical pressure region in APROS.

### 2.2.2 Heat transfer

Heat transfer to fluids at supercritical conditions has been studied in numerous experiments since the 1960's. Despite the great amount of work put into the research, a single heat transfer correlation that would predict the heat transfer at supercritical pressures reliably doesn't exist. The failure to find such a correlation is most likely caused by the very complex phenomena, such as the *heat transfer deterioration* to name just one, that occur in a supercritical fluid when its enthalpy passes the pseudo-critical line [5, 6]. Besides, because most of the experimental work on heat transfer to supercritical fluids was made during the 60's and 70's, using the steam tables of that time, the available data may have an error as high as 15 % and more [6]. Even further error can be introduced into calculations when the correlations that were derived using older steam tables are applied using modern formulations such as the IAPWS-IF97.

The heat transfer correlation of Jackson and Hall [7] has been showed to agree best with new experimental data [8], and thus it was implemented in APROS:

$$\mathrm{Nu_b} = 0.0183\,\mathrm{Re_b^{0.82}}\,\mathrm{Pr_b^{0.5}}\left(\frac{\rho_\mathrm{w}}{\rho_\mathrm{b}}\right)^{0.3}\left(\frac{\overline{c_p}}{c_{p,\mathrm{b}}}\right)^{n}$$

$$n = \begin{cases} 0.4, & \text{if } T_\mathrm{b} < T_\mathrm{w} < T_\mathrm{pc} \quad \text{or} \quad 1.2T_\mathrm{pc} < T_\mathrm{b} < T_\mathrm{w} \\ 0.4 + 0.2\left(\dfrac{T_\mathrm{w}}{T_\mathrm{pc}} - 1\right), & \text{if } T_\mathrm{b} < T_\mathrm{pc} < T_\mathrm{w} \\ 0.4 + 0.2\left(\dfrac{T_\mathrm{w}}{T_\mathrm{pc}} - 1\right)\left(1 - 5\left(\dfrac{T_\mathrm{b}}{T_\mathrm{pc}} - 1\right)\right), & \text{if } T_\mathrm{pc} < T_\mathrm{b} < 1.2T_\mathrm{pc} \quad \text{and} \quad T_\mathrm{b} < T_\mathrm{w} \end{cases} \tag{6}$$

Recently, there has been an effort to develop this correlation further to better agree with experimental data by taking into account the effects of flow acceleration and buoyancy observed when passing the pseudo-critical line [9]. Fixing the constants in this new Jackson correlation by fitting the correlation to experimental data will hopefully prove it to be more accurate and widely-applicable than any currently available heat transfer correlation.

### 2.2.3 Interfacial friction and heat transfer

Because the 6-equation model treats the fluid at supercritical pressures as a two-phase fluid, an interfacial friction factor has to be defined even when it has no physical counterpart in the real world. On one hand, a high interfacial friction factor would ensure that the velocities of both the pseudo-phases would be equal, which is desirable, but on the other hand this would cause some of the kinetic energy to be changed into heat, which is undesirable. Thus the interfacial friction should have minimal effect on the flow, which can be accomplished be ensuring that the time both the fluid phases are present in a node is minimal, i.e. the pseudo-phase transition is handled as fast as possible.

Like the interfacial friction factor neither the interfacial heat transfer coefficients have physical counterparts in the real world, and thus they can be chosen rather arbitrarily to yield the desired result of "fast-as-possible" pseudo-phase transition. The evaporating mass flow per unit area Γ is calculated based on the requirement that the energy production on the interface is zero, and on the assumption that the interface is at saturated state:

$$\Gamma_i = \frac{K_{i1}\left(h_{l,stat} - h_{l,sat}\right) + K_{ig}\left(h_{g,stat} - h_{g,sat}\right) - q_{wi}}{L_{pe}} \tag{7}$$

Here $K_{il}$ and $K_{ig}$ are the interfacial heat transfer coefficients of liquid and gas, $h_{l,stat}$ and $h_{g,stat}$ static enthalpies (solved enthalpies minus the kinetic terms) of liquid and gas, $h_{l,sat}$ and $h_{g,sat}$ the pseudo-saturation enthalpies ($h_{l,sat} = h_{pc} - L_{pe}/2$, $h_{g,sat} = h_{pc} + L_{pe}/2$), $q_{wi}$ the heat flux directly from wall to the interface and $L_{pe}$ the pseudo-evaporation heat. Based on experimentation it was find out that coefficients should be only functions of void fraction and flow velocity. The formulas currently implemented in APROS need still some refinement to cause the void fraction to change from zero to unity (and vice versa) as fast as possible, but without introducing any numeric instabilities to the solution.

### 2.3 Steam tables

The thermophysical properties of the fluid, such as density, heat capacity or viscosity, have to be known accurately at every thermodynamic state that the fluid may go through during the simulation. Formulations for the calculation of the thermophysical properties are for historical reasons called *steam tables*. For the simulation of the thermal hydraulics to be meaningful, the implementation of the steam tables has to be accurate and consistent, and give properties that are continuous.

APROS uses an approximative implementation of the IAPWS-IF97 formulation for the calculation of the thermophysical properties [11], which defines the properties of water accurately over a wide range of operation parameters. The implementation of APROS's steam tables was double-checked to ensure that the properties are adequately accurate over the whole parameter range of interest, and that they are continuous functions of pressure and enthalpy. As a result of the double-check, a few inconsistencies related to the definition of the pseudo-critical temperature, and artificial limitation of some properties were identified and resolved.

### 2.4 Extension of the two-phase variables

Because the 6-equation model treats the fluid as a two-phase fluid even at the supercritical pressures, all the variables based on the existence of two separate phases have to be redefined in a consistent and reasonable manner at supercritical pressures. Such variables include the void fraction $\alpha$, and saturation enthalpies $h_{sat,liq}$ and $h_{sat,gas}$.

For the homogeneous model, the definition of the void fraction was extended by letting it attain the value *zero* when the temperature is below the pseudo-critical line, and the value *one*, when it is above it:

$$\alpha \equiv \begin{cases} \dfrac{V_{gas}}{V_{liq} + V_{gas}}, & \text{if } p < p_{crit} \\ 0, & \text{if } p \geq p_{crit} \;\&\; T \leq T_{pc} \\ 1, & \text{if } p \geq p_{crit} \;\&\; T > T_{pc} \end{cases} \tag{8}$$

For the 6-equation model the void fraction at supercritical pressures is simply the volume fraction of the pseudo-gas phase, and the pseudo-phase transition is handled internally by the same mechanisms that APROS uses for boiling and condensation at subcritical pressures, discussed above. This leads to a situation where the fluid exists temporarily in both the pseudo-phases when passing the pseudo-critical line, but this should have no effect on the other fluid properties.

## 3 TESTING AND VALIDATION

To test the software modifications, a series of fundamental test cases was simulated. In the first one, the conservation of mass and energy were verified by simulating the steady-state behavior of flow through a heated pipe, first with both ends exposed to supercritical pressures by boundary conditions, and second time with the inlet at a supercritical pressure and the outlet at a subcritical pressure. The heating power of the pipe was adjusted to cause the fluid to be fully (pseudo)evaporated at the outlet. This fundamental test proved that the implementation of the pseudo-void fraction doesn't break the conservation laws.

As a second test a modified version of the *Edwards-O'Brien blowdown experiment* was simulated. In this test a straight closed horizontal pipe of 4.096 m length and 0.073 m inner diameter was initially filled with water at 25.0 MPa. One of the pipe ends was then opened abruptly to cause a rapid depressurization, flashing and emptying of the pipe. This test was run with three different initial temperatures (580 K, 700 K and 780 K).

As a result it was verified that APROS is able to simulate a rapid transition between the supercritical and subcritical pressure regions. The simulation results are presented in figures 2 and 3. Because experimental data on these modified tests doesn't exist, it is impossible to evaluate how realistic the simulation results are. Nevertheless, the results seem reasonable, and in any case they are very close to results of the same tests acquired with other thermal hydraulic system codes [1].

While APROS passed all these tests, there is still room for improvement: at some points during these validation simulations APROS was forced to use really tiny time steps to find a convergent solution, which is inconvenient because it increases the overall computational time needed to perform a simulation.

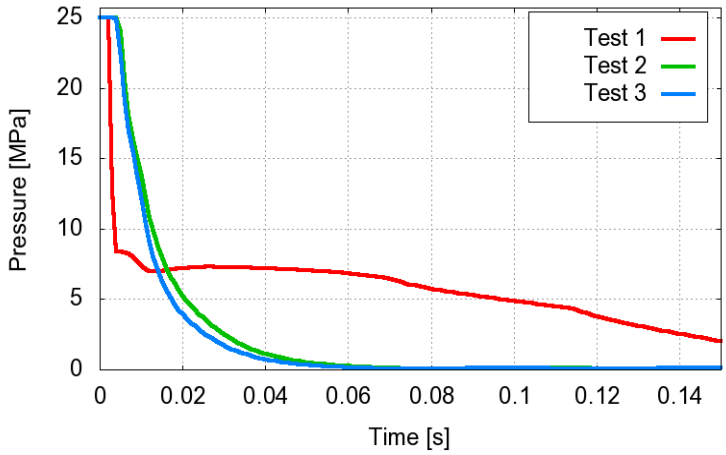


*Figure 2: Results of the Supercritical Edwards-O'Brien simulations. The initial temperatures were 580 K, 700 K and 780 K.*

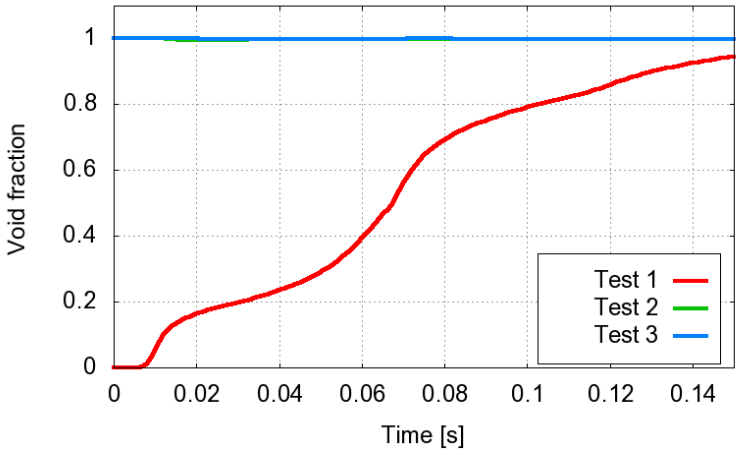


*Figure 3: Results of the Supercritical Edwards-O'Brien simulations. The initial temperatures were 580 K, 700 K and 780 K.*

## 4 CONCLUSION

The changes implemented in APROS thus far have made the simulation at supercritical pressures possible: the implementation of the pseudo-phase transition doesn't break the conservation laws, and the supercritical Edwards-O'Brien blowdown simulations proved APROS's capability to simulate a fast transition from the supercritical pressure region to the two-phase region. However, because there's much uncertainty in the constitutive equations – especially in the the wall-to-supercritical fluid heat transfer correlation – currently implemented in APROS, the simulation results have to be interpreted with appropriate caution whenever these correlations may play an important role.

Additional work is still needed to enhance the robustness and efficiency of the solution algorithm, and to solve any remaining issues that may come up as the system is thoroughly tested. More reliable constitutive equations are also required before APROS can be used for any serious safety analyses at supercritical pressures.

## NOMENCLATURE

LETTERS AND SYMBOLS

| | |
|---|---|
| *c* | specific heat capacity |
| *F* | force |
| *g* | gravitational acceleration |
| *h* | total specific enthalpy (i.e. including kinetic energy) |
| *K* | heat transfer coefficient |
| *L* | evaporation heat |
| Nu | Nusselt number |
| *p* | pressure |
| Pr | Prandtl number |
| *q* | heat transfer rate |
| Re | Reynolds number |
| *t* | time |
| *T* | temperature |
| *u* | velocity |

SUBSCRIPTS

| | |
|---|---|
| b | bulk |
| g | gas |
| h | hydraulic |
| i | interface |
| *k* | phase *k* (l or g) |
| l | liquid |
| pc | pseudo-critical |
| pe | pseudo-evaporation |
| sat | saturation |
| stat | static (without kinetic energy) |
| w | wall |

$z$ location
$\alpha$ void fraction (volume fraction of the gas phase)
$\Gamma$ mass transfer rate
$\mu$ dynamic (absolute) viscosity
$\rho$ density

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