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Thermal Hydraulics Modelling

Apros[®] thermal hydraulics model library contains three different thermal hydraulic models for one dimensional water/steam/gas flow (homogenous, 5-equation and 6-equation), one for single phase flow, one for the containment and one for the steady state flow with tank dynamics. Thermal hydraulics is described using the conservation equations for mass, momentum and energy and correlations for friction and heat transfer. This presentation and common features presented here concern only the thermal hydraulic models for homogenous, drift flux (5-equation) and separated two-phase flow (6-equation) models unless otherwise stated.

All except steady state model employ the staggered grid discretization scheme. In this scheme the state variables such as pressure and enthalpy are calculated in the middle of the mesh, i.e. in a node. The flow related variables are calculated at the border of two nodes, i.e. in a branch. The water and steam properties are obtained as a function of pressure and enthalpy by using a fast look-up table. All models include the effects of pumps and valves as well as the calculation of boron concentration. A unified model for non-condensable gases and transport of chemicals and radioactive species is used in all the two phase flow models.

All the thermal hydraulic models include several correlation sets, which can be changed, according to the plant modelling needs. The heat conduction solution can be connected to all the thermal hydraulic models by defining model specific heat transfer modules. The heat flows between solid heat structures and fluid are calculated from empirical correlations. The heat transfer regimes are defined on the basis of wall, fluid and saturation temperatures. Separate parts of a simulated system can be described with different thermal hydraulic models. The different models can be interconnected by using special connection modules.

Homogenous model

The one dimensional homogeneous two phase flow model (the three-equation model) is based on the mass, momentum and energy conservation equations of the mixture. Hence, in this model water and steam/gas have equal velocities and temperatures. For large vertical volumes, where the flow velocities are usually small, a special node can be used in which the water and steam are fully separated.

Five-equation model

The five-equation model is based on the conservation equations of mass and energy for gas and liquid phases and a conservation equation of momentum for the mixture of the phases. The pressures and volume flows as well as the enthalpies of the phases are solved from the equations. A separate drift-flux model is used to solve the velocities of the two phases.

The five-equation model has its own correlation package for the calculation of friction and heat transfer. In the five-equation model no iterations are needed and thus the calculation speed is fast also in large applications.

Six-equation model

The six-equation model is based on the conservation equations of mass, momentum and energy for the two phases. The equations are coupled with empirical correlations describing

various two-phase phenomena, like friction and heat transfer for wall and interface. The pressures and velocities, volume fractions and enthalpies of each phase are solved from the discretized equations using an iterative procedure.

The six-equation model is especially suitable for accurate simulation with dense nodalization in fast transients required in safety analysis and design calculations.

Steady state model with tank dynamics

The steady state model is based on the conservation equations of mass and energy. The solver is a sequential modular one.

The steady state model is suitable in situations where fully dynamic pressure-flow solution or two-phase flow is not needed and input data for the process components is scarce. In the simplest case only process topology and tank dimensions are needed to use the model. This enables fast model building. Thus the steady state model can serve as the first stage of a modelling project. Later the parts of the model that need more accurate calculation can be converted to be solved with more advanced flow solvers.

Containment

The containment model is based on the conservation equations of mass, momentum and energy. The simulated containment is described by subvolumes (nodes) and flow

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paths between the subvolumes (branches). The containment model can be arbitrarily divided into nodes and branches. Each node includes a gas region and may also include a liquid pool. In the gas phase, steam and non-condensable gases have a uniform temperature, but the liquid and gas phases may have different temperatures. The gas branch is assumed to connect the gas regions of two nodes and only gas flows are calculated. For liquid flows, a liquid branch is available. The gas region of a node can be connected to one or more heat structures. The containment model calculates the heat transfer between the gas region and the heat structure surface. The heat conduction is calculated by using the general heat conduction model available in Apros.

The sprinkler spray or a leakage flow from other systems can be introduced into any node. The leakage can be specified either as a time dependent table of the leakage mass flow and enthalpy or by defining a flow path between the thermal hydraulic nodes and the containment nodes. A model for the condensation pool is included. The containment spray system model is based on the complete mixing droplet model, which assumes a uniform droplet temperature. The droplet surface temperature is considered separately due to its strong effect on the combined heat and mass transfer. It is iterated using the energy balance of the interface between the droplet and the gas phase. The model takes into account the change in the droplet size due to steam condensation or water evaporation, the influence of non-condensable gases on the mass transfer coefficient and the temperature dependency of physical properties. The spray cooling can also be specified for the outer surface of the containment.

Non-condensable gases

In 5-equation and 6-equation model the non-condensable gas spreading is calculated. In 6-equation model the mass conservation equation of non-condensable gas is solved and the effect of non-condensable gas properties is taken into account in pressure and enthalpy solutions.

In homogeneous model the air can be defined to be in a node, but it can not flow from one node to another. The air mass is taken into account in calculation of pressure.

Discretization

The flow solution of Apros is based on staggered grid discretization scheme. In this scheme the state variables such as pressure and enthalpy are calculated in the middle of the mesh, i.e. in a node and the flow related variables are calculated at the border of two nodes, i.e. in a branch. These nodes and branches form the calculation level of the thermal hydraulic solution.

Fluid section structure

Alongside with the thermal hydraulic network Apros creates also so called composition network or section level. This network takes care of concentrations of substances and material properties flowing in the thermal hydraulic network. This way the thermal hydraulic and material properties solution data can be defined and solved separately. The module, where the fluid property data is specified, is called the fluid section and network itself consist of composition branches and nodes. Every node has a section attribute. The section defines the simulated fluid and its properties. Furthermore the section defines the system to be used for pressure-flow solution.

On the section level the material properties are searched as a function of pressure, enthalpy and mass fractions of substances in a fluid. Furthermore, the concentration solution is made on the section level.

In composition network the concentrations are solved by using the flows obtained from the thermal hydraulic solutions. The heat transfer correlations must be selected on the section level, because certain correlations cannot be used for different fluids. The chemical reactions between substances are calculated on section level.

When defining a process model using process component modules, the modules of the composition network and thermal hydraulic network are automatically created. Their parameters are generated from the user given input data of the process components.

Boundary conditions

The flexible definition of boundary conditions in the Apros models has been achieved by defining several variables that are used only as a boundary condition. The normal boundary conditions for flow models are the pressure or/and mass flow boundaries. The heat flow boundary condition in a thermal hydraulic node can be defined directly or with the aid of the heat transfer coefficient between thermal hydraulic node and heat structure surface. The heat flux to or from heat structure surface and heat generation can also be defined. The surface temperature of a heat structure can defined to be constant.

The boundary condition variables can be controlled by a special boundary condition module. It is a useful tool, which can be used to move data in the database and to calculate new variables with the aid of existing database variables during the simulation. The boundary condition definitions can be applied to a larger group of variables through the subprocess system. The boundary condition module includes different functions

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that change the value of the variable to be transferred. The typical application of boundary condition module is in defining the values for thermal hydraulic boundaries, but it is not in any way limited to any physical model of Apros.

Interconnection of the thermal hydraulic models

Separate parts of a simulated system can be described with different thermal hydraulic models. The different models can be interconnected by special connection modules.

In all connection modules, the lower level model uses the pressures of the higher level as boundary conditions and calculates the mass flows between the two levels. The pressure solution of the higher level uses the mass flows as boundary conditions. The enthalpy and concentration solutions use the enthalpies and boron concentrations of the other level according to the flow direction between the levels. The connection is not implicit as default (iterative solution can be forced) and therefore division between different solution systems should be made in locations where the systems to be connected are not highly dependent on the flow.

Although the connection modules calculate the flow of a homogeneous mixture, 5-and 6-equation models need information about both phases. The flows, enthalpies, volume fractions and densities of the phases are therefore calculated. Because all properties of the gas phase are not available in the single-phase model, it is not advisable to connect it to a true two-phase system.

Interconnection rules

When a single phase model or homogeneous model is connected into 5-or 6-equation model nodes, the following rules should be followed:

- From the single phase or a homogeneous model the sections simulated by the 5-or 6-equation model are considered as external points and a quasi-stationary pressure behavior is expected in this kind of points.
- Small 5-or 6-equation model nodes cannot be isolated behind a valve, which can be completely closed.
- Small single phase and homogeneous model nodes can be located behind a closed valve. Their pressure follows smoothly the 5-or 6-equation model pressure.
- If a pipe described with a single phase or a homogeneous model is connected from both ends into a 5-or 6-equation model, the pipe must have enough flow inertia ($\text{length}/\text{area} > 100 \text{ m}/\text{m}^2$).

Nodalization principles

The general rules concerning the nodalization of the thermal hydraulic models have been listed below:

- Node sizes in the same size class (e.g. 1 to 30 m³ nodes for a real reactor processes) are recommended.
- Sometimes different nodes should be used for the horizontal and vertical sections in the 3-and 5-equation models.
- Denser nodalizations are needed in sections, where the axial enthalpy (core, steam generator, pressurizer) or axial void fraction distribution (core, upper plenum, loop seals) is significant. In loop seals, upper plenum, downcomer and pressurizer the dense nodalization may be avoided by using special node types.
- In the steam generator the liquid separation must be described by a special separating node or branch.
- Flow restrictions and pressure drops are described by branch properties. A diminished flow area and an increased pressure loss coefficient increase the pressure drop in a similar way.
- The phase separation characteristics are described by the branch flow area. A greater flow area allows for a better phase separation in 5-and 6-equation models.

Heat structure models

A one-dimensional solution of heat conduction in heat structures can be used together with all thermal hydraulic models. A two-dimensional heat conduction model is also provided for tasks, which require greater accuracy, but it can only be used in the cylindrical coordinate system. Each thermal hydraulic model has its own heat transfer correlation package and a separate heat transfer module to connect the solutions. The heat structures connected with different thermal hydraulic models are all defined using the same module types. The heat structures are automatically divided into separate parts, which are solved together with the corresponding fluid system.

The heat conduction model includes material property data as a function of temperature for many common materials. New material properties can be added easily without code modifications

General features of the numerical methods used in thermal hydraulic models

The numerical solution of the PDEs is based on the implicit or semi-implicit time integration (implicit Euler). The control

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volume approach is used in the space discretization and staggered grids are adopted, i.e. control volumes of the momentum equation are displaced with respect to the control volumes of the pressure and enthalpy equations. Upwind scheme is used in convective terms. The implicit time integration results in solving a set of algebraic equations for each time step. The algebraic equations are linearized and then solved iteratively (for 3-and 6-equation models). The thermohydraulic solution algorithm is an adaptation of the SIMPLER method. The 5-equation model uses a predictorcorrector algorithm without iteration.

Boron transportation

Boron concentration and transport is calculated in homogeneous, 5-equation and 6-equation models. The boron is assumed to stay in liquid phase (5-equation and 6-equation models).

Thermal hydraulic library is included in the following products

- *Apros[®] Combustion*
- *Apros[®] Nuclear*

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Comparison of different thermal hydraulic modelling approaches: basic conservation equations

The calculation of thermal hydraulics is based on the conservative equations of mass, momentum and energy for both phases. The equations are written in an Eulerian form by neglecting the diffusion term.

The equations in the following table are solved for different approaches. The most relevant approaches for the thermal hydraulic simulation are the homogeneous model (3 conservation equations), drift flux model (5 conservation equations) and two-fluid model (6 conservation equations).

Conservation equations	Homogeneous model	Drift-flux model	Two-fluid model
1: Vapour mass		x	x
2: Liquid mass		x	x
1&2: Mixture mass	x		
3: Vapour momentum			x
4: Liquid momentum			x
3&4 Mixture momentum	x	x	
5: Liquid energy		x	x
6: Vapour energy		x	x
5&6 Mixture energy	x		

Additional equations are needed if the noncondensable gas components in vapour (nitrogen, hydrogen, radioactivity) and dissolved substances in liquid (boric acid, impurities) are included in the models.

Two-fluid model

The discretized conservation equations are solved in an iterative solver. The physical content in 6-equation model is described as closure relationships for:

- wall heat transfer in all heat transfer modes
- interfacial heat transfer between liquid and vapour
- wall friction for vapour and liquid separately
- interfacial friction between liquid and vapour.

The formulation of physics is built in a mechanistic way by considering each phenomenon through the elementary relationships.

Drift flux model

In the 5-equation model the liquid and vapour momentum equations (3 and 4) are replaced by the mixture momentum equation. In drift-flux model the momentum equation is solved only for the mixture and the phase separation is solved by a diffusion equation of void fraction.

The physical content in 5-equation model is described as closure relationships for:

- wall heat transfer in all heat transfer modes
- interfacial heat transfer between liquid and vapour
- wall friction for vapour and liquid mixture
- drift flux model parameters.

Homogeneous model

Simplified equations are achieved by assuming same velocities for both phases (= mixture momentum equation) and one energy equation for the mixture. This homogeneous model is practical for small diameter pipeline networks. Due to the simplicity the calculation is faster than that of the 5-and 6-equation models. The physical content in 3-equation (homogeneous) model is described as closure relationships for:

- wall heat transfer in all heat transfer modes (if structures are described)
- wall friction for vapour and liquid mixture.

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The 3-equation model can be improved by assuming a complete phase separation in large volumes like tanks and pipes with a large flow area.

Applicability of different models

In general the homogeneous model (3-equation model) is a practical solution for auxiliary systems, feedwater systems, main steam system after the turbine control valve etc. The model can also describe the phase change due to flashing or condensation, but does not take into account different phase velocities. On the other hand the phase separation in small diameter piping is negligible. And in large diameter tanks also these features can be described. Like other models, the 3-equation model can be expanded for noncondensable gas and soluble components in the liquid.

5-equation or 6-equation models are suitable to describe the primary circuit of the nuclear power plant, water circulation in the boiler plant etc... It is not easy to give any direct recommendation whether to use 5- or 6-equation model. The arguments regarding different approaches can be described as follows.

Driftflux model features

- The solution of the phase separation for mixture makes the solution more stable and allows more simple (clear) solution algorithms (+)
- Only few analysis codes (ATHLET) apply 5-equation solution. The comparison of phase separation models on the correlation basis is more difficult than for two-fluid models. In drift flux model typically many subphenomena are tailored in (-). A good reference for comparing the model is the full range drift flux model developed by EPRI (+).
- Due to limited instrumentation in experiments the results are typically measured for mixture, not separately for phases. Thus drift flux correlation can be easier to determine using the experimental data (+).
- Stratification in long pipes (water on the bottom, steam flows freely above the water level) cannot be described well enough with the 5-equation model (-). The modelling is not a big problem in reactor piping (+).
- The momentum added into liquid phase is not modelled properly (ECCS-injection in hot leg, entrainment of liquid droplets in core during emergency core cooling,

spray injection into BWR core) (-)

- Water level void profile is sharper than with two fluid model. The drift flux formalism works best for continuous water with rising bubbles. Thus it naturally predicts best the physics where the water level is essential (core uncover, steam generator secondary side, pressuriser, loop seals) (+).

Two-fluid model features

- The solution of the phase separation separately for both phases is more difficult than for 5-equation model (-), but with present knowledge possible (+). Two approaches, iterative solution (longer solution time (-), clear structure (+) and twostep SETS-method (fastest solution (+), complicated structure (-) can be mentioned.
- The most of well-known analysis codes (TRAC, RELAP5 and CATHARE) apply 6-equation solution. Thus the physical content is easy to compare to other analysis codes. Because the physics in two-fluid models is described typically in a mechanistic way also for phase separation, the comparison of elementary pieces is easier than the comparison of complex drift flux formulations (+). The problems in numerical algorithms may cause that the physical response of a twofluid model cannot be predicted from the correlation (-)
- Because the parameters in experiments are typically measured for mixture, not separately for phases, the interfacial friction and heat transfer relationships have to be based on additional assumptions.
- Stratification in long pipes (water on the bottom, steam flows freely above the water level) can be described also in long pipes with the 6-equation model (+).
- The momentum added into a single phase is modelled properly. If ECCS water in hot leg is injected towards pressure vessel, the flow water can reach upper plenum in spite of large steam velocity. In BWR the spray injection into the core can be described more physically with two-fluid model. In PWR the water entrainment during reflooding is described more physically (+)
- Water level void profile needs more nodes than the drift-flux model (-).

Fortum, Nuclear and Thermal Power Division

Thermal Production and Power Solutions,
P.O.Box 100, 00048 Fortum, Finland, Tel. +358 10 4511
www.fortum.com/powersolutions, www.apros.fi

For further information, please contact:

Sami Tuuri, Product Manager
sami.tuuri@fortum.com, Tel. +358 40 354 5604
Matti Paljakka, Key Account Manager
matti.paljakka@vtt.fi, Tel. +358 20 722 6423

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