SH2705 Simulation Course

Computer codes, validation & verification

COMPUTER CODES AND APPLICATIONS

- Computer codes are main tools to perform the Deterministic Safety Analysis, by determining the response of the reactor to such transients.
- Computer codes are a collection of models needed to simulate the behavior of a nuclear plant (or of a part of it) during a transient or accident.
- Models are representations of thermo-hydraulic (TH), reactor dynamic, thermo-mechanical, structural, radiological, etc.

COMPUTER CODES AND APPLICATIONS

Codes used in conservative DSA are different from that used in best-estimate DSA:

- Conservative DSA: conservative codes (i.e., codes with pessimistic models, used with pessimistic assumptions). Are often proprietary codes.
- Best Estimate DSA: BE or realistic codes (those with realistic models). They are mainly system codes.

The same code may have the capability to be used both for Conservative and BEPU DSA analysis

COMPUTER CODES AND APPLICATION

- System codes: large codes that can model the entire reactor system to simulate certain accidents,
- Reactor dynamic Codes: codes that can model the reactor core in detail to simulate the neutron kinetic response of the plant,
- Severe accident codes: codes design to analyze beyond design basis accidents

COMPUTER CODES AND ASSUMPTION USED IN DSA

Applied codes	**Input & BIC (boundary and initial conditions)**	**Assumptions on systems availability**	**Approach**
Conservative codes	Conservative input	Conservative assumptions	Deterministic*
Best estimate (realistic) codes	Conservative input	Conservative assumptions	Deterministic
Best estimate codes + Uncertainty	Realistic input + Uncertainty	Conservative assumptions	Deterministic
Best estimate codes + Uncertainty	Realistic input + Uncertainty	PSA-based assumptions	Deterministic + probabilistic

COMPUTER CODES AND APPLICATION
SYSTEM CODES

- The thermal-hydraulic system codes have been developed and used for analysis of loss of coolant accidents (LOCAs) for 60 years. At the end of the sixties and beginning of the seventies the capabilities of the codes were strongly limited by lack of experimental data, details of modelling and the capacity of the computers. Since then, the situation has improved significantly on all these areas.
  - New generations of the system codes have been developed in many countries.
  - Thermal-hydraulic system codes of the current generation are based on solving mixed hyperbolic-elliptic system of six conservation equations (conservation of mass, energy and momentum for the vapor and liquid phases).
  - Experimentally based correlations that are often called ‘constitutive laws’ are incorporated to describe the needed boundary conditions for each of the phases, such as friction between the phases and the wall.
  - The codes are typically developed for one dimensional modelling. However, there have been many efforts to introduce simulation of multidimensional behavior and effects into these two-fluid codes.

COMPUTER CODES AND APPLICATION
SYSTEM CODES

RELAP5, TRACE, APROS, POLKA-T, CATHARE, ATHLET, RETRAN….

- They are realistic, state-of-the-art codes.
- Control volume approach, big nodalization.
- State-of-the-art TH models (multi-fluid models).
- Core model approach varies from relatively simple, represented by an average channel and/or a hot channel to advanced, to half or full core model. The output can be input to a sub-channel analysis code.
- Typically, simple neutronic models (e.g., point kinetics).
- Despite the development made in the advanced codes, they are not yet fully capable of a realistic description of the physical phenomena that occur during the accidents. The complex phenomena due to their multidimensional and micro scale features cannot be modeled in detail

NEED FOR COUPLING TO A NEUTRONIC CODE

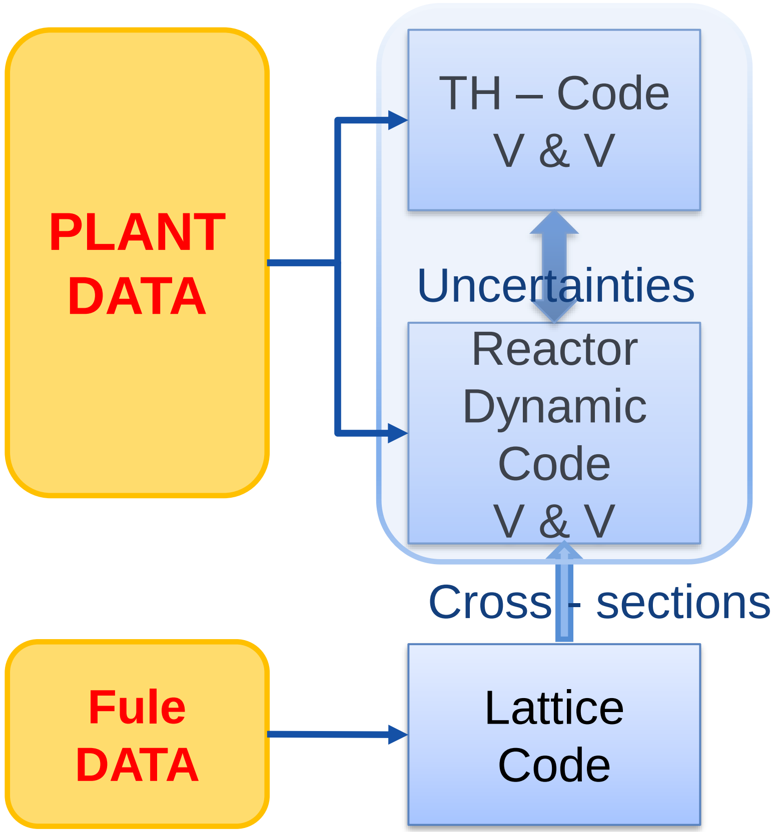
COMPUTER CODES AND APPLICATION
REACTOR DYNAMIC CODES

PARCS, SIMULATE3K, POLKA7, DYN3D…

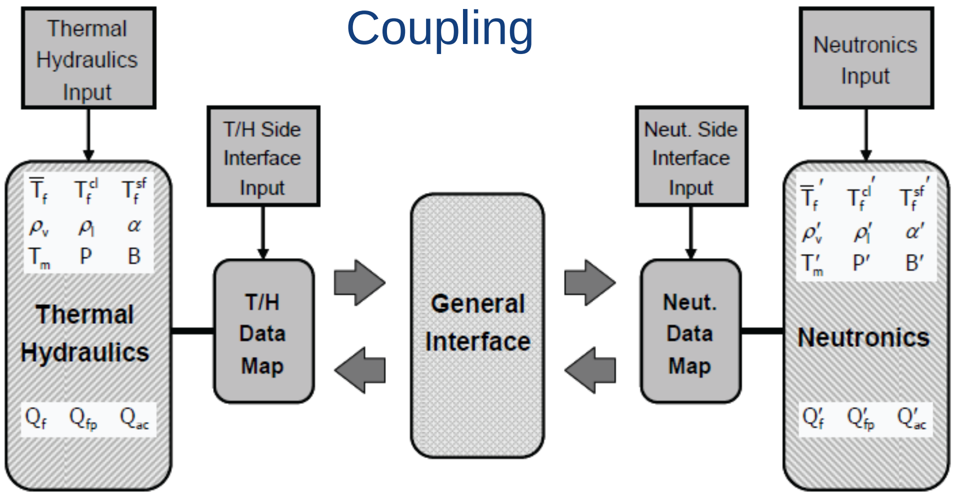
- Simulate transients and accidents, with criticality concerns,
- Need a detailed presentation of the core neutron kinetics,
- Does not include the detailed thermal-hydraulics for the reactor circuit due to computer capacity limitations in the past,
- Lack of detailed TH is not limiting if there is a well-mixed single-phase flow in the primary circuit.

The analysis needs for more complicated thermal-hydraulic progressions with the criticality concerns gave an incentive to couple the 1-D and 3-D reactor dynamics models with an advanced thermal-hydraulic modelling

COUPLED CODE STRATEGY



Coupling



COMPUTER CODES AND APPLICATION
SEVERE ACCIDENT CODES

MELCORE, MAAP, ASTEC….

- Deterministic severe accident codes are used for detailed modelling of physical phenomena,
- Realistic modelling has been the strategy of the severe accident code development from the early phases by utilizing the existing knowledge of physical phenomenology.
- Sometimes, a severe accident code can be linked to a system code to provide an integrated view of the entire accident (e.g., RELAP/SCDAP).

COMPUTER CODES AND APPLICATIONS

- Codes which take part on Safety Analysis must undergo:
  - a development and assessment process, performed by the methodology developer.
  - a parallel verification and validation process.
- Analysts and users of the codes should be trained, qualified, and experienced.
- Codes should draw on:
  - accumulated operating experience from similar nuclear plants.
  - Relevant experimental data and accumulated data for anticipated operational occurrences.

COMPUTER CODES at NPS

- The U.S. NRC. codes RELAP5/PARCS, TRACE/PARCS and MELCORE have been chosen to perform safety analysis and transient calculations by SSM.
- Additional codes such as Gothics, APROS, CFD codes, etc. are used by industry and university

Advanced simulation software for multiple purposes (APROS)

ADVANCED SIMULATION SOFTWARE FOR MULTIPLE PURPOSES

APROS is a tool that claims to be excellent for everything.

- Safety analyses of fast transients at nuclear power plants,
- Operator training at nuclear and conventional power plants,
- Research and development by universities and research institutes.

A comprehensive APROS model of a plant consists of all the main process, automation and electric systems and can be used for:

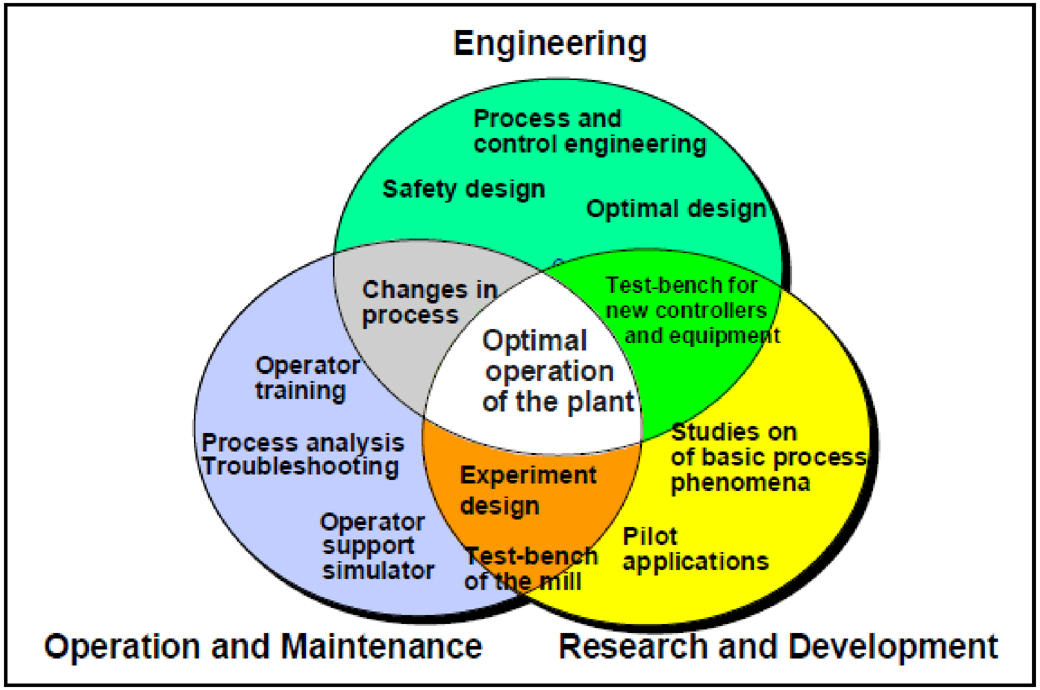
- Safety analyses,
- Dynamic process and automation testing,
- Training simulators,
- Optimization
- etc.

APROS can even be used as a simulation tool for testing of simple process change before building the actual system.

THE ADVANCED PROCESS SIMULATION ENVIRONMENT

- The modular and hierarchical approach of APROS allows flexibility of process analysis at various conceptual levels, from small computational experiments to models for full scope training simulators.
- APROS benefits from a fully graphical user interface.
- User enters only process related input data, model equations and choice of solution methods are done automatically.
- APROS has an online-feature, which allows the user to make any changes in parameter values or even the model structure and immediately continue the simulation.
- APROS allows the inclusion of the user's own models in the calculation.
- APROS allows connection to external models, automation systems or control room equipment.

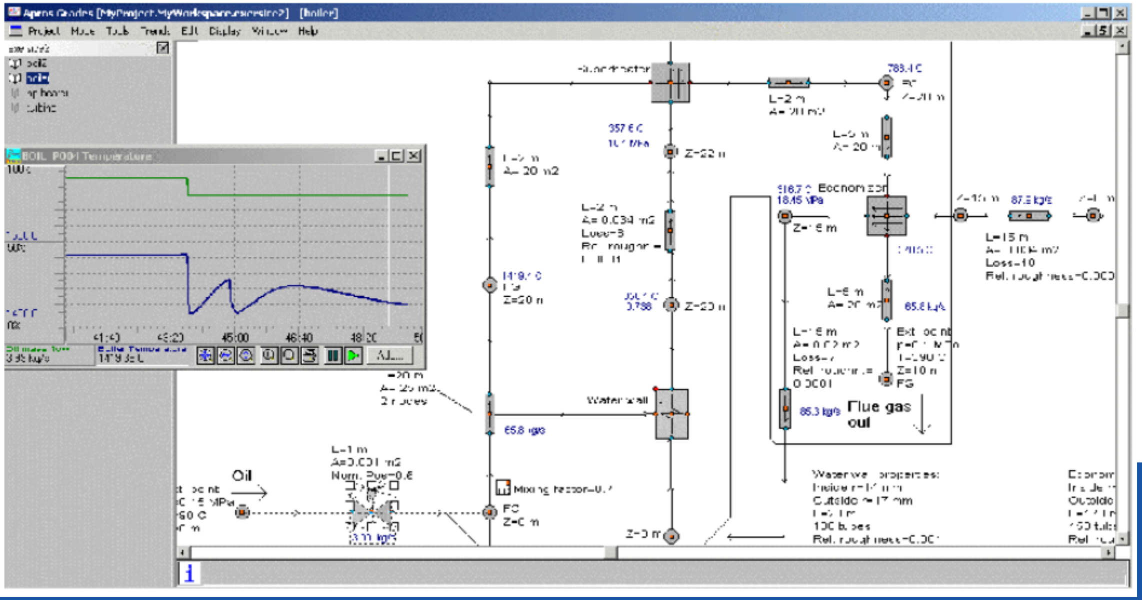
WIDE RANGE OF APPLICABILITY



- APROS can be used for simulation during the whole life span of the process, from the conceptual design to the operation and maintenance of the process.
- The same simulation model can be used for versatile tasks, thus avoiding unnecessary data transfer and reconfiguration of the simulation model.

EASY MODEL DEFINITION

- Simulation models are created graphically through the user interface presented in the figure.
- The user drags and drops components from model library palettes, draws connections between them,
- The user enters input data using component specific dialog windows.
- As a result, the user gets a P&I diagram with simulation specific additions, e.g., the values of the calculated variables can be monitored.

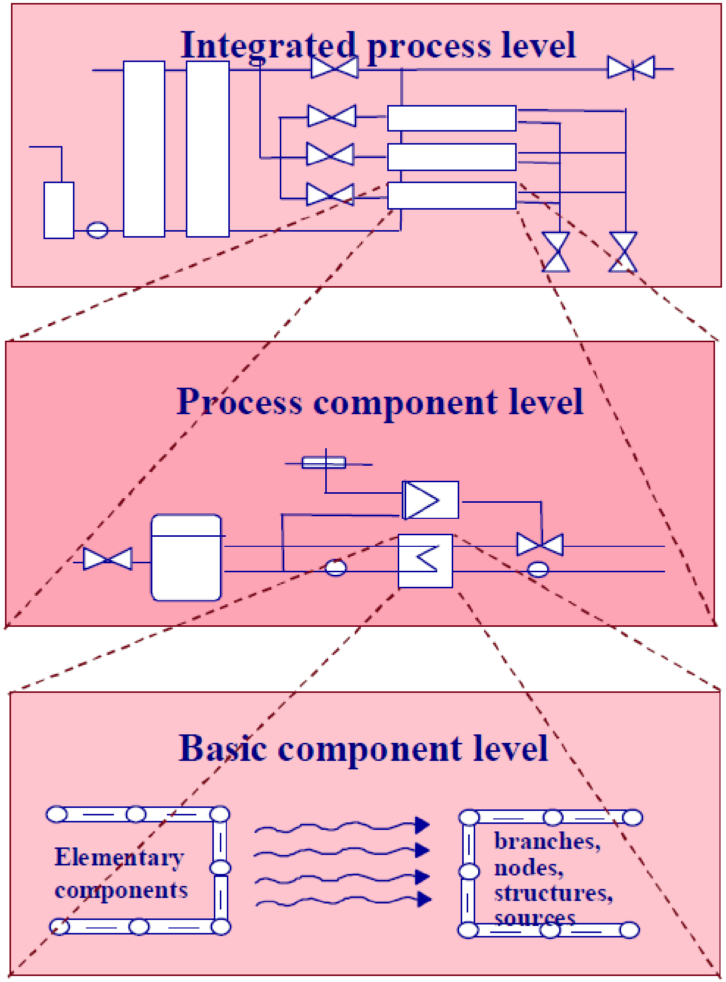


COMPREHENSIVE MODEL LIBRARIES

The APROS database structure supports hierarchical model presentation. Models are divided into tre levels:

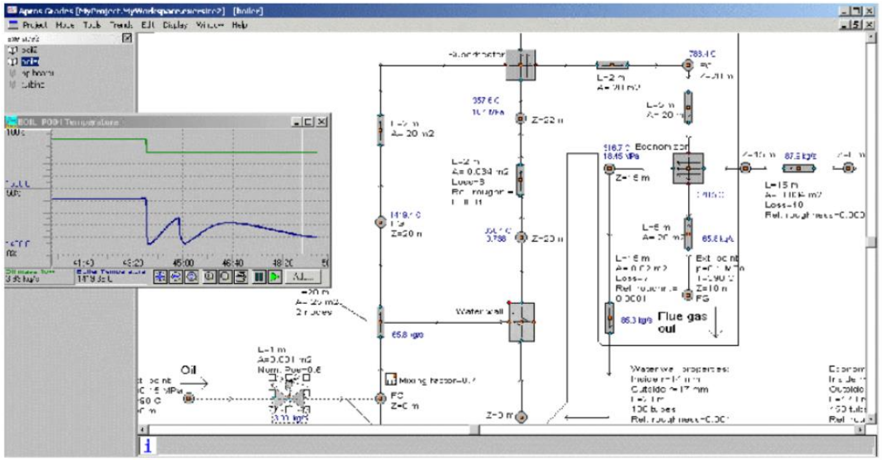
- Integrated process level (conceptually one-to-one corresponding with actual devices and hide all solution algorithms)
- Process component level (pipes, valves, pumps, heat exchangers, reactors, tanks, measurements, PID controllers, electric generators etc.)
- Basic component level (physical models which describe the component)

Most of the time, the user operates on the process component level using predefined components, like a heat exchanger, provided in model libraries. The process component automatically creates all necessary calculation level objects (nodes and branches). Components can be composed together to form a sub process, which in turn can be used as a part of an integrated process model.



MODEL ORGANIZATION AND RE-USE

- A large process model can be divided into several flow-sheet diagrams. This can be done both in a hierarchical and a horizontal way.
- At any time, the complete model information can be saved into a model snapshot file containing the full model configuration and its momentary state data at the time instant.



- At any time, the user can backtrack to a snapshot once saved in the past.
- Any part of the simulation model can be exported to a file, which can be merged to another model.

THERMAL HYDRAULIC FLOW MODELS

The APROS thermal hydraulic model library contains three different thermal hydraulic models for one dimensional water/steam/gas flow

- **homogenous,**
- **5 equation (drift flux model),**
- **6 equation (two fluid model).**

Thermal hydraulics uses the conservation equations for mass, momentum and energy and correlations for friction and heat transfer.

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.
- In this model, water and steam/gas have equal velocities and temperatures.
- Used 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.

5-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.

6-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.

APPLICABILITY OF DIFFERENT MODELS

- 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 consider different phase velocities.
  - The phase separation in small diameter piping is negligible.
  - In large diameter tanks can these features be described.
  - The 3 – equation model can be expanded for non-condensable 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…

STEADY STATE MODEL WITH TANK DYNAMICS

- The steady state model is based on the conservation equations of mass and energy.
- The steady state model is suitable when:
- fully dynamic pressure flow solution or two-phase flow is not needed,
- Input data for the process components is scarce.
- A simple model only consist of process topology and tank dimensions.
- This allows fast model building.
- Therefore, steady state model can be used as 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

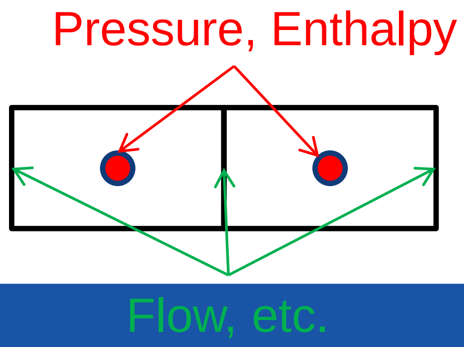
- The conservation equations of mass, momentum and energy. Described by sub-volumes (nodes) and flow paths between the sub-volumes (branches).
- The containment model can be arbitrarily divided into nodes and branches.
- Each node includes a gas region and may also include a liquid pool.
- In the gas phase, steam and non-condensable gases have a uniform temperature,
- The liquid and gas phases may have different temperatures.
- The branch is assumed to connect the gas regions of two nodes (only gas flows are calculated).
- For liquid flows, a liquid branch is available.
- 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.

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.
- In 6 equation model, the effect of non-condensable gas properties is considered in pressure and enthalpy solutions.
- In homogeneous model the air can be defined to be in a node, but it cannot flow from one node to another node. The air mass is considered in calculation of pressure.

DISCRETIZATION

- The flow solution of APROS is based on “staggered grid discretization scheme”.
  - the state variables (pressure, enthalpy, etc.) are calculated in the middle of the node,
  - 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.

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 define to be constant.

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 (length/area > 100 m/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 m^3 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 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

NUCLEAR REACTOR MODELS

APROS includes one- and three-dimensional core neutronics models.

- Based on time dependent two-group neutron diffusion equations computing the local flux at each time step, (accuracy comparable to the codes used for core supervision at a nuclear power plant).
- The models are valid for both BWR and PWR cores with either square or hexagonal fuel lattice.
- The reactivity level and the axial power distribution of the core can be tuned in both models.

What to consider while writing the report

1. time-line of the event
2. Use a correct language! "… After simulating the scenario in the APROS the behaviours of the parameter were observed. Figure 1, Figure 2, Figure 3 and Figure 4 illustrate those behaviours."
3. Explain how the plant behaves correctly! " …In the beginning the recirculation flow drops sharply due to loss of feedwater. After few seconds the drop rate is not as fast as the initial response since the main steam isolation valves are closed."
4. Use the correct nomenclature! "…Bleed valves closes"

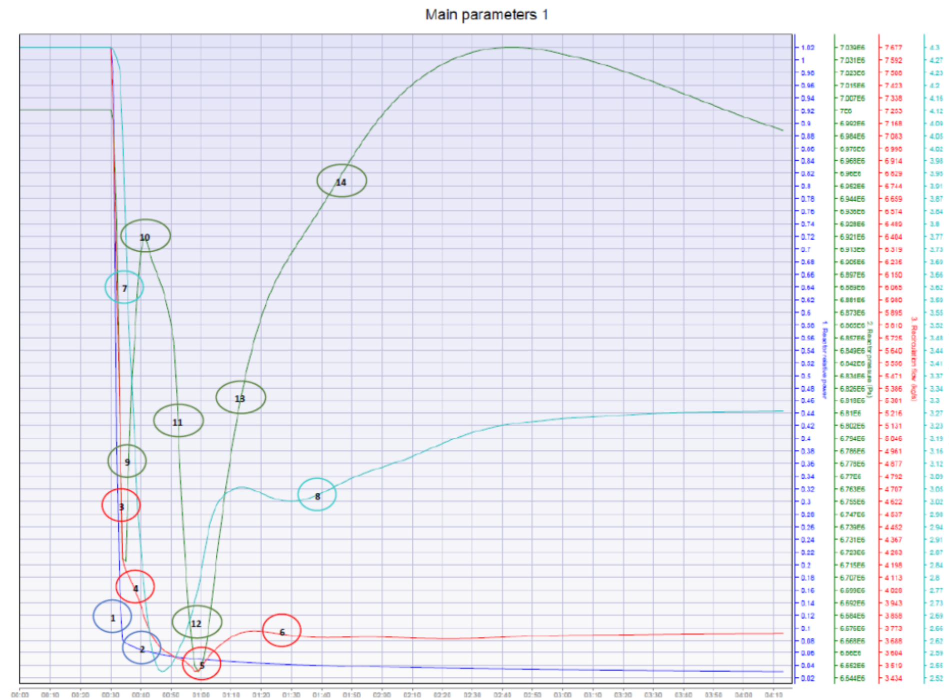


Figure 1. Behaviour of the Main Parameters 1 with respect to time

Verification and Validation

Verification and Validation (V&V) of computer codes for safety analysis:

- Systematic approach for improving reliability of computer codes and reduce risk of incorrect application.
- Activities that can be performed in parallel with the code development process, or a posteriori.
- The project sponsor should determine the level and modality of V&V efforts.

Verification and Validation

- Verification: process of evaluating a model during the software development phase to provide assurance that they meet the requirements defined for them.
- Validation: process of testing and evaluating the results of a code to ensure compliance with specified requirements.
- Testing carried out by the code developer, must be evaluated, supplemented or independently performed by a separate V&V team.

Verification and Validation

VALIDATION

REALITY → MATH MODEL → CODE DESIGN → CODE RESULT

VERIFICATION

Verification and Validation

- The code is validated when tests results are shown to meet criteria stated in advanced.
- V&V activities are performed by the code developer or by an independent V&V team.
- Model/user qualification is considerably simplified if the codes involved have been adequately V&V.

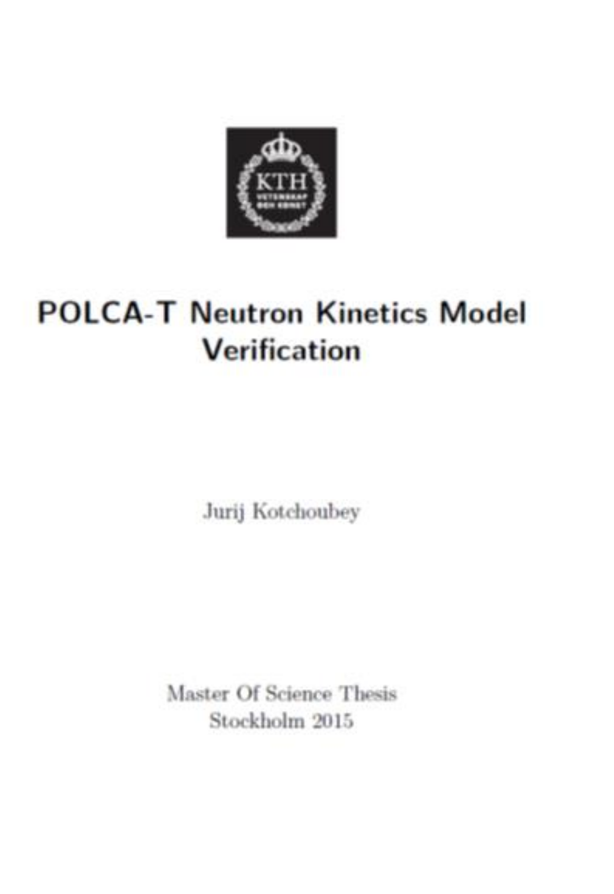
Verification and Validation

- Details of the V&V process:
  - Results should be documented and reported.
    - Each V&V activity should produce a report describing both the positive and negative results of the analysis or testing performed.
  - If V&V findings require revisions to the documents and products that are being verified, the modified ones should be re-verified before the next phase begins.
  - Checklists (containing questions that must be answered) should be used in the verification process.

Verification and Validation

- Verification and validation of computer codes are an important step of quality assurance procedure for successful application.
- Quality Assurance of computer codes
  - The quality assurance program should be established by the code developers to ensure the planned and systematic actions to provide confidence that the code developed meets technical requirements.
  - The quality assurance program should at least address
    - design control,
    - document control,
    - configuration control and testing,
    - corrective actions.

Example



POLCA-T Neutron Kinetics Model Verification

Jurij Kotchoubey

Master Of Science Thesis
Stockholm 2015

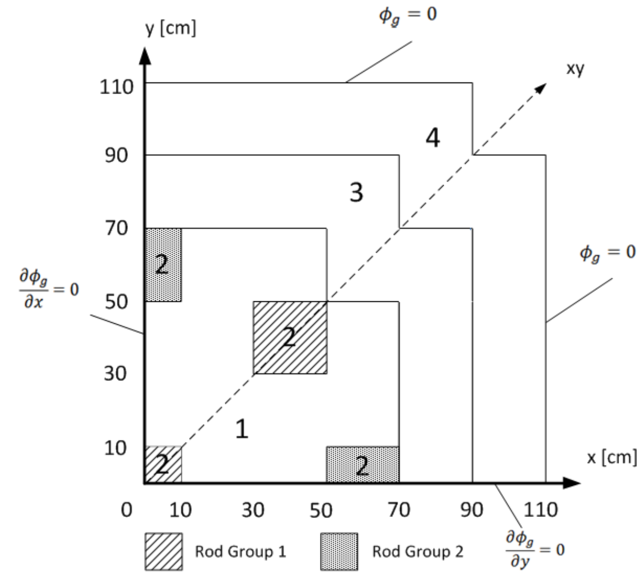
- The objective of the work was to verify of neutron kinetics employed in POLCA-T, Version 2.1.
- The verification was done by solving several widely used two- and three-dimensional kinetics problems. The results are then compared to those of other, established and well-proven spatial kinetics codes.

The Langenbuch-Maurer-Werner (LMW) benchmark problem

- Reflects an operational transient initiated by control rod movements in a highly simplified PWR.
- Later, the problem was extended such that it included even the thermal-hydraulic feedback effects. In this presentation, however, the latter are not considered.

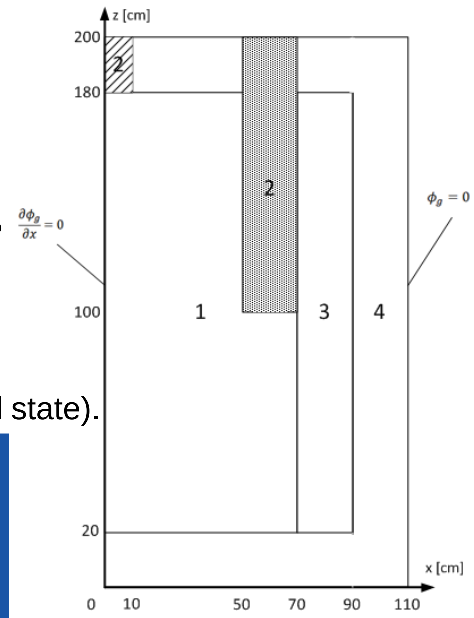
Example of Verification of Kinetic models

Horizontal cross-section.



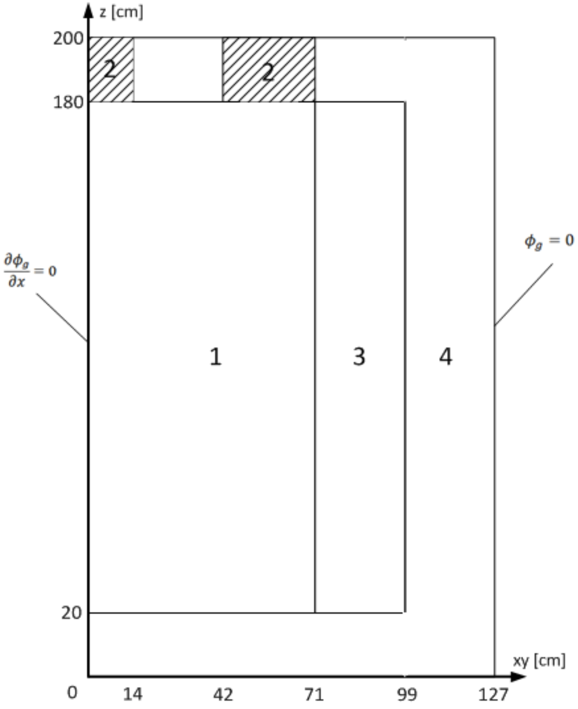
Langenbuch–Maurer–Werner (LMW) bench Operational Transient

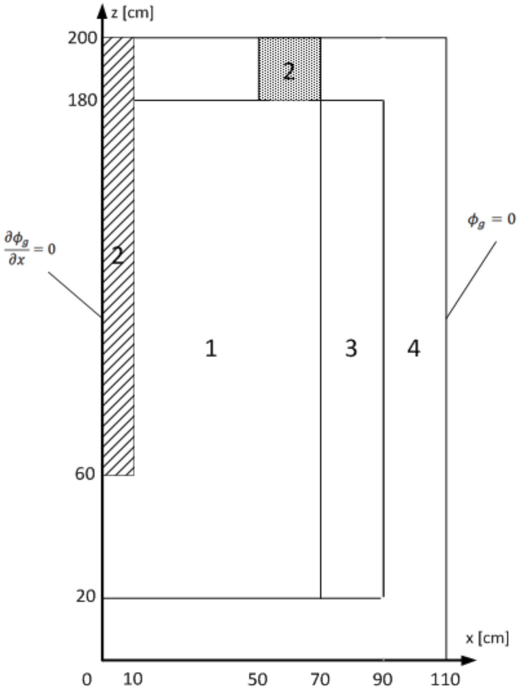
- quarter-symmetric PWR reactor core
- initial reactor core power is 739.2 MW_{th}
- two different fuel types
- initial core power density 150.0 W/cc.
- 77 fuel assemblies in the full core
- surrounded radially by an explicit water reflector
- fuel assembly's cross-section area 20x20 cm^2
- two energy groups and six delayed neutron families
- two CR banks

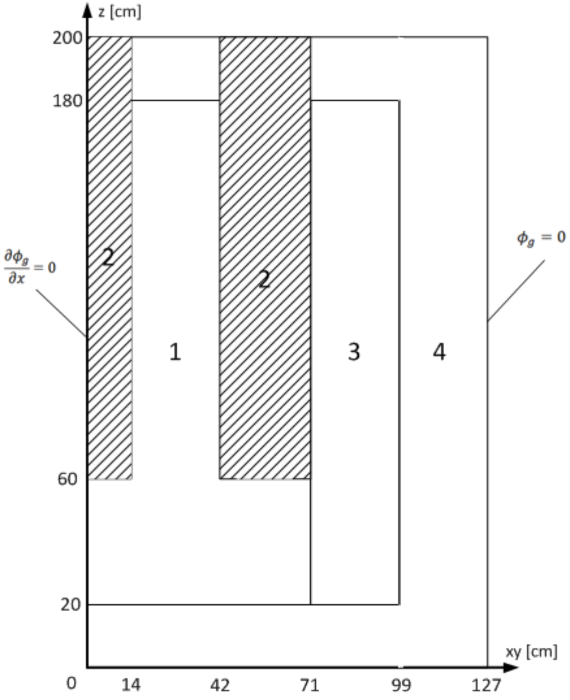


Vertical cross-sections (initial state).

LMW Operational Transient







LMW Operational Transient

Table 6.2.1: LMW benchmark: Eigenvalue results for both the initial and the final core state.

Code	Tested Code	QUANDRY	AETNA	SPANDEX	MGRAC
Node size* [cm^3]	20x20x20	20x20x20	10x10x5	5x5x2.5	4x4x4
Initial state	0.99970	0.99974	0.99971	0.99964	0.99964
Final state	0.99672	-	-	-	0.99666

*The node size (or node volume) is defined as $h_x \times h_y \times h_z$ where h is the node width in the respective direction.

- The MGRAC code is a three-dimensional nodal simulator
- Applied to neutron kinetic problems and recently extensively to research reactor, and in particular swimming-pool type materials testing reactor simulation.
- In the applied version of MGRAC, the core nodal neutronic and the fuel exposure meshes are identical and the selected mesh is fixed for all fuel assemblies and for all cycle depletion calculations.

Tested Code
MGRAC (Ref.)
ϵ (%)

			865 860 0,6	433 435 -0,5
		1126 1125 0,1	983 982 0,1	629 628 0,2
	1591 1593 -0,1	1397 1398 -0,1	1085 1085 0,0	708 709 -0,1
1556 1557 -0,1	1657 1658 -0,1	1441 1442 -0,1	982 982 0,0	728 728 0,0

Figure 6.2.1: LMW benchmark, initial condition: Normalized assembly power densities in comparison with MGRAC (octal symmetry is applied).

Tested Code

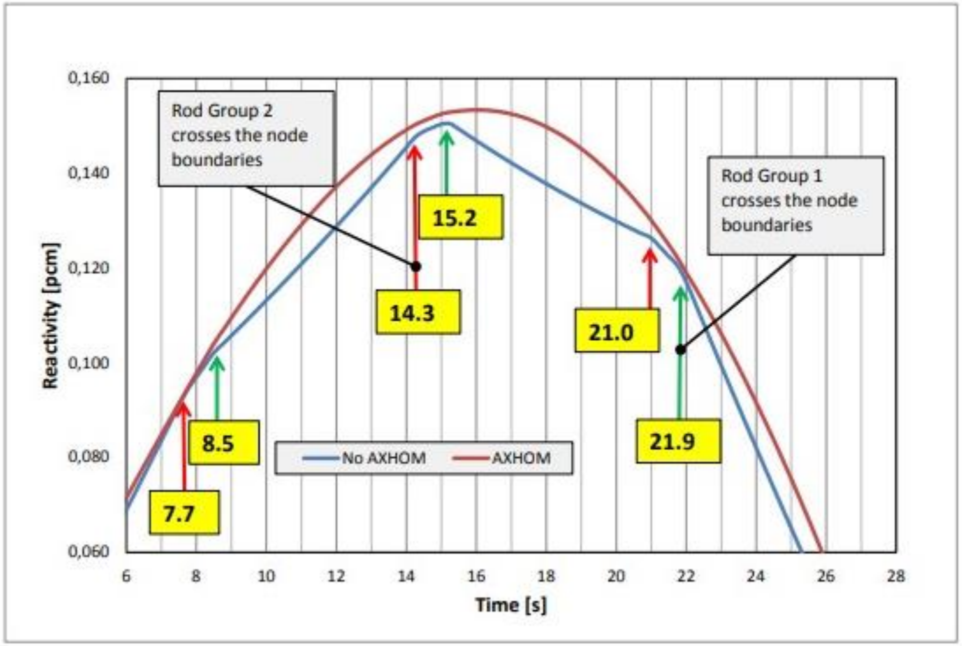
MGRAC (Ref.)

ϵ (%)

			859 855 0,5	437 439 -0,5
		1050 1052 -0,2	970 968 0,2	639 638 0,2
	1556 1557 -0,1	1382 1382 0,0	1109 1109 0,0	738 738 0,0
1427 1428 -0,1	1606 1606 0,0	1455 1455 0,0	1045 1047 -0,2	771 772 -0,1

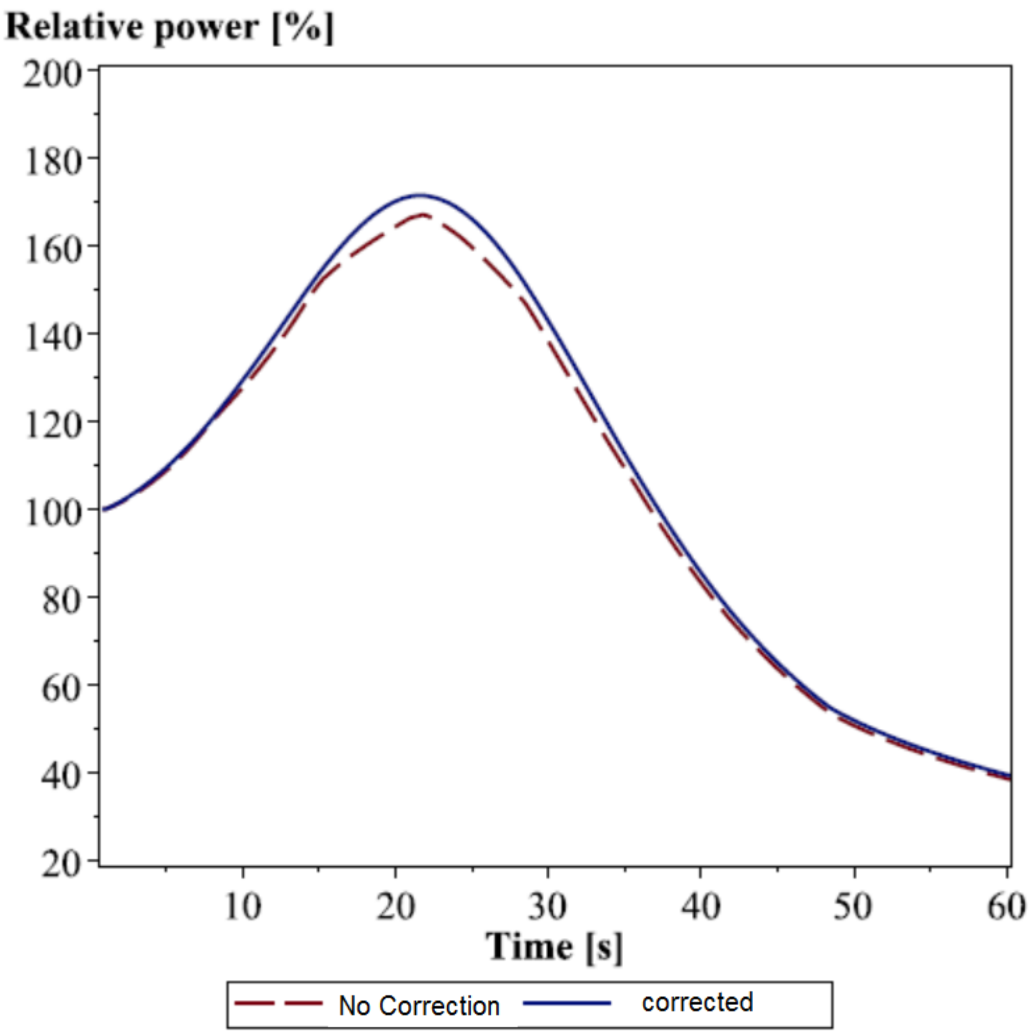
Figure 6.2.2: LMW benchmark, final condition: Normalized assembly power densities in comparison with MGRAC (octal symmetry is applied).

Errors in cross-section homogenization are also caused by the presence of spacers, burnable absorbers, etc. In this case, a special scheme (called AXHOM) is employed in order to minimize errors caused by these heterogeneities.



- As already pointed out by Smith and other authors, the so-called control rod cusping effect is especially pronounced in the LMW transient.
- That is, the error in determination of volume-weighted, homogenized cross-sections for partially rodded nodes can become significant. The error results then in an unphysical behavior of the total reactivity,
- This behavior leads consequently to an underestimation of the total reactivity and core power.
- Error in cross-section homogenization are also caused by the presence of spacers, burnable absorbers, etc. In POLCA7,
- The “uncorrected” power profile shows a clear underestimation of power, especially in the aforementioned power peakregion.

LMW Operational Transient



LMW Operational Transient