AER Benchmark Solution Sheet

1. Test ID: AER-DYN-005 (Draft 1)

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Date: 27.12.2000

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3. Code or Program Applied: DYN3D/ATHLET

4. Short description of the Code:

The code complex DYN3D/ATHLET consists of the advanced thermohydraulics code ATHLET and the 3D neutron kinetics core model DYN3D. The code ATHLET has been developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS). An overview on the capabilities of ATHLET is given in [1]. It can be applied to the whole spectrum of operational and accident transients, small and intermediate leaks up to large breaks of coolant loops or steam lines at PWRs and BWRs. The code includes basic modules for thermohydraulics, heat transfer and heat conduction, neutron kinetics (point kinetics and 1D neutron kinetics) and balance of plant simulation. Within the General Control and Simulation Module (GCSM) a general interface is available, that allows to couple other independent modules to ATHLET without changes of the code architecture. The fluiddynamics is described by a six-equation model, with separate conservation equations for liquid and vapour mass, energy and momentum. In the code, the 1D thermohydraulics is used. The code DYN3D [2] consists of the 3D neutron kinetic model and an own thermohydraulics module (FLOCAL). The neutron kinetics of DYN3D is calculated by using a nodal expansion method (NEM) for hexagonal geometry. The developed method solves the neutron diffusion equation for two energy groups. Stationary state and transient behaviour can be calculated. The thermohydraulics module FLOCAL consisting of a two-phase coolant flow model, a fuel rod model and a heat transfer regime map up to superheated steam is coupled with neutron kinetics by the neutron physical constants. One coolant channel per fuel assembly and additional hot channels can be considered.

In accomplishing the coupling of ATHLET and DYN3D two basically different ways were pursued [3]. The first one uses only the neutron kinetic part of DYN3D and integrates it into the heat transfer and heat conduction model of ATHLET. This is a very close coupling, the data have to be exchanged between all core nodes of the single models (internal coupling). In the second way of coupling the whole core is cut out of the ATHLET plant model (external coupling). The core is completely modelled by DYN3D. The thermohydraulics is split into two parts: the FLOCAL module of DYN3D describes the thermohydraulics of the core and ATHLET models the coolant system. As a consequence of this local cut it is easy to define the interfaces. They are located at the bottom and at the top of the core. The pressures, mass flow rates, enthalpies and concentrations of boron acid at these interfaces have to be transferred. So the external coupling needs only a few parameters to be exchanged between the codes and is therefore easy to be implemented. It is effectively supported by the above mentioned GCSM of the ATHLET code.

5. Known Approximations:

- Thermohydraulics of the plant

  - modular network approach for the representation of the thermohydraulics system
  - 1D six equation model for two phase coolant flow
  - finite-volume approach for solving the equations inside the objects of the network
  - assignment of heat conduction objects to all thermofluiddynamics objects of the network

- Neutron Kinetics

  - Neutron diffusion theory
  - Two group theory
  - Nodewise homogenized cross sections

- Thermohydraulics of the core

  - One-dimensional four equation model for two phase coolant flow
  - (momentum equation of mixture, energy equation of mixture, mass balance of mixture and mass balance of vapour phase)
  - Constituitive laws
  - Radial heat conduction equation in fuel pin
  - Map for heat transfer from fuel to coolant

- Coupling

  - Replacement of the point kinetics model in ATHLET by the 3D neutron kinetics model of DYN3D (internal coupling)
  - Replacement of the complete ATHLET core model by the whole DYN3D model (3D neutron kinetics and core thermohydraulics); coupling at the core in- and outlet (external coupling)

6. Mathematical Model:

- ATHLET

The time integration of the thermofluiddynamics is performed with the general purpose ODE-Solver FEBE (Forward-Euler, Backward-Euler). It provides the solution of a general nonlinear system of differential equations of first order, splitting it into two subsytems, the first being integrated explicitly, the second implicitly. Generally, the fully implicit option is used in ATHLET. The linearization of the implicit system is done numerically, by calculation of the Jacobian matrix. A block sparse matrix package is available to handle in an efficient way the reapeated evaluation of the Jacobian matrix and the solution of the resulting system of linear equations. A rigorous error control is performed based on an extrapolation technique.

- DYN3D (Neutron Kinetics)

The 3D neutron kinetic model is based on the solution of the 3D 2-group neutron diffusion equation by a nodal expansion method which is specific for the geometry of fuel assemblies [2,4]. It is assumed that the macroscopic cross sections are spatially constant in a node being a part of the hexagonal fuel assembly. The stationary diffusion equation in the node is solved by factorizing the space dependency of neutron fluxes in the radial plane and the axial direction. A 2D diffusion equation in the radial plane and a 1D equation in axial direction are obtained. The two equations are coupled by the transversal bucklings. In the hexagonal plane the fluxes are expanded by using Bessel functions being the solutions of the Helmholtz equation. The low order coefficients are expressed by the node averaged fluxes and the incoming partial currents averaged over the interface of the hexagon. In this way, the outgoing partial currents at the interfaces are given by the node fluxes and the incoming partial currents. The matrix elements of these relations depend on the transversal buckling and the eigenvalue k_{eff}. The 1D equation in axial direction is solved by a polynomial expansion up to the fourth order. The outgoing partial currents in axial direction are given by the averaged fluxes, incoming partial currents and higher order coefficients. The equations for the 3rd and 4th order polynomials are obtained by Galerkin weighting. The outgoing partial currents at a node interface are the incoming currents in the neighbouring nodes. The steady state diffusion equation is solved by an inner and outer iteration process. The outer iterations are the fission source iterations accelerated by a Chebychev extrapolation scheme. A small number of inner iterations (3-5) are sufficient for the convergency. During the outer iteration process the matrix elements are recalculated few times (3-5).

Concerning the time integration over the neutronic time step an implicite difference scheme with exponential transformation is used. The exponents in each node are calculated from the previous time step or during the iteration process. For the calculation of matrix elements describing the relation between partial currents and averaged fluxes it is assumed that the time behaviour of the neutron fluxes in the nodes is exponential and the local variation of the source of delayed neutrons is proportional to the source of prompt neutrons. These assumptions allow the same treatment of diffusion equation in the nodes as in the steady state. In the iteration process we have to solve an inhomogeneous problem. Similar methods as used for the steady state are applied.

- DYN3D (Thermohydraulics)

The thermohydraulics model of the reactor core and the fuel rod model are implemented in the module FLOCAL [5] being a part of DYN3D. The reactor core is modelled by parallel cooling channels which can describe one or more fuel elements. The parallel channels are coupled hydraulically by the condition of equal pressure drop over all core channels. Additionally, so- called hot channels can be considered for the investigation of hot spots and uncertainties in power density, coolant temperature or mass flow rate. Thermohydraulic boundary conditions for the core like coolant inlet temperature, pressure, coolant mass flow rate or pressure drop must be given as input for DYN3D. Applying the coupled DYN3D - ATHLET code they are provided by the ATHLET code. Mixing of coolant from different loops before entering the core can be modelled by applying several options. Homogeneous mixing can be assumed for each reactor type and number of loops. For VVER-440 type reactors, an analytical mixing model for the downcomer and the lower plenum is implemented in the code. The model is based on the analytical solution of the Navier-Stokes equations in the potential flow approximation in 3D cylindrical geometry and the diffusion equation for heat transport or soluble poison. Turbulent Peclet numbers for the downcomer and the lower plenum are parameters of the model, which are used for a best fit adaptation to experimental results. The mixing model represents an interface between the cold legs of the primary loop and the core inlet. The two-phase flow model is closed by constitutive laws for heat mass and momentum transfer, e.g. vapour generation at the heated walls, condensation in the subcooled liquid, phase slip ratio, pressure drop at single flow resistance's and due to friction along the flow channels as well as heat transfer correlations. The heat transfer regime map which is implemented in FLOCAL ranges from one-phase liquid convection up to superheated steam. The occurrence of heat transfer crisis is stated by different correlation's for the critical heat flux. The transient boiling region is described by the KIRCHNER and GRIFFITH interpolation for the heat flux. In the stable post-crisis region for inverted annular or dispersed flow the GROENEVELD - DELORME or a modified BROMLEY correlation's are used. After full evaporation of coolant, heat transfer to superheated steam is estimated by a forced convection correlation [5].

- Coupling DYN3D to ATHLET

In both cases of coupling, the DYN3D model is called at the end of each thermohydraulics ATHLET time step. In the internal coupling, the fuel temperature, coolant density and temperature and boron concentration are transferred for each node to DYN3D to calculate the power distribution. This distribution is then used for the next thermohydraulics time step. In the case of external coupling, the pressure drop over the core together with the enthalpy and boron concentration at the core inlet are transferred to DYN3D. Using these parameters, a whole core calculation is carried out. The calculated mass flow rate, core outlet enthalpy and boron concentration are transferred to ATHLET.

7. Features of Techniques Used:

For the calculation of the benchmark, the external coupling of DYN3D to ATHLET was used. An option for constant decay heat during transient calculation has been developed and implemented into the code.

8. Computer, Operational System: SUN workstation, Solaris

9. References:

[1] V. Teschendorff, H. Austregesilo, G.: "Lerchl: Methodology, status and plans for development and assessment of the code ATHLET" *Proc. OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements*, Annapolis, USA, Nov. 5-8, 1996, p. 112, NUREG/CP-0159, NEA/CSNI/R(97)4

[2] U. Grundmann and U. Rohde: "DYN3D/M2 - a Code for Calculation of ReactivityTransients in Cores with Hexagonal Geometry", *Proc. of IAEA Technical Committee Meeting on Reactivity Initiated Accidents*, Wien (1989)
Rep. FZR 93-01, Research Center Rossendorf (1993)

[3] U. Grundmann, D. Lucas, S. Kliem and U. Rohde: “Coupling of the Thermohydraulic Code ATHLET with the 3D Neutron Kinetic Model DYN3D“, *Proc. 6th Symposium of AER*, pp. 179-191, KFKI Atomic Energy Research Institute, Budapest (1996)

[4] U. Grundmann: “A NEM for Solving Time-Dependent 3-Dimensional Diffusion Equation for Hexagonal Geometry”, *Proc. International Conference on the Physics of Reactors PHYSOR'90*, Marseille (1990)

[5] U. Rohde: “Modelling of Fuel Rod Behaviour and Heat Transfer in the Code FLOCAL for Reactivity Accident Analysis of Reactor Cores”, 1st Baltic Heat Transfer Conference, Göteborg, (1991), published in: Transport Processes in Engineering, 2: Elsevier Publ., Amsterdam (1992)

[6] S. Kliem: “Solution of the Fifth Dynamic AER Benchmark Using the Coupled Code DYN3D/ATHLET“, *Proc. 8th Symposium of AER*, pp. 357-367, KFKI Atomic Energy Research Institute, Budapest (1998)

[7] S. Kliem: “Comparison of the Results of the Fifth Dynamic AER Benchmark - A Benchmark for Coupled Thermohydraulic System/3D Hexagonal Neutron Kinetic Core Models“, *Proc. 8th Symposium of AER*, pp. 429-469, KFKI Atomic Energy Research Institute, Budapest (1998)

[8] S. Kliem, S. Danilin, R. Kyrki-Rajamäki, J. Hadek, A. Keresztury, P. Siltanen: “A Benchmark for Coupled Neutron Kinetics/Thermohydraulics System Codes – Main Steam Header Break in a NPP with VVER-440 Reactor”, *Proc. Int. Conf. On Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications (MC ’99)*, v. 2, pp. 1794-1803, Senda Editorial, S.A., Madrid (1999)

10. Results:

All requested results are in the ASCII-file DYN005_FZR.RES. The solution of the benchmark is described in [6]. The comparison with other solutions is presented in the specification document DYN-005 and in [7, 8].

11. Comparison to Recommended Solution:

No reference solution does exist so far. The comparison with solutions of other coupled codes is presented in the specification document DYN-005 and in [7, 8].