# LOOP2: COMPREHENSIVE TRANSIENT CODE FOR ADVANCED NUCLEAR REACTORS

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## ABSTRACT

**1. Program Name and Title:** LOOP2: comprehensive transient code for advanced nuclear reactors.

**2. Computer for Which Program is Designed and Other Machine Versions Available:** The code was prepared for personal computer.

**3. Problem Solved:** LOOP2 code [1,2] simulates transient processes in the core and system of circuits of advanced nuclear reactors of various types, including liquid-metal, molten-salt, gas-cooled reactors, etc. A structure of the model includes three main blocks: 1) reactor neutron and isotopic kinetics; 2) thermal hydraulics and mass transfer in a system of circuits, and 3) thermal mechanics of fuel rods and structural elements. Information flows between main blocks of LOOP2 code are shown in Figure 1.

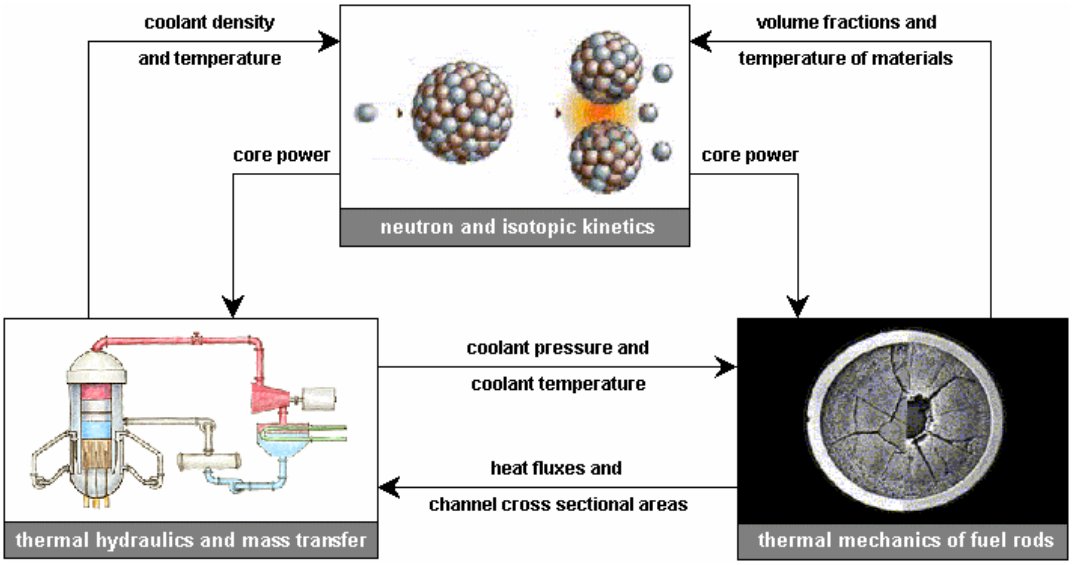


Figure 1. Information flows between main blocks of LOOP2 code

A block of reactor neutron and isotopic kinetics calculates transient 3-D fields of concentrations of isotopes, neutron cross sections, neutron fluxes, and concentrations of delayed neutron precursors under diffusion multigroup approximation for square, hexagonal or cylindrical geometry. For transient calculations a set of ordinary differential equations, including transient multi-group equations of neutron transport in diffusion approximation, transient group equations for precursors of delayed neutrons and transient equations of isotopic kinetics for atomic density of isotopes are solved:

$$\frac{1}{v^g}\frac{\partial \Phi^g}{\partial t} = \sum_{g' \neq g}^{N^g} (\Sigma_i^{g' \to g} + \Sigma_e^{g' \to g} + 2\Sigma_{n2n}^{g' \to g})\Phi^{g'} - \sum_{g' \neq g}^{N^g} (\Sigma_i^{g \to g'} + \Sigma_e^{g \to g'} + \Sigma_{n2n}^{g \to g'})\Phi^{g} - \nabla J^g - \Sigma_a^g \Phi^g + \tag{1}$$
$$+ \chi_P^g \sum_{g'=1}^{N^g} \nu_P^{g'} \Sigma_f^{g'} \Phi^{g'} + \sum_{m=1}^{N^d} \chi_D^{gm} \lambda^m C^m + S^g;$$

$$\frac{\partial C^m}{\partial t} = \sum_{g'=1}^{N^g} \chi_D^{g'm} \nu_D^{g'} \Sigma_f^{g'} \Phi^{g'} - \lambda^m C^m; \tag{2}$$

$$\frac{\partial c^i}{\partial t} = \sum_{j=1}^{N^i} \left[ \lambda^{j \to i} c^j - \lambda^{i \to j} c^i + \sum_{g'=1}^{N^g} y_{ij}^{g'} \left( \sigma_{j \to i}^{g'} - \sigma_{i \to j}^{g'} \right) \Phi^{g'} \psi \right]; \tag{3}$$

where $g=1,\ldots,N^g$–energy group number, $m=1,\ldots,N^d$–delayed neutrons group number; $v^g$–neutron velocity; $\Phi^g$–neutron flux density; $J^g$–neutron current; $S^g$–external neutron source; $\chi_P^g$ and $\chi_D^{gm}$–prompt and delayed fission neutron spectrum; $\Sigma_i^{g' \to g}$, $\Sigma_e^{g' \to g}$ and $\Sigma_{n2n}^{g' \to g}$–inelastic, elastic and (n,2n) scattering cross sections; $\Sigma_a^g$ – absorption cross section; $\nu_P^g \Sigma_f^g$ and $\nu_D^g \Sigma_f^g$ – prompt and delayed neutron production cross sections; $C^m$ – concentration of delayed neutron precursors;

Diffusion coefficient is calculated as $1/3\Sigma_{tr}$, where $\Sigma_{tr}$ is transport cross section, estimated as $\Sigma_{t,l}$–$\Sigma_{i,l}^{g \to g}$–$\Sigma_{e,l}$. When calculating $\Sigma_{e,l}$ both scattering in the same group and downscattering were accounted for all isotopes, but hydrogen. For hydrogen only scattering in the same group $\Sigma_{e,l}^{g \to g}$ is taken into account. A neutron flux density and current is approximated either by finite-difference approach or with the use of effective nodal technique [3].

Neutron microscopic cross sections and constants are prepared with the use of evaluated nuclear data files in ENDF-6 format processed with NJOY-94 system [4]. A Russian CONSYST/ABBN system [5] developed for fast reactors was also included in the LOOP2 code as an option for preparation of cross section on the basis of the ABBN-93 library.

Neutron macroscopic constants are re-calculated during a transient, when the value of temperatures and/or nuclear densities of core materials, computed in thermal hydraulics and thermal mechanics blocks of the code, is changed by the specified values since previous re-calculation.

Spatial thermal hydraulics and mass transfer block of LOOP2 code calculates in a system of circuits the transient spatial fields of velocities, pressures, enthalpies, and concentrations of soluble admixtures for single-phase or two-phase equilibrium homogeneous coolant flow. An opportunity to combine for selected sections of circuits 1-, 2- or 3-D nodalization schemes with the use of square, hexagonal or cylindrical geometry allows for flexible modeling of spatial distribution of calculational thermal-hydraulic parameters in a system of circuits.

The spatial thermal hydraulics and mass transfer model is based on four equations for a mass velocity vector $\mathbf{w}$ (kg/m$^2$s), coolant pressure P (Pa), coolant enthalpy h (J/kg) and concentrations of soluble admixtures $c^j$ (kg/m$^3$).

Conservation laws:

for coolant mass:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) = 0\,, \qquad (4)$$

for coolant momentum:

$$\frac{\partial w_i}{\partial t} + \nabla(w_i \mathbf{v}) = -\frac{\partial P}{\partial x_i} + \rho \mathbf{g}\cdot\mathbf{i} - \nabla \boldsymbol{\phi}, \qquad (5)$$

for coolant energy:

$$\frac{\partial(\rho h)}{\partial t} + \nabla(\rho h \mathbf{v}) = -\nabla \lambda \nabla T + \frac{q_w \Pi_w}{A} + q_v\,, \qquad (6)$$

for soluble admixtures:

$$\frac{\partial c^j}{\partial t} + \nabla(c^j \mathbf{v}) = \frac{q_m^j \Pi_m^j}{A} + w_+^j - w_-^j\,, \qquad (7)$$

where $\rho$ – coolant density (kg/m$^3$);
$\mathbf{v}$ – coolant velocity (m/s).
$\mathbf{g}$ – gravitational constant (m/s$^2$);
$\boldsymbol{\phi} = \mu \nabla \mathbf{v}$ – tensor of viscous stresses (Pa);
$\lambda$ – coolant thermal conductivity (W/mK);
T – coolant temperature (K);
$q_w$ – heat flux from heat transfer surfaces (W/m$^2$);
$\Pi_w$ – heat transfer perimeter (m);
A – channel flow cross section area (m$^2$);
$q_v$ – power density in coolant (W/m$^3$);
$q_m^j$ – mass flux of j-th soluble admixture from mass transfer surfaces (kg/m$^2$s);
$\Pi_m$ – mass transfer perimeter (m);
$w_+^j$ and $w_-^j$ – rates of chemical reactions in which j-th soluble admixture is generated and disappears, respectively, (kg/m$^3$s).

Two-phase flow in all equations is approximated by a homogeneous equilibrium two-phase mixture of liquid and vapor, i.e. both phases are assumed to be at saturation and have equal pressure and the same velocity.

Data base of the code on coolant properties includes thermal-physical properties and closure relations for liquid-metal coolants (lead, eutectics lead-bismuth and lead-magnesium, sodium), molten fluoride salts, gas coolants, including helium and air, as well as water and vapor.

Boundary conditions on heat fluxes as well as channel cross section areas are calculated in the thermal-mechanical block. When modeling of volume heat generation in coolant, thermal power field calculated in reactor kinetics block is used.

Transient thermal mechanics block FRED [6] was included in LOOP2 code and calculates in r-z geometry coupled change in fields of temperatures, heat fluxes, stresses, strains and failure probability for such structural elements as fuel rods, steam generator tubes, reactor vessel, etc. Main equations, solved in thermal mechanics block, are given in Table 1.

Table 1. Equations solved in thermal mechanics block

| Cauche equations | Hooke's laws | Equilibrium equations |
|---|---|---|
| $\varepsilon_r = \frac{\partial u_r}{\partial r}$ | $\varepsilon_r = \frac{1}{E}\left[\sigma_r - \nu(\sigma_\theta + \sigma_z)\right] + \varepsilon_r^{TCP}$ | $\frac{\partial \sigma_r}{\partial r} + \frac{1}{r}\frac{\partial \tau_{r\theta}}{\partial \theta} + \frac{\partial \tau_{zr}}{\partial z} + \frac{\sigma_r - \sigma_\theta}{r} = 0$ |
| $\varepsilon_\theta = \frac{1}{r}\left(\frac{\partial u_\theta}{\partial \theta} + u_r\right)$ | $\varepsilon_\theta = \frac{1}{E}\left[\sigma_\theta - \nu(\sigma_z + \sigma_r)\right] + \varepsilon_\theta^{TCP}$ | $\frac{\partial \tau_{r\theta}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_\theta}{\partial \theta} + \frac{\partial \tau_{\theta z}}{\partial z} + \frac{2}{r}\tau_{r\theta} = 0$ |
| $\varepsilon_z = \frac{\partial u_z}{\partial z}$ | $\varepsilon_z = \frac{1}{E}\left[\sigma_z - \nu(\sigma_\theta + \sigma_r)\right] + \varepsilon_z^{TCP}$ | $\frac{\partial \tau_{zr}}{\partial r} + \frac{1}{r}\frac{\partial \tau_{\theta z}}{\partial \theta} + \frac{\partial \sigma_z}{\partial z} + \frac{1}{r}\tau_{rz} = 0$ |
| $\varepsilon_{r\theta} = \frac{1}{r}\frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r}$ | $\varepsilon_{r\theta} = \frac{\tau_{r\theta}}{G} + \varepsilon_{r\theta}^{TCP}$ | **Boundary conditions** |
| $\varepsilon_{\theta z} = \frac{1}{r}\frac{\partial u_z}{\partial \theta} + \frac{\partial u_\theta}{\partial z}$ | $\varepsilon_{\theta z} = \frac{\tau_{\theta z}}{G} + \varepsilon_{\theta z}^{TCP}$ | $\sigma_r \cos(n,k_r) + \tau_{zr}\cos(n,k_z) = f_r$<br>$\tau_{r\theta}\cos(n,k_r) + \tau_{\theta z}\cos(n,k_z) = f_\theta$<br>$\tau_{zr}\cos(n,k_r) + \sigma_z\cos(n,k_z) = f_z$<br>or specified $u_r$, $u_\theta$, $u_z$ |
| $\varepsilon_{zr} = \frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}$ | $\varepsilon_{zr} = \frac{\tau_{zr}}{G} + \varepsilon_{zr}^{TCP}$ | |

Nomenclature in Table 1: r, θ and z – radial, hoop and axial coordinates; $u_r$, $u_\theta$ and $u_z$ – radial, hoop and axial displacements; $\varepsilon_r, \varepsilon_\theta, \varepsilon_z, \varepsilon_{r\theta}, \varepsilon_{\theta z}, \varepsilon_{zr}$ – components of total deformation; E – elasticity modulus; ν – Poisson ratio; G – shear modulus; $\varepsilon_\theta^{TCP}, \varepsilon_r^{TCP}, \varepsilon_z^{TCP}, \varepsilon_{r\theta}^{TCP}, \varepsilon_{\theta z}^{TCP}, \varepsilon_{zr}^{TCP}$ – components of thermal-viscous-plastic deformation; $\sigma_r, \sigma_\theta, \sigma_z, \tau_{r\theta}, \tau_{\theta z}, \tau_{zr}$ – stress components; n – normal to boundary surface; $k_r$ and $k_z$ – orts of the corresponding axes, $f_r$, $f_\theta$ and $f_z$ – components of surface loading.

Other equations are solved in the model, including energy conservation equation for temperature calculation, correlation for fuel-clad gap conductance [7], inner gas pressure model similar to [8], Hill equation for effective stress, empirical function for creep calculation [9], Prandtl-Reuss flow rules for components of plastic and creep strains, equation for stress-strain curve [10,11], etc. Several independent fuel rod failure criteria are used, including overstress failure criterion [10,11], creep rate/time-to-failure criterion [12], strain energy density criterion [13], melting criterion. A library of thermal-mechanical material properties includes data for Zry [10], Zr-1%Nb [11], advanced Zr-alloys for high burnup fuel, several types of stainless steel, some nickel-based alloys, $UO_2$ [10], MOX [14], UN-PuN, etc.

The thermal mechanics block uses fields of temperatures and pressures in surrounding fluid calculated in the thermal hydraulics block as well as thermal power distribution calculated in the neutron and isotopic kinetics model.

**4. Method of Solution:** Implicit scheme of the first order is used for approximation of time derivatives in neutron kinetics equations (1) and (2). The obtained set of linear algebraic equations is solved by the Gauss-Zeidel iteration method. The other velocity equations are solved with the use of a common standard integration procedure LSODES based on a BDF method (Backward Differentiation Formula) with automatic step, error and method order control [15]. A Jacobi matrix of the system in this procedure is generated automatically and processed in a general sparse form.

**5. Restrictions on the Complexity of the Problem:** There are no other restrictions except those, defined by hardware parameters.

**6. Typica1 Running Time:** Several minutes up to several days, depending on the problem and accuracy.

**7. Unusual Features of the Program:** The main feature of the LOOP2 code is ability to perform coupled dynamic calculations of neutronics, thermal hydraulics and thermal mechanics of advanced nuclear reactors.

**8. Related and Auxiliary Programs:**
Neutron microscopic cross sections and constants are prepared with the use of evaluated nuclear data files in ENDF-6 format processed with NJOY-94 system [4]. A Russian CONSYST/ABBN system [5] developed for fast reactors was also included in the LOOP2 code as an option for preparation of cross section on the basis of the ABBN-93 library. The code also uses water property package prepared with the use of the STGH2O code [16].

**9. Status:** Second version released October 2001.

**10. References:**

1. K. Mikityuk, "The LMFBR and MSR Transient Analysis Code LOOP-1/MOD1: System Models and Solution Methods", Preprint IAE-5667/4, Moscow, June 1993.
2. K. Mikityuk, P. Alekseev and V. Ignatiev, "Verification of the LOOP Code Against the Experiments with Natural Circulation of a Molten Fluoride Salt Fuel", Proceedings of Annual Meeting on Nuclear Technology '95, Nürnberg, Germany, May 1995.
3. A. Vasiliev, L. Yaroslavtseva, P. Alekseev, P. Fomichenko."Development and Evaluation of an Effective Nodal Diffusion Method for Perturbation Theory", Proc. of Annual Meeting on Nuclear Technology-97, Aachen, Germany, May 13-15, 1997.
4. R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System, Version 91" Los Alamos National Laboratory Report LA–12740–M, October 1994.
5. G. Manturov, M. Nikolaev, A. Tsibulya, "ABBN-93 Group Data Library. Part 1. Nuclear Data for Calculation of Neutron and Photon Radiation Fields". Vienna, IAEA, INDC(CCP)-409/L, August 1997.
6. K. Mikityuk and P. Fomitchenko. "FRED: Calculational Model of Fuel Rod Behavior Under Accident Conditions Coupled with RELAP5/MOD3", ICONE-8101, Proc. of ICONE-8, 8th International Conference on Nuclear Engineering, April 2-6, 2000, Baltimore, MD USA.
7. A.M. Ross and R.L. Stoute, "Heat Transfer Coefficient Between $UO_2$ and Zircaloy-2", AECL-1552, 1962.
8. L.J. Siefkin, Ch. Allison, M. Bohn, S. Peck. "FRAP-T6: Computer Code for the Transient Analysis of Oxide Fuel Rods", NUREG/CR-2148 EGG-2104, May 1981.
9. Rosinger, H.E., et.al., 1978, "Steady-State Creep Fuel Cladding from 940 to 1873", Journal of Nuclear Materials, v.82, p.286-297.
10. Hagrman, D.L., et al., 1980, "MATPRO-Version 11 (revision 1): A Handbook of Material Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior", NUREG/CR-0497 TREE-1280, Rev 1.
11. L. Yegorova, et.al. "Data Base to Characterize Behavior of High-Burnup Fuel Rods with Zr-1%Nb Cladding and $UO_2$ Fuel (VVER Type)", International Agreement Report NUREG/IA-0156, 1999.
12. B. Burton, et al., "Tensile Creep of Beta-Phase Zircaloy-2", Journal of Nuclear Materials v.73, p.70-76, 1978.
13. O. Ozer, et al., "Assessment of Reactivity Transient Experiments with High Burnup Fuel", Proceedings of Specialists Meeting on Transient Behavior of High Burnup Fuel, Cadarache, France, 1995.
14. S.G.Popov, J.J.Carbajo, V.K.Ivanov, G.L.Yoder, Thermophysical Properties of MOX and $UO_2$ Fuels Including the effect of Irradiation, report ORNL/TM-2000/351, 2000.
15. A. C. Hindmarsh, "ODEPACK, A Systematized Collection of ODE Solvers," in Scientific Computing, R. S. Stepleman et al. (eds.), North-Holland, Amsterdam, 1983 (vol. 1 of IMACS Transactions on Scientific Computation), pp. 55-64. Also available as LLNL Report UCRL-88007, August 1982.
16. R. J. Wagner, "STH2O, A Subroutine Package to Compute the Thermodynamic Properties of Water", Idaho National Engineering Laboratory, Internal Report (1973)

**11. Hardware Requirements:** There are no special requirements to hardware.

**12. Programming Language(s):** FORTRAN language.

**13. Operating System:** MS Windows OS.

**14. Other Programming or Operating Information or Restrictions:** none.

**15. Name and Affiliation of Author or Contributor:**

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**16. Material Available:** The content of the software package, which will be made available upon request to the authors:

1. A set of FORTRAN subroutines. The files are ready for translation by Compaq Visual Fortran Version 6.6.
2. Data base on 25-group neutron constants for a number of isotopes.
3. Executable module.
4. Sample input decks.
5. Utilities for postprocessing of the results and converting them to the ASCII tables.
6. Sample output files.

**17. Category:**

**Keywords:** advanced reactors, dynamic calculations, neutronics, thermal hydraulics, thermal mechanics

**18. Sponsor:**

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