

5.10 REACTOR DESIGN SOFTWARE

5.10.1 Introduction

Most of the design results have been obtained by using computer codes and programmes either developed by INVAP or other recognised organisations. This Section describes the computer codes and programmes used for reactor design. Software validation and verification has been performed against a range of experiments in operating reactors, and against IAEA benchmarks. When additional software validation or verification is required, a description of the corresponding programme for validation or verification is provided.

5.10.2 Nuclear Design Codes

The CONDOR cell code and the CITVAP core code are used as computer codes to formulate the fuel management strategy, including the following:

- FA loading requirements
- FA powers and maximum rating
- Burnup of each FA
- Isotopic content of each FA
- Prediction of excess reactivity of the reactor throughout a fuel cycle

These codes are included in the MTR_PC system (MTR_PC, 1995). Codes included in the MTR_PC system generate and handle a database with macroscopic cross-sections which reduces interfaces between cell and core calculations, thus handling information in an efficient manner.

The system has several auxiliary programmes that are useful for:

- a) input preparation;
- b) facilitating output analysis;
- c) one or two-dimensional plotting, e.g. fluxes or power densities;
- d) plotting time-dependent variables such as reactivity and maximum and average burnup.

In addition, the system has a microscopic cross-section nuclear data library. Its structure was specifically designed for multi-group calculations in thermal reactors. Users may select different parameters based on the type of calculations to be performed.

5.10.2.1 MTR_PC System

5.10.2.1.1 Introduction

The MTR_PC system was developed by INVAP to perform neutronic, thermal-hydraulic and shielding calculations of MTR-type reactors on personal computers (PCs). The MTR-PC v3.0 code system has a complete set of programmes to perform calculations, manage data and plot results. It can also run on Unix workstations.

The system offers the following capabilities:

- a) Steady-state neutronic and thermal-hydraulic studies
- b) Time and burnup dependent calculations
- c) Perturbation calculations (kinetic parameters)

- d) Fuel management
- e) Control rod plate positioning calculations
- f) Transient calculations
- g) Accident calculations
- h) Calculations of production, decay and processing of radioactive materials
- i) Calculations of shielding against gamma radiation

5.10.2.1.2 Software and Hardware Requirements

The programmes are written in FORTRAN. Two different platforms can be used: Windows 95 operating system (or later versions thereof) for PCs or UNIX workstations.

5.10.2.1.3 MTR_PC Technical Documentation

The documentation includes the following items:

- Installation instructions
- Introduction to the MTR_PC System
- Description of the different INVAP codes, including the mathematical and calculation techniques wherever applicable
- Description of the modified parts, if applicable, for the International Codes
- Input descriptions
- Output descriptions
- Sample problems

5.10.2.2 Macroscopic Cross Section Handler: HXS V4.2

The HXS programme (Cross section handler) is a major utility. It handles macroscopic cross sections (identified by a name) in library form.

This programme has the following functions:

- Creation of a library
- Adding cross-sections (xs) with various formats (anisn, wims)
- Extracting xs with formats for various programmes (citvap, dioxybar)
- Listing of xs names
- Displaying of xs
- Deleting a set of xs
- Renaming a set of xs
- Mixing of different XS sets

5.10.2.3 Cell Calculations

5.10.2.3.1 CONDOR v2.5

The CONDOR Code (CONDOR, 1995) can be used to perform fuel cell calculations for fuel plates in slab geometry, single fuel rods and fuel rods in cluster geometry.

The flux distribution within the region of interest is calculated using the collision probability method in a multi-group scheme with various types of boundary conditions available.

The code incorporates free format input and uses its own nuclear data library. Nuclear data used by CONDOR (ESIN type) is described in Section 5.7.6.5. This data includes cross sections (P_0 and P_1), resonance parameters and burnup information.

For MTR-type reactors, calculations are conducted in one-dimensional geometry (1D), applying the collision probability method.

The user can plot different variables, such as: burnup-dependent variables (multiplication factor, atom densities, peaking factor, fluxes); spatial-dependent variables (fluxes, power densities), in 1 or 2 dimensions; energy-dependent fluxes; and a geometric representation of the system under calculation.

The main purpose of the code is to prepare cross-section libraries to be used by the CITVAP code.

This code is not included in the free version of the MTR_PC system (v 2.6).

5.10.2.4 Core Calculations

5.10.2.4.1 CITVAP v3.2

The CITVAP reactor calculation code (CITVAP, 1995) is a new version of the CITATION-II code, developed by INVAP's Nuclear Engineering Division.

The code was developed to improve CITATION-II performance. In addition, programming modifications were performed for its implementation on personal computers.

The code solves 1, 2 or 3-dimensional multi-group diffusion equations in rectangular or cylindrical geometry. Spatial discretisation can also be achieved with triangular or hexagonal meshes.

Nuclear data can be provided as microscopic or macroscopic cross-section libraries.

CITVAP maintains all the original CITATION options and implements the following relevant features:

- a) Burnup dependent calculations can be made with macroscopic cross sections (MXS).
- b) FA management can be modelled, also with MXS.
- c) Changes of control rod plate position can be simulated during the calculation of a reactor with MXS.
- d) It has a great versatility in the input data format due to the inclusion of a pre-processing module. Input data are free-format and fully compatible with standard CITATION formatted data. This feature improves 3-D problem description and makes it easier to describe fuel management and fuel element movements with axial discretisation.
- e) The MXS are dependent on two parameters: burnup (to take into account time dependence of fissile and fission product concentrations), and power density (to consider specific fission product concentrations, such as Xe-135).
- f) It allows a fast search for the equilibrium core (BOC and EOC).
- g) It is easy to replace materials during calculation.

- h) The calculation may be interrupted at user specified conditions, for instance, for FA replacement when the core excess reactivity is lower than a fixed value.
- i) It automatically generates an auxiliary file with time dependence of selected variables.
- j) It has a user-friendly graphic display.
- k) It can store a given core state, for instance, BOC or EOC state.
- l) It is easy to define the initial core state.
- m) It has easy to use restart capabilities.
- n) It permits fast and easy access to MXS libraries generated with HXS 4.0 and HXS_PC programmes.

5.10.2.5 Monte Carlo Codes

5.10.2.5.1 MCNP

This is a well-known Monte Carlo transport code (Briesmesiter, J., et al., 1992) for neutron, gamma and electron calculations. It uses ENDF/B-VI cross sections and performs calculations in 3-dimensions. It is used to verify neutronic parameters through an independent calculation method. This code is not included in any version of the MTR_PC system.

5.10.2.6 Validation of Nuclear Design Codes

The calculation method chosen for the neutronic design has been validated against measurements taken at various reactors and an additional validation against an IAEA computational benchmark (IAEA TECDOC 233) has also been performed.

5.10.2.6.1 Experimental Measurements

5.10.2.6.1.1 RA-2 Measurements

A set of neutronic measurements was performed on the RA-2 reactor (Buenos Aires, Argentina) in 1983. The analysed configurations of the core had between 20 to 30 FAs.

Different reflectors were employed, e.g.; water, graphite and beryllium.

The FAs are composed of 90% enriched uranium with a loading of 147 g of U²³⁵ per FA.

Reactivities of different core configurations were obtained from these measurements.

5.10.2.6.1.2 RA-6 Measurements

A set of neutronic measurements was performed on the RA-6 reactor (Bariloche, Argentina). The configurations of the core are fixed to 20 FA.

The FAs are composed of 90% enriched uranium.

The reactivity worth of a small piece of ternary alloy of Ag-In-Cd absorber material was obtained from these measurements.

5.10.2.6.1.3 NUR Measurements

A set of neutronic measurements was performed on the NUR reactor in Argel in 1989. They include core configurations up to 16 FAs.

The FAs are composed of 20% enriched uranium, with a loading of 290.7 g of U²³⁵ per FA.

The following data was obtained from these measurements:

- a) Excess reactivity of various cores.
- b) Reactivity worth of various control rods with different insertion percentages in the core.
- c) Subcritical reactivity of various control rods with the rod-drop method.
- d) Flux profiles.

5.10.2.6.1.4 ETRR-2 Measurements

Numerous neutronic measurements were performed on the ETRR-2 reactor during the commissioning in 1997/1998.

Various core configurations were assembled for the low power tests during the commissioning. Various validation tests were carried out including measurements and calculations for the following:

- a) Critical states for different core configurations.
- b) The reactivity worth of the ETRR-2 SSS, based on the insertion of gadolinium into the core.
- c) CR calibration.
- d) Reactivity excess of the cores analysed, shutdown margins and reactivity worth of the shutdown system for the different core configurations.
- e) Power Peaking Factor.

5.10.2.6.2 Theoretical Verification – Benchmark Calculation

The MTR reactor benchmark proposed by IAEA in 1980 in the IAEA TECDOC-233 "Research Reactor Core Conversion from the use of Highly Enriched Uranium to the use of Low Enriched Uranium fuels", and the 1985 annex were calculated.

The following contributing organisations performed this benchmark:

Argonne National Laboratory	ANL	USA
Australian Atomic Energy Commission	AAEC	Australia
Comisión Nacional de Energía Atómica	CNEA	Argentina
Commissariat a l'Energie Atomique	CEA	France
Eldg. Institut für Reaktorforschung	EIR	Switzerland
Internationale Atomreaktorbau F.R. GmbH	INTERATOM	Germany
Japan Atomic Energy Research Institute	JAERI	Japan
Junta de Energía Nuclear	JEN	Spain
Kyoto University Research Reactor Institute	KURRI	Japan
Riso National Laboratory	RISO	Denmark

The core has 25 FAs with BOC and EOC states, with graphite reflector.

There are two types of FA:

- a) HEU: 90 % enrichment with 280 g of U^{235} in each FA
- b) LEU: 20 % enrichment with 390 g of U^{235} in each FA

The following results were obtained from this calculation:

- a) Multiplication factor.
- b) Fluxes and flux ratios along the two axes of symmetry of the core in three groups for BOC and EOC conditions.
- c) Neutron generation time and delayed neutron fraction.
- d) Isothermal reactivity feedback coefficients versus:
 - (i) Water temperature
 - (ii) Water density
 - (iii) Core void fraction
 - (iv) Local void fraction
 - (v) Radial and Local PPF
 - (vi) Control Rod worth:
 - with Ag-In-Cd absorber
 - with Hafnium absorber
 - with B_4C absorber

5.10.3 Thermal-hydraulic Design Codes

5.10.3.1 Steady-State Calculations

5.10.3.1.1 TERMIC4.0

The TERMIC code is part of the MTR_PC system described above. It is a steady-state thermal-hydraulic code developed to perform core thermal hydraulic design using plate type fuel assemblies. TERMIC is intended to calculate maximum allowable powers and heat fluxes using selectable limiting criteria of onset of nucleate boiling (ONB), CHF and Flow Instability as a function of the coolant velocity. The coolant is light water, in upward or downward flow.

Despite the capability of the code is limited to single-phase condition, it includes two-phase limits, such as Flow Instability and CHF in the coolant. In the analysis coolant channels are assumed bounded by flat plates with a width equal to the fuel plate span.

A single channel is split into axial cells. An energy balance and dynamic and frictional pressure gradients are calculated across each axial cell.

Losses resulting from entrance and exit effects are accommodated in the code using specific loss coefficients, while frictional pressure drop is calculated using a friction factor correlation appropriate for narrow channels. All coolant property values are assumed to vary with temperature and pressure along the channel.

As TERMIC was programmed as an engineering code, it includes a multiplicative and statistical treatment for uncertainty factors of the input data. The first method combines in a multiplicative way the different uncertainty factors that affect the data appearing on the calculation expressions. In the statistical evaluation method it is assumed that most of the uncertainties are independent and as the probability of the extreme values of the

deviations, all occurring at the same point in the core, is quite remote, uncertainties are combined in a statistical manner.

5.10.3.1.2 CAUDVAP

CAUDVAP is part of the MTR_PC system. This isothermal hydraulic programme calculates the coolant velocity distribution in steady state regime through different type of channels connected in a parallel array between inlet and outlet common plenums. Bypass mass flow can be calculated with detail for each channel in addition to pressure drop within the core.

The code establishes correlations for laminar and turbulent regimes as well as improved correlations for rectangular-shaped channels.

The program can solve two different situations depending on whether the total fluid flow is known or whether the total pressure drop is given.

5.10.3.1.3 CONVEC

CONVEC is a steady-state thermal-hydraulic code developed to perform core thermal-hydraulic evaluation under natural circulation conditions.

Its unique features have been specially tailored to the geometry of the rectangular channels of MTR fuel elements.

Due to the Natural Circulation characteristics, the hydraulic problem is highly coupled with the thermal problem. A single coolant channel is split into axial cells, and a balance between buoyant and frictional forces is performed to determine the flow.

Given the power to be removed from a fuel element, the program calculates: mass flow and velocity in the channel, coolant temperature distribution, wall and fuel temperatures

The effect of a chimney (or riser) located in the upper part of the core is also included in the calculation, as the pressure drop of the inlet pipe from the flap valves to the core inlet.

Despite the capability of the code is limited to single-phase condition, it includes the calculation of two-phase limits, such as margin to bulk boiling and to CHF. Correlation to predict ONB and Pulsed Boiling are also included.

This code is included in the MTR_PC system.

5.10.3.2 Transient Analysis

5.10.3.2.1 PARET-PC

This thermal-hydraulic programme was designed to calculate fuel and coolant behaviour during transients or accidents initiated by reactivity or power changes.

It solves the energy balance and heat transfer equations for coolant and fuel. The coolant may be in the single or two-phase states.

Power is calculated following the point-kinetics model, while reactivity feedback terms are taken into account through expansion in each of the following variables: coolant temperature, moderator density and fuel temperature.

The programme can be interrupted at any given point to plot the state of certain variables and the calculation can then be restarted.

Additional details on this code including validation and verification information is provided in Chapter 16, Section 16.3.

5.10.3.2.2 RELAP-5-mod 3.2

The light water reactor (LWR) transient analysis code, RELAP5, was developed at the Idaho National Engineering Laboratory (INEL) for the U.S. Nuclear Regulatory Commission (NRC). Code uses include analyses required to support rulemaking, licensing audit calculations, evaluation of accident mitigation strategies, evaluation of operator guidelines, and experiment planning analysis.

The RELAP5 code has been developed for best-estimate transient simulation of light water reactor coolant systems during postulated accidents.

It models the coupled behavior of the reactor coolant system and the core for accidents such as but not limited to loss-of-coolant accidents and operational transients such as anticipated transient without scram, loss of offsite power, and loss of flow.

RELAP5 is a highly generic code that, in addition to calculating the behavior of a reactor coolant system during a transient, can be used for simulation of a wide variety of hydraulic and thermal transients in both nuclear and non-nuclear systems involving mixtures of steam, water, non-condensable, and solute.

Control system and secondary system components are included to permit modeling of plant controls.

The development of the models and code versions that constitute RELAP5 has spanned approximately 17 years from the early stages of RELAP5 numerical scheme development to the present.

5.10.3.3 Validation of Thermal-hydraulic Design Codes

5.10.3.3.1 TERMIC 4.0

The TERMIC code has been verified against, theoretical data from the IAEA TECDOC – 233 and RELAP code results and validated against experimental data.

A wide variety of cases were simulated using TERMIC. In most cases resulting differences were less than 10 % when temperatures results are compared with experimental values or other code results like RELAP. In cases with larger differences the TERMIC calculations were conservative. This last observation and the acceptable prediction of calculated values make TERMIC an appropriate tool for core thermal design purposes.

5.10.3.3.2 CAUDVAP

CAUDVAP code has been verified by comparing its results against those obtained with RETRAN, theoretical data from the IAEA TECDOC–233 and validated against experimental data performed ad hoc for the RRR .

A wide variety of cases were simulated using this program. CAUDVAP results indicated deviations around 10% from the experimental values used as reference and, moreover, the results were conservative. Thus, the CAUDVAP code features make it appropriate for hydraulic design purposes of research reactor cores in the forced convection regime.

5.10.3.3.3 CONVEC

The CONVEC code has been verified by comparing its results against those obtained with RELAP , SPCONVEC, theoretical data and validated with experimental data from French Laboratories.

SPCONVEC is a finite element programme developed for forced and natural convection regimes for incompressible flow inside cooling channels, in the transient state. This code

has also been tested against problems having analytical solutions with accurate results obtained in each case.

A wide variety of cases were simulated using CONVEC and results were verified against RELAP and SPCONVEC as well as against analytical values. Validation was carried out comparing CONVEC results against experimental data from the Argentina RA-3 reactor and OSIRIS mock-up experiments. Several variables were analysed including heat flux, coolant, channel thickness, channel width, fuel plate length and chimney height. Various parameters were calculated and compared including total core flow rate, maximum coolant temperature, maximum wall temperature and coolant velocity. The maximum deviations observed were 10% from the reference values. Considering the results obtained from the validation and verification analysis it was concluded that the CONVEC code is appropriate for core thermal analysis purposes in the natural circulation regime.

5.10.4 Shielding Calculations

A collection of various codes using different calculational methods is used to design and verify shielding against ionising radiation. This includes:

- a) Determination of radiation source parameters.
- b) Transport calculations for the proposed shielding and evaluation of the desired response (dose and energy deposition) at points of interest.

5.10.4.1 ORIGEN-2

This is one of the most widely used programmes for calculating radioactive-material production and decay of radioisotopes and processing calculations.

The code uses nuclear data from the ENDF-B/IV library.

5.10.4.2 MERCURE

This programme uses the point-kernel method following the Monte Carlo technique for integration over the energy and spatial domain of a distributed source. It features vast geometric 3-D versatility that enables the user to represent practically any source-shielding configuration with the desired degree of approximation.

The programme uses two data libraries, namely:

- a) MER-BIB10, which contains build-up coefficients and complementary data.
- b) MER-BIB09, which contains attenuation coefficients and dose and heating-response functions for 32 materials in a 36-energy-group structure. This library was created using the VITAMIN-C (ENDF-B/IV) library.

Both libraries are included in the module, as well as graphic facilities for plotting the results.

5.10.4.3 ANISN

ANISN is a 1-dimensional discrete ordinates transport code for neutron and gamma calculations, (CCC-650 Oak Ridge National Laboratory, RSIC, august 1996). It uses anisotropic cross sections of any order and can calculate fluxes for any quadrature.

5.10.4.4 DORT

DORT is a 1 and 2-dimensional discrete ordinates transport code for neutron and gamma calculations. It uses anisotropic cross sections of any order and can calculate fluxes for any quadrature.

5.10.4.5 MCNP

MCNP is a Monte Carlo code for the transport of neutrons, photons and electrons. It allows explicit 3-dimensional representation of the geometry of any problem. A comprehensive collection of variance reduction techniques is available to reduce the calculation time of large or deep penetration problems. A cross-section library based on ENDF/B-VI data is provided with the code.

5.10.5 Safety Analysis Software

Several computational codes are required for the safety analysis.

Most of these codes are included in the MTR_PC package, outlined previously in the section devoted to the nuclear design software.

1. TERMIC, CONVEC and CAUDVAP are used for the detailed thermal-hydraulic design and analysis of a fuel assembly in steady state.
2. PARET and RELAP are used for coupled thermal-hydraulic and neutron kinetics reactor transient analysis.
3. CONDOR and CITVAP are used to calculate reactor physics parameters.
4. MCNP is used for the criticality assessment of fuel transport and storage arrangements.
5. ORIGEN II, ANISN, DORT, MERCURE and MCNP are used for shielding.
6. COSMOS/M for Windows Ver. 1.75A and MSC/NASTRAN for Windows Ver. 2.1 are used for stress analysis.
7. ORIGEN II with the IAEA recommended transfer factors is used for analysis of fission product release from the containment.
8. For atmospheric dispersion analysis, PC COSYMA and PC CREAM are used for accidents and normal releases, respectively.

A detailed description of the software used for the safety analysis, including validation and verification information, is given in Chapter 16, Section 16.3.

5.10.6 Auxiliary Programmes

5.10.6.1 Pre-processors

5.10.6.1.1 PRE-CIT

This programme interprets the free-format input for CITVAP.

5.10.6.1.2 HGEO

This graphic input programme allows the generation of very complicated inputs files. The interactive graphic capability makes input preparation for the CITVAP code a very simple task.

5.10.6.2 Post-processors and Plotters

5.10.6.2.1 CITVAP Post-processors

CITVAP has several post-processors:

- a) FLUX: This programme plots fluxes and power densities in 1 or 2D plots.

- b) GENGRA: This programme plots the CITVAP input file.
- c) FLUXHC: This interactive programme homogenises and/or condenses fluxes and average power densities from CITVAP auxiliary files.
- d) POST-CIT: This programme enables the plotting of neutronic variables versus time during burnup calculations. It is possible to plot the following variables: multiplication factor, reactivity, peaking factors (according to zone or mesh) and burnup (average or maximum).
- e) CNV_SV: This programme handles the information stored in the CITVAP state files. The information available is: burnup, power density, control rod position, fuel temperature, coolant density and temperature.

5.10.6.2.2 CONDOR Post-processors

CONDOR has several post-processors:

- a) POS_CON: This programme plots fluxes and power densities in 1 or 2-dimensions. It can plot burnup-dependent variables such as effective and infinite multiplication factors, power peaking factor, numerical density, power densities and fluxes. The geometry of the system can also be plotted.
- b) NDDUMP: This programme allows reconstruction of the numerical densities of any material from a CITVAP state file.
- c) POS_LIB: This programme generates a microscopic CITVAP cross-section library with different materials from a CITVAP state file.

5.10.6.2.3 TERMIC 4.0 Post-processor (POS-TER)

This post-processor of the TERMIC programme (POS-TER) allows plotting the following variables versus coolant flow: maximum heat flux, redistribution phenomena ratios, ONB and DNB.

5.10.6.2.4 PARET Post-processor (POS-PAR)

This post-processor of the PARET_PC programme (POS-PAR) enables plotting the following variables versus time: power, net reactivity, coolant flow, outlet temperature, maximum cladding and fuel temperature and energy.

5.10.7 References

Briesmesiter J. et al., MCNP v4.2, Monte Carlo Code and Photon Transport Code System, RSIC Computer Code Collection, CCC-200 A, Oak Ridge National Laboratory, November 1992.

CITVAP, v3.1, Improved Version of CITATION II, Subgerencia de Sistemas INVAP SE, MTR_PC v2.6 system, User Manual, July 1995.

CONDOR, v1.3, Users Manual, September 1995 (in Spanish).

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End of Section