6

A Literature Survey of Neutronics and Thermal-Hydraulics Codes for Investigating Reactor Core Parameters; Artificial Neural Networks as the VVER-1000 Core Predictor

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1. Introduction

In this chapter, we investigated an appropriate way to predict neutronics and thermal-hydraulics parameters in a large scale VVER type nuclear reactors. A computer program is developed to automate this procedure using Artificial Neural Network (ANN) method. The neutronics and thermal-hydraulics codes are connected to each other and then the neural network method use results with different configuration of a suggested core for prediction. The main objective of this research is to develop fast and first estimation tool (a software) based on ANNs which allows large explorations of core safety parameters. This tool is very useful in reactor core design and in-core fuel management or loading pattern optimization. Therefore, herein, an overview study on the multiphysics/multiscale coupling methods for designing current and innovative VVER systems by coupling neutronics parameters (using MCNP 5) and thermal-hydraulics simulator (e.g., COBRA-EN) are carried out. This work is aimed to extend the modeling capabilities of coupled Monte Carlo/Subchannel codes for whole core simulations based on pin-level in order to address many problems e.g. higher burn-up, Mox-fuels, or to improve the performances and accuracy of reactor dynamics.

Verification and validation of the above development are the main concern and important procedures and therefore taking into account using experimental data or another code-to-code benchmarking. Finally the extended simulation capabilities should be applied to analyze a selected VVER reactor and we present our input computer codes for interested readers. Also, our future designed user friendly Artificial Neural Network (ANN) software would be given for everyone who wants to get it.

Bushehr Nuclear Power Plant (BNNP), a VVER-1000 Russian model, was simulated during the first plant operational period using WIMS and CITATION codes (Faghihi et al., 2007). Modelling of all rods (including fuel rods, control rods, burnable and non-burnable poison rods) and channels (including central guide channel, measuring channel) were carried out using the WIMS code. Moreover, modelling of the fuel assemblies and reactor core is completed using the CITATION code. The multi-group constants generated by WIMS for different fuel configurations are fed into CITATION. In our past mentioned article, average burn ups and calculated reactivity coefficients from Beginning of Cycle (BOC) to Middle of Cycle (MOC) for the VVER-1000 BNPP were carried out. A thermal-hyraulics analysis for the VVER-1000 were employed using COBRA-EN code (Mirvakili et al., 2010). Moreover, a 13×13 square array fuel assembly core of a 1000 MWe Westinghouse reactor was investigated and its “Prompt reactivity coefficient”, which is an important factor in the study of nuclear power excursions, and also “power coefficient of reactivity” were calculated using MCNP-5 (Faghihi and saidinezhad, 2011). MCNP 5 has seven new features with respect to the older ones and complete description along with a list of bug fixes are listed in its release notes (MCNP-5 Team, 2008).

In the incoming sections we will investigate ANNs theory and then we introduce with MCNP and COBRA-EN code as our toolboxes for the reactor neutronics and thermal hydraulics feedbacks

2. Neutronics codes

A literature review of available coupled codes for application to LWR's analysis has been conducted to investigate their capabilities for VVER applications. In order to identify the types of codes coupled, different types of methods implemented into neutronics codes and thermal-hydraulics codes need to be discussed. The neutron flux can be predicted with diffusion codes, deterministic codes and Monte Carlo methods.

2.1 Diffusion and transport codes

Diffusion codes solve the neutron diffusion equation to obtain the neutron flux, from which the power distribution is computed. They use macroscopic cross section data for neutron particles, processed usually from two or more energy groups. The modeling of a reactor core or fuel assembly is homogenized for the diffusion approximations to be valid. Diffusion codes have been well suited to analyze reactors, which are designed with relatively homogeneous distributions of fuel, moderator and absorber materials. However, with higher heterogeneity such as in the VVER or HPLWR (High-Performance Light-Water Reactor) fuel assembly, the simplified model will produce inaccurate results. Details of the VVER fuel assembly such as coolant density in different sub-channels and power distribution of different fuel rods, which are needed in the coupling, cannot be obtained.

Until now, coupling experience for PWR and BWR reactor have been with diffusion codes coupled with system codes, which have been applied for various transient analysis. For transient analysis diffusion codes and system codes are restricted to simplified geometries and their application cannot be extended to complex geometries such as for fuel assembly design of a VVER. The neutronic code PARCS (Purdue Advanced Reactor Core Simulator) developed at the Purdue University is used to predict the dynamic response of the reactor to reactivity perturbations such as control rod movement or change in temperature/fluid conditions in the reactor core. A coupling interlace of PARCS with TRAC-M, a system code, was completed by Miller et al. The coupled code was tested using the OECD PWR main steam line break (MSLB). The coupled TRAC-M/PARCS was also applied for turbine trip (TT) transient analysis of the OECD/NRC BWR by Lee et al. The PARCS code has also been coupled with the system code RELAP5 for analysis of the peach bottom turbine trip (TT), Salah et al.

DYN3D is a neutron kinetic code developed to investigate reactivity transients in the reactor core with hexagonal or quadratic fuel assembly. The neutron diffusion equations are solved for two groups. An internal coupling approach of DYN3D with ATHLET is a system code that has been developed by Grundmann et al. The coupled code DYN3D/ATHLET has been applied for analysis of BWR TT transient.

The SKETCH-N code solves neutron diffusion equation in x-y-z geometry for steady state and neutron kinetic problems. The code treats an arbitrary number of neutron energy group and delayed neutron precursors. The SKETCH code has been implemented into thermal-hydraulic code TRAC for analysis of rod injection transients Asaka et al.

NEM (Nodal Expansion Method) is a 3-D multi-group nodal code developed and used at the Pennsylvania State University for modeling both steady state and transient core conditions. The code has options for modeling 3-D Cartesian, cylindrical and hexagonal geometry. NEM has been coupled to the system code TRAC-PF for MSLB transient analysis of a PWR Ivanov et al. and Ziabletsev et al. and for BWR core transient, NEM has been coupled with TRAC-BFI by Fu et al.

NESTLE is a multi-dimensional neutron kinetic code developed at the North Carolina State University. It solves the two group or four group neutron diffusion equations in Cartesian or hexagonal geometry.

QUABOX is a neutron kinetic code developed in the 70s at GRS in Germany for 3-D core neutron flux and power calculations in steady state and transient conditions. It solves the two-group neutron energy diffusion equation through local polynomial approximation of the neutron flux. The QUABOX code has been coupled with ATHLET internally for analysis of the OECD/NRC BWR turbine trip benchmark by Langenbuch et al. A serial coupling is applied. The T-H code ATHLET makes the first calculation step and when it is finished the core model QUABOX/CUBBOX calculates the same step for the neutronics on the same computer.

PANBOX is a three dimensional neutron kinetics code coupled with a multidimensional core thermal-hydraulics module, developed to perform PWR safety analysis and transients in which power distribution is significantly affected. The time-dependent few-group diffusion equation is solved in Cartesian geometry using a semi-analytical nodal expansion method (NEM). The PANBOX code system has been coupled with the thermal-hydraulics system code RELAP for analysis of the OECD/NEA PWR MSLB, Sanchez-Espinoza et al. Verification of the coupled PANBOX /RELAP was performed by Jackson et al. for core transient analysis.

CITATION code is a three dimensional, multi group diffusion code (Oak Ridge National Laboratory, 1972), is used for core simulation. This code was designed to solve problems involving the finite-difference representation of diffusion theory treating up to three space dimensions with arbitrary group-to-group scattering. Explicitly, finite-difference approximation in space and time has been implemented. The neutron flux-eigenvalue problems are solved by direct iteration to determine the multiplication factor or the nuclide densities required for a critical system. In the input file of this code the macroscopic cross-sections are required which are prepared by running WIMSD-4 code (Winfrith, 1982). As this code uses the transport theory in its calculations, the results have a high degree of accuracy.

2.2 Discrete-ordinate codes

Deterministic codes are most commonly based on the discrete ordinates method. They solve the Boltzmann transport equation for the average particle behavior to calculate the neutron flux. With discrete ordinate methods, the phase space is divided into many small boxes and particles are moved from one box to another. If this approach is to be used for modeling a VVER fuel assembly, the guide tubes, the coolant sub-channels, and fuel rods will be homogenized and the medium is discretized to solve the transport equation. This type of geometry modeling will not accurately represent the important design details essential for the VVER fuel assembly. Deterministic codes use macroscopic cross section data, which are processed from multi-group energies. Processed macroscopic cross section data from microscopic scale are required for different parts in the geometry. For complicated geometries with varying parameters such as coolant and moderator density, preparation of the macroscopic cross section data would also require a lot effort. Therefore deterministic codes need to be homogenized for complex geometries. The global solutions are obtained with truncated errors. Computer codes based on deterministic methods include DORT, two dimensional (X-Y, and R-Z) geometries, TORT, a three-dimensional discrete transport code DORT-TD, a transient neutron transport code, KARPOS, a modular system code developed by Broeders et al.

2.3 Monte-Carlo method

A Monte Carlo method does not solve an explicit equation like the deterministic code, but rather obtains the answers by simulating individual particles and recording some aspects (tallies) of their average behavior. Monte Carlo codes use a continuous energy scale to represent the variation of cross section data. They are widely used because of the capability of complex geometries modeling and accurate solution produced with the continuous energy scale used to represent the cross section data. Computer codes based on the Monte-Carlo methods include: MCNP (Monte Carlo N-Particle) is a general-purpose, continuous-energy, generalized-geometry, coupled neutron/photon/electron transport code. The MCNP code for neutronics analysis is described by Briesmesiter, 2000 from the Los Alamos National laboratory. Different versions of MCNP have been developed, for example MCNP4C for low energy calculation and MCNPX for higher energies. The application of the Monte Carlo codes in nuclear energy is increasing for fuel assembly and core design analysis typically in BWR where the density varies in the core. Mori et al. has already coupled the Monte-Carlo MCNP has been successfully coupled with a thermal-hydraulics system code for power and reactivity analysis of a supercritical fast reactor (SCFR) core that does not include moderator tubes, hence a simplified design.

3. Thermal-hydraulics codes

3.1 System codes or lumped approach

System codes are based on a lumped parameter approach. This means, for nuclear power plant (NPP) application the components in the primary and secondary system are represented by a one-dimensional model. Details of a fuel assembly such as moderator rod, individual sub-channels for density variation study cannot be revealed through such means. The basic equations for continuity, momentum and energy are applied and averaged and the thermal-hydraulics properties for each component are obtained. The smallest volume is typically a total core or major parts of it. System codes are commonly used in LWR

application for different types of transient and safety analysis. Widely used system codes include:
ATHLET, (Analysis of Thermal-hydraulics of LEaks Transient) has been developed by the Gesellschaft für Reaktorsicherheit (GRS) for analysis of anticipated and abnormal plant transients, small and intermediate leaks and large breaks in light water reactors. The concept of ATHLET for analysis of PWR and BWR system has been described by Burwell et al. The ATHLET code has been coupled with the 3-D core model neutronic code DYN3D for analysis of BWR turbine trip benchmark, Grundmann et al. Validation of the ATHLET thermal-hydraulics code for PWR and BWR was presented by Glaeser. The coupling interlace of ATHLET with the neutronic core model DYN3D has been reported by Langenbuch et al. The coupled code ATHLET- QUABOX/CUBBOX has been used by Langenbuch et al. for analysis of the OECD/NRC BWR turbine trip benchmark.
RELAP (Reactor Excursion and Leak Analysis Program) is used for transient simulation of LWRs. It is widely used for LWR transient analysis in PWR and BWR. The RELAP5 code has been coupled with point kinetic code for analysis of OCED/NEA PWR MSLB by Sanchez-Espanioza and Nigro et al. Bovalini et al. reported coupled application of RELAP and comparison with different codes for TMI-MSLB. The CATHARE code is used for transient analysis of PWR plants, VVER and BWR. The CATHARE code has been coupled with CRONOS2-FLICA4 for BWR turbine trip analysis Mignot et al.

3.2 Sub-channel codes

Sub-channel codes are used for multi-component modeling in the core. A core is represented by the sub-assemblies and the sub-assembly by different sub-channels and other water channels and fuel rods. The basic equations are solved for control volumes in the scale of sub-channels. The sub-channel codes are capable of three-dimensional geometry modeling. Codes that are based on this approach include:
COBRA (Coolant Boiling in Rod Arrays) is a public computer code used for thermal-hydraulics analysis with implicit cross-flow between adjacent sub-channels, single flow and homogeneous two-phase fluids. It is used world-wide for DNBR (departure from nucleate boiling ratio) analysis in LWR sub-channels as well as for 3-D whole PWR core simulation with one or more channels per fuel assembly, Wheeler et al.
MATRA (Multi-channel Analyzer for steady states and Transient in Rod Arrays) is a sub-channel analysis code developed at KAERI (Korea Atomic Energy Research Institute), Yoo et al. The main concept of the MATRA code is based on COBRA.
The STAFAS (Sub-channel Thermal-hydraulics Analysis of Fuel Assembly under Supercritical Conditions) code was developed by Cheng et al. It is based on the concept of the COBRA code but includes special features of the HPLWR such as: downward flow of the moderator water and incorporates steam table that allows the prediction of supercritical water properties. The code is flexible and allows for complex geometry modeling. Heat transfer from solid surfaces can be easily implemented. The present version of the STAFAS code is for steady state conditions and single-phase flow only.
FLICA-4 is a thermo-hydraulic code developed at the French Atomic Energy Commission (CEA) for computing three-dimensional, transient or steady, two-phase flows in nuclear reactors. The code is described in the paper by Allaire for 3-D transient computation. The FLICA code has been coupled with the system code CATHARE and CRONOS2, a 3D neutronics code for computation of a BWR turbine trip, Mignot et al.

No.	Title and authors	Coupled codes	NPP	Transient type ef.
1	*Coupling of the Thermal-hydraulics Code TRAC with 3-D Neutron Kinetics Code SKETCH-N* H. Asaka, V.G. Zimin, T. Iguchi, Y. Anoda	J-TRAC *TRAC-BF1* Sketch-N	PWR *BWR (Ringhals*-1) BWR	RIA Stability benchmark cases Instabilities
2	*Core-wide DNBR Calculation for NPP Krško MSLB* I-A. Jurkoviá, D. Grgiá, N. Debrecin	RELAP5/ MOD3.2 COBRA III C QUABOX/CUBBOX	PWR (NPP Krško)	MSLB
3	*MSLB Coupled 3-D Neutronics/Thermal-hydraulics Analysis of a Large PWR Using RELAP5-3-D* F. D'Auria, A. Lo Nigro, G. Saiu, A. Spadoni	RELAP5/MOD3.2 NESTLE	PWR B&W TMI-1 AP-1000	MSLB
4	*TMI-1 MSLB Coupled 3-D Neutronics/ Thermal-hydraulics Analysis: Application of RELAP5-3-D and Comparison with Different Codes* R. Bovalini, F. D'Auria, G.M. Galassi, A. Spadoni, Y. Hassan	RELAP5/MOD3.2.2 PARCS RELAP5/MOD3.2.2 QUABBOX RELAP5/3-D NESTLE	PWR (B&W TMI-1)	MSLB
5	*PWR REA Sensitivity Analysis of TRAC-PF1/NEM Coupling Schemes* N. Todorova, K. Ivanov	TRAC-PF1 NEM	PWR (B&W) TM-1	REA
6	*Coupled 3-D Neutronic/Thermal-hydraulics Codes Applied to Peach Bottom Unit 2* A. Mª Sánchez, G. Verdú , A. Gómez		BWR (Peach Bottom Unit 2)	TT
7	*Study of the Asymmetric Steam Line Break Problem by the Coupled Code System KIKO3D/ATHLET* Gy. Hegyi, A. Keresztúri, I. Trosztel	ATHLET KIKO3D	VVER 440	MSLB
8	*Development of Coupled Systems of 3-D Neutronics and Fluid-dynamic System Codes* and their *Application for Safety Analysis* S. Langenbuch, K. Velkov, S. Kliem U. Rohde, M. Lizorkin, G. Hegyi, A. Kereszturi	ATHLET *DYN3D* BIPR-8	*VVER-1000*	LOFW Station black out MCP stop
9	*VIPRE-02 Subchannel Validation Against NUPEC BWR Void Fraction Data* Y. Aounallah, P. Coddington	VIPRE-02 ARROTTA	BWR	Void fraction validation study
10	*High Local Power Densities Permissible at Siemens Pressurised Water Reactors* K. Kuehnel, K.D. Richter, G Drescher, I. Endrizzi	PANBOX	PWR	Maximum local heat flux investi-gation

ATWS: Anticipated Transient without Scram; RIA: Reactivity Induced Accident;
REA: Rod Ejection Accident; MCP: Main Coolant Pump; LOFW: Loss Of proper Feed Water

Table 1. Overview of 3-D coupled neutronics/thermal-hydraulics calculations available from the literature

No.	Title and authors	Coupled codes	NPP	Transient type ef.
11	*Analysis of a Boron Dilution Accident for VVER-440 Combining the Use of the Codes DYN3D and SiTap* U. Rohde, I. Elkin, V. Kalinenko	SiTap DYN3D	VVER 440	RIA
12	*RELAP5-PANTHER Coupled Code Transient Analysis* B.J. Holmes, G.R. Kimber, J.N. Lillington, M.R. Parkes	RELAP5 PANTHER	PWR (Sizewell-B)	Grid frequency error injection test Single turbine trip event
13	*TACIS R2.30/94 Project Transient Analysis for RBMK Reactors* H. Schoels, Yu. M. Nikitin Nikiet	FLICA GIDRA SADC DINAO CRONOS QUABOX/CUBOX	RBMK (Smolensk 3)	RIA
14	*PWR Anticipated Transients Without SCRAM Analyses Using PVM Coupled RETRAN and STAR 3-D Kinetics Codes* M. Feltus, K. Labowski	RETRAN STAR 3-D	PWR	ATWS
15	*Development and First Results of Coupled Neutronic and Thermal-hydraulics Calculations for the High -performance LWR* C.H.M. Broeders, V. Sanchez-Espinoza, A. Travleev	RELAP5 KAPROS	HPLWR	FA tests
16	*Analysis and Calculation of an Accident with Delayed Scram on NPP Greifswald using the Coupled Code DYN3D-ATHLET* S. Kliem	ATHLET DYN3D	VVER-440 (Greifswald)	Delayed scram
17	*Multi-dimensional TMI-1 Main Steam Line Break Analysis Methodology using TRAC-PF/NEM* K. Ivanov, T. Beam, A. Baratta, A. Irani, N. Trikouros	TRAC-PF NEM	PWR (B&W TMI-1)	MSLB
18	*Realistic and Conservative Rod Ejection Simulation in a PWR Core at HZP, EOC with Coupled PARCS and RELAP Codes* J. Riverola, T. Núñez, J. Vicente	RELAP PARCS	Three-loop PWR	Peripheral rod ejection
19	*OECD/NRC BWR Benchmark 3rd Workshop*	ATHLET QUABOX/CUBBOX	BWR Peach Bottom	TT
ATWS: Anticipated Transient without Scram; RIA: Reactivity Induced Accident; REA: Rod Ejection Accident; MCP: Main Coolant Pump; LOFW: Loss Of proper Feed Water				

Table 1.(continues) Overview of 3-D coupled neutronics/thermal-hydraulics calculations available from the literature

3.3 Computational Fluid Dynamics (CFD) codes

The strategy of CFD is to replace the continuous domain with a discrete domain using a grid. The geometry is discretized with a typical mesh size of less than a volume and the thermal-hydraulics properties are computed for every grid point defined. The conservation equations for mass momentum and energy are solved in a discrete form. Any complex geometry is possible, the extremely fine resolution costs computation time. The CFD approach is mostly preferred for small geometries. Existing CFD codes include: FLUENT, CFX.

4. Coupled neutronic and thermal-hydraulics computer codes for LWR

An overview of available coupled neutronics/thermal-hydraulics code published up to now has been reported in table 1. This table summarizes a list of coupled codes for PWR, BWR to date, with the computer codes described in the previous chapters.

4.1 Requirements to the coupling algorithm

Detailed description of the interlace requirement to couple thermal-hydraulics code to 3-D neutronic code has been reported by Langenbuch et al. The objective to couple neutronics code with a thermal-hydraulics code is to provide an accurate solution in a reasonable amount of CPU time. For the present study, the basic components that are considered for the coupling methodology include:

4.2 Coupling method

There are two different ways of coupling, internal and external coupling. With internal coupling the neutronics code is integrated within the thermal-hydraulics code. While with external coupling, the two codes run externally and exchange information between each other.

4.3 Spatial mesh overlay

Accurate mapping of mesh or volumes between the two codes is important to exchange information between each other.

4.4 Coupled convergence schemes

A convergence scheme of the two codes needs to be defined. For a final convergence of the coupled codes, independent convergence in the individual codes is required.

5. Theory of Artificial Neural Network (ANN)

An ANN consists of simple computational units called neurons and it is characterized by a network structure. The neurons connected to each other with different connection strengths. The strength of a connection between neurons is called weight. The types of ANNs are different and associated with applications. The artificial neural networks have a wide variety of applications in nuclear engineering. Some of the basic related researches are listed below:

- Fuel management optimization (Faria and Pereira, 2003)
- Prediction of core parameters (Gazula and Bohr, 1992)
- Plant control and monitoring (Uhrig, 1995)

- Nonlinear dynamics and transient diagnosing (Adali et al., 1997)
- Two-phase flow study (Tambouratzis and Pazsit, 2009)
- Signal validation method (Ikonomopoulos and Van Der Hagen, 1997)

In some investigations to speed up effectively optimization process a very fast estimation system of core parameters has been introduced and developed using cascade feed forward type of artificial neural networks.

5.1 ANN designing

Among the literature, there are different types of available network architectures. The most popular neural network is Multi-Layer Perceptron (MLP) network. This later has been chosen because of its high performance in predictive tasks (Erdogan and Geckinli, 2003; Souza and Moreira, 2006) and to let comparison with the results issued from our calculations. In MLP, various neurons are arranged in different layers called input, hidden, and output. Fig. 1 shows a typical scheme of the three layers neural network. The neurons in the first layer correspond to independent input variables of the problem and transmit the input values to the succeeding layer. After the input layer, there may be one or more hidden layers. They receive the weighted combination of input values from the preceding layer and produce an output depending on their activation function (Jodouin, 1994). As shown in figure 1, the weights are determined and adjusted, through an iterative and a back-propagation process, minimizing a quadratic error function. Thus, to make use of an appropriate Artificial Neural Network, one must fine-tune the following items as their incidence on the prediction parameters are of a crucial importance.
The items of interest are as follow:

1. Activation function,
2. Performance function,
3. Training algorithms.

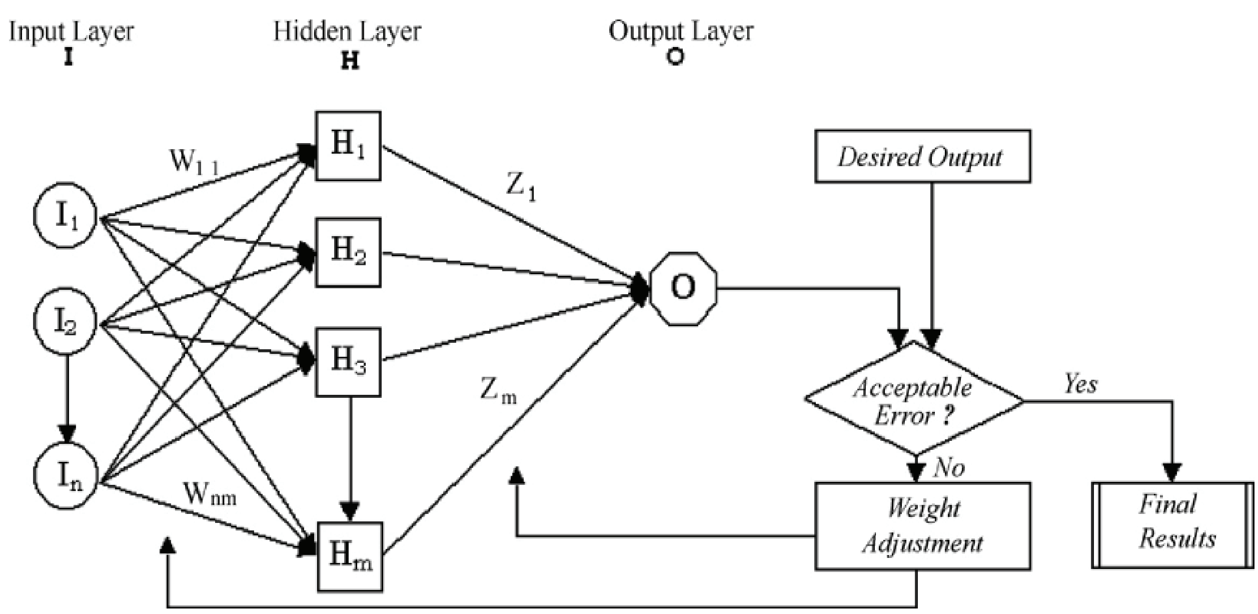

Fig. 1. Typical architecture of Multi-Layer Perceptron (MLP) neural network

5.2 Cascade feed forward neural networks

A general type of feed-forward ANNs consists of a layer of inputs, a layer of output neurons, and one or more hidden layers of neurons. Figure 2 shows a general type of a three layers feed-forward ANN. Typically feed-forward ANNs are used to parameter prediction and data approximation.

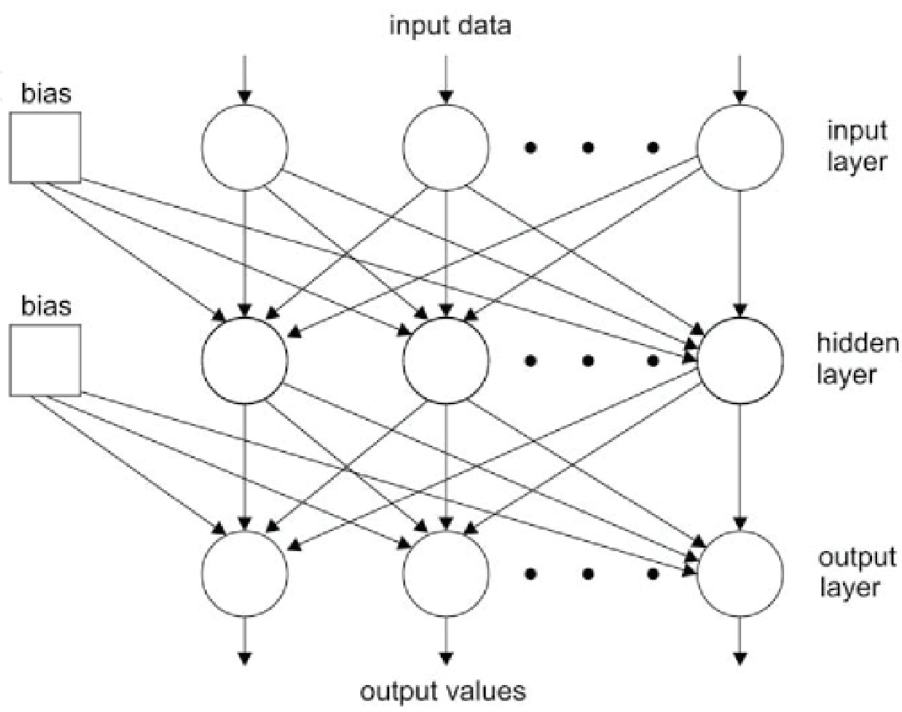

Fig. 2. A general type of three layered feed-forward ANNs

A cascade type of feed-forward ANNs consists of a layer of input, a layer of output neurons, and one or more hidden layers. Similar to a general type of feed-forward ANNs, the first layer has weights coming from the input. But each subsequent layer has weights coming from the input and all previous layers. All layers have biases. The last layer is the network output. Each layer's weights and biases must be initialized. A supervised training method is used to train considered cascade feed forward ANNs.

5.3 Training and activation functions

The training process determined through a back propagation algorithm which minimizes a quadratic error between the desired and network outputs. The gradient descent method with momentum weight/bias learning rule has been used to train considered ANNs. It is a developed algorithm of the basic back propagation algorithm (Hagan et al., 1995; Rumelhart et al., 1986a,b). A net input (V_j) to a neuron in a hidden layer k is calculated by this formula (Eq. (1)).

$$V_j = \sum_{i=1}^{n} W_{ji}\theta_i + \theta_j \quad (1)$$

Where n is the number of k-1 layer neurons for a general type of feed-forward ANNs and the number of all of the previous layer neurons for a cascade type of feed-forward ANNs. Weights are noted by W_{ji}; and the threshold offset by θ_j.

The output of the neuron O_j is given by an activation function. An activation derivative function effects on neuron outputs to compress propagated signals and simulate the nonlinearity of the complex systems. Many different activation functions are used in feed-forward ANNs. There are several types of activation functions such as Linear (Eq. (2)), Log-Sigmoid (Eq. 3), Tan-Sigmoid (Eq. 4) functions, etc.

$$O_j = Pureline(V_j) \tag{2}$$

$$O_j = Logsig(V_j) = 1 / \left(1 + e^{-(V_j)}\right) \tag{3}$$

$$O_j = Tansig(V_j) = \left(1 - e^{-2(V_j)} / (1 + e^{-2(V_j)}\right) \tag{4}$$

In this learning method, which is a batch training method, weights and biases are only updated after all the inputs and targets are presented to ANNs. Then the average of system error (Eq. 5) should be minimized to increase learning performance.

$$E_{AV} = \frac{1}{2N} \sum_{i=1}^{N} \sum_{j=1}^{M} \left(d_j(n) - O_j(n) \right)^2 \tag{5}$$

Where $d_j(n)$ is the desired output; and $O_j(n)$ is the network output. N and M are the total number of training data sets and the number of neurons of the output layer. In the gradient descent method improved values of the weights can be achieved by making incremental changes Δw_{ji} proportional to $\partial E_{AV}/\partial W_{ji}$ (Eq. 6).

$$\Delta W_{ji} = -\eta \frac{\partial E_{AV}}{\partial W_{ji}} \tag{6}$$

Where the proportionally factor η is called the learning rate. Large values of η in the gradient descent formulation may lead to large oscillation or divergence. One attempt to increase the speed of convergence while minimizing the possibility of oscillation, or divergence, involves adding a momentum term to the basic gradient descent formulation. In this case the weight vector at time index (k+1) is related to the weight vectors at time indexes (k) and (k-1) by this formula (Eq. 7).

$$W(k+1) = W(k) - \left[\eta \frac{\partial E}{\partial W} + \beta \Delta W(k-1) \right] \tag{7}$$

Then the new weights for step (k+1) are given by:

$$\Delta W_{ji}(k+1) = \eta \delta_j O_j + \beta \Delta W_{ji}(k) \tag{8}$$

Where a momentum coefficient, or an acceleration parameter β is used to improve convergence. The expression of δ_j is given by:

$$\delta_k = 0.5(d_k - O_k) f'(v_k) \tag{9}$$

$$\delta_j = f'(v_k) \sum_k \delta_k W_{kj} \quad \text{for hidden neurons} \tag{10}$$

It should be noted that the technology of ANNs has been still developing. The determination of minimum number of necessary hidden neurons and hidden layers is completely practical. If the hidden neurons are chosen very small, the network will classify its input in a small number of classes (Wilde, 1997). If the hidden neurons are selected extremely large, the time of learning process increases ineffectively. Presently, the best method is making an educated guess. In this work, after primarily studies some practical tests are suggested and used to adjust the main parameters and properties of the ANNs' structures and used training rule (Eqs. 1 through 10).

5.4 ANN development strategy

The motivation in using such a computational procedure lies in the fact that it will let us use just hundreds of configurations rather than the thousands, in the learning stage, that are usually required in typical calculations to ensure reasonable predictions. Hence, as shown in Fig. 3, a suitable neural networks development strategy can be tested based on executing the following two main calculational stages, in an independent way: learning stage and prediction stage.

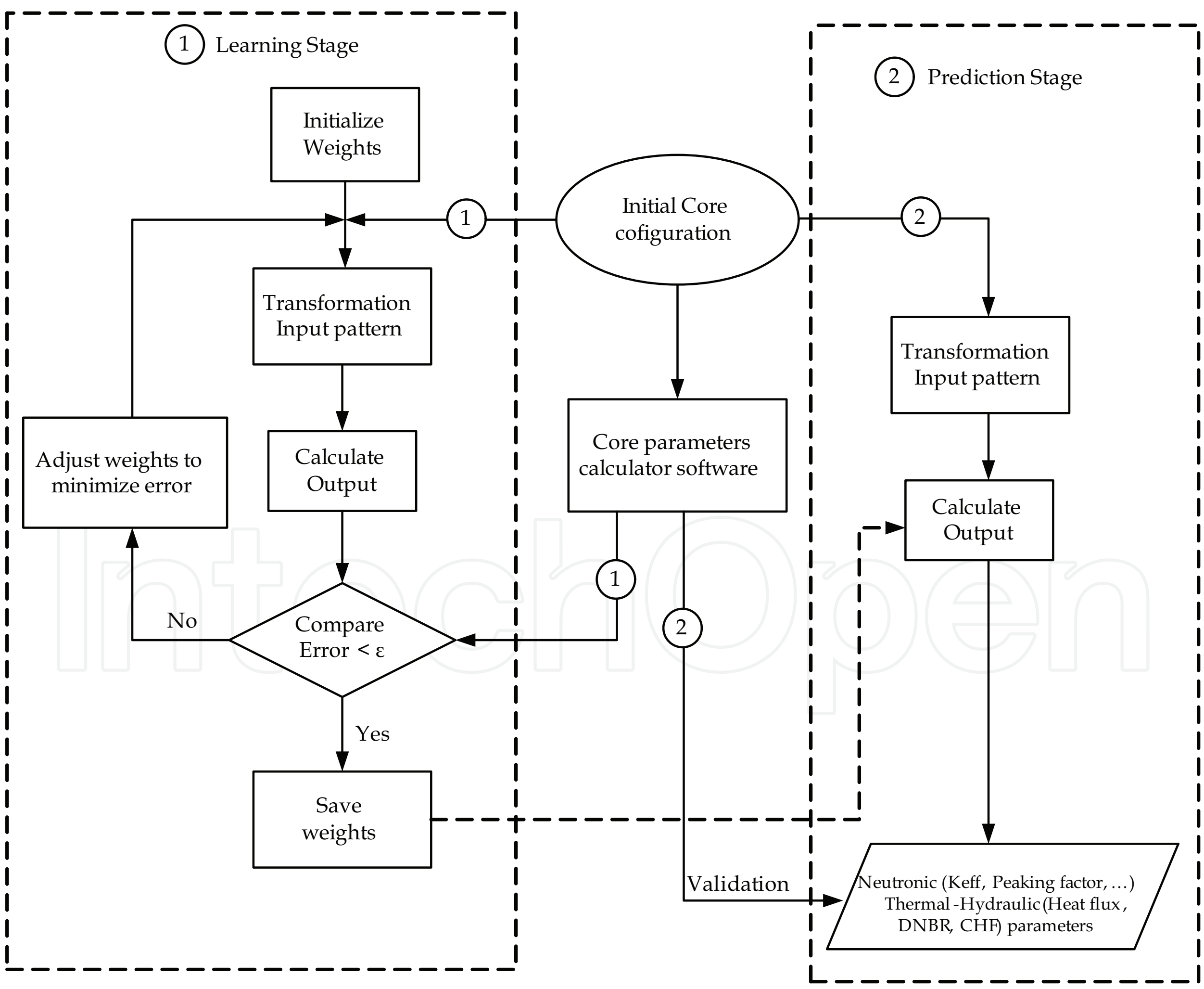

Fig. 3. Overall back-propagation computational strategy for the core parameter prediction

The first stage of computational procedure consists of creating suitable networks by applying an appropriate learning rule using a desired database. The information required in the related database will contain coupled input values with the corresponding target output values. These values are used to train the networks until the error reaches a desired value stated at the beginning of the learning process. It becomes evident that the quality of the results obtained will depend on how well knowledge is capitalized in this database. Hence, significant attention will be focused on how well this database will be created. The main steps required in the learning process are:

1. Create the database for training;
2. Construction of networks for training;
3. Choosing a learning function;
4. Train the developed networks;

The second stage is the prediction one where the weights, from the inter-connected neurons, have been adjusted to the desired error in the previous calculations stage. These weights will be used in a global computational sequence, to predict the networks outputs when unseen data will be presented to the developed networks. This is the power of the network approach and one of the reasons for using it. The net is said to have been generalized from the training data. This stage is necessary to test the performance of the developed neural network.

5.5 Create data-base for training

A wide variety of completely different core arrangements are needed to train effectively considered ANNs. In this work, the fuel assembly positions are considered changeable in calculations. Core calculations have been done by a supporting software tool that will be able to calculate neutronic and thermal hydraulic parameters of a typical reactor core. This program uses a coupling method to calculate reactor core parameters for desired core configuration. Needed parameters for training should be extracted from the software calculations. They must be converted to a compatible format to feed desired ANNs. Doing this manually takes a long time while some human errors are possible. In this research, a data base builder program is designed and used. It is used to create data sets necessary to train and test considered ANNs.

In this research, a software package (Core Parameters Calculator) is developed and used. The random state of the software is used to create data sets necessary to train and test used ANNs. Many strings composed of specific integer numbers are chosen randomly to form different core configurations. For each different state (configuration), Core Parameters Calculator software uses MCNP and COBRA-EN code to extract needed neutronic and thermal-hydraulics core parameters. During calculation process, MCNP code uses cross sections library provided by NJOY program. Then calculated fission powers of fuel rods send to Thermal-hydraulics code for calculating of density and temperature distribution of fuel and coolant. Finally the results (consist of neutronic and thermal- hydraulic parameters) are stored on a local data base table. Figure 4 shows the main diagram of creating desired data.

5.6 Developing of a supporting tool for core parameters calculation

Due of the strong link between the water (moderation) and the neutron spectrum and subsequently the power distribution, a coupling of neutronics and thermal-hydraulics has

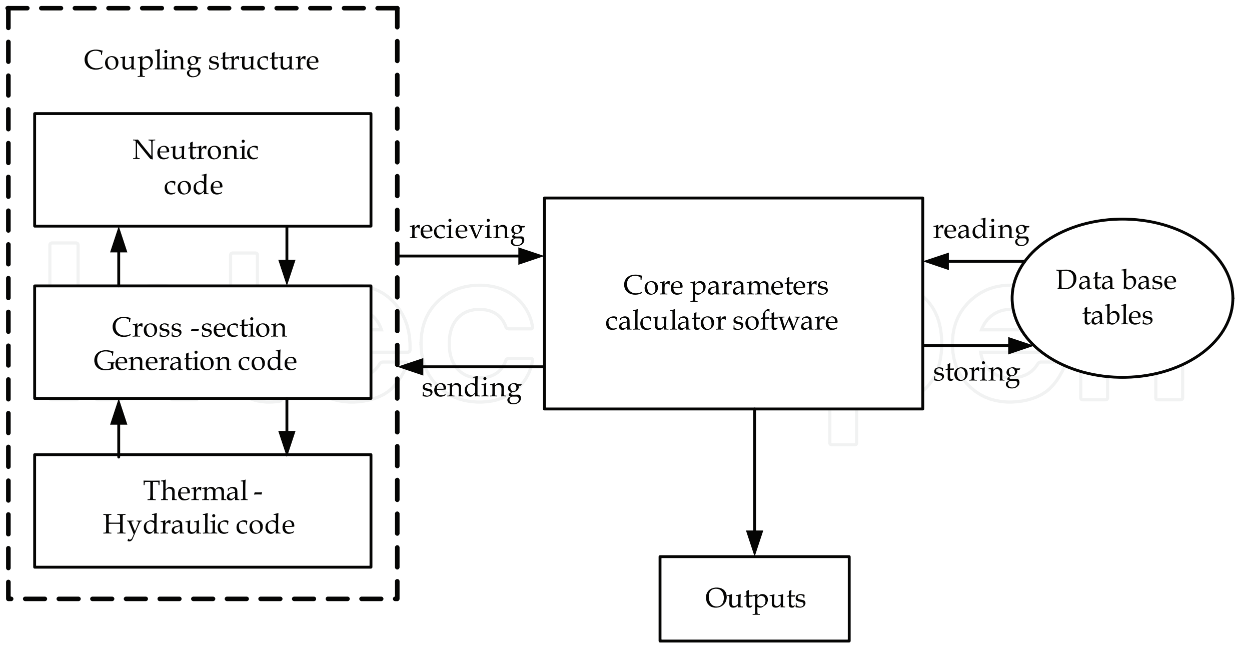

Fig. 4. The main diagram of creating desired data

become a necessity for reactor concepts operating at real conditions. The effect of neutron moderation on the local parameters of thermal-hydraulics and vice-verse in a fuel assembly has to be considered for an accurate design analysis. In this study, the Monte Carlo N-Particle code (MCNP) and the sub-channel code COBRA-EN (Sub-channel Thermal-hydraulics Analysis of a Fuel Assembly for LWR) have been coupled for the design analysis of a fuel assembly and core with water as coolant and moderator. Both codes are well known for complex geometry modeling. The MCNP code is used for neutronics analyses and for the prediction of power profiles of individual fuel rods. The sub-channel code COBRA for the thermal- hydraulics analyses takes into account the coolant properties as well as separate moderator channels.

The coupling procedure is realized automatically. MCNP calculates the power distribution in each fuel rod, which is then transferred into COBRA to obtain the corresponding thermal-hydraulics conditions in each sub-channel. The new thermal-hydraulics conditions are used to generate a new input for the next MCNP calculation. This procedure is repeated until a converged state is achieved. The parameters that are exchanged between the two codes for the coupling are: power distribution from MCNP code, water density distribution, water temperature distribution and fuel temperature distribution from COBRA code, as shown in Figure 5. The COBRA-EN code, which is written in FORTRAN language, is modified to include the power distribution obtained from neutronics analysis and to be able modeling of Russian fuel type.

The nuclear cross section data library of MCNP must be provided for additional temperatures and must be added to MCNP data directory. The cross section data for neutron interaction are obtained from the evaluated MCNP libraries ENDF/B. Cross section data provided with the MCNP are for a limited number of temperatures. An additional library must be constructed from NJOY code with more temperatures (300 K, 500 K, 600 K, 760 K, 800 K, 1000 K, 1500 K) and is added to the MCNP data directory. The coupled code system was tested on a proposed fuel assembly design of a VVER-1000. The coupling procedure presented will also be applicable to other types of reactors with a density variation in the core such as in BWR.

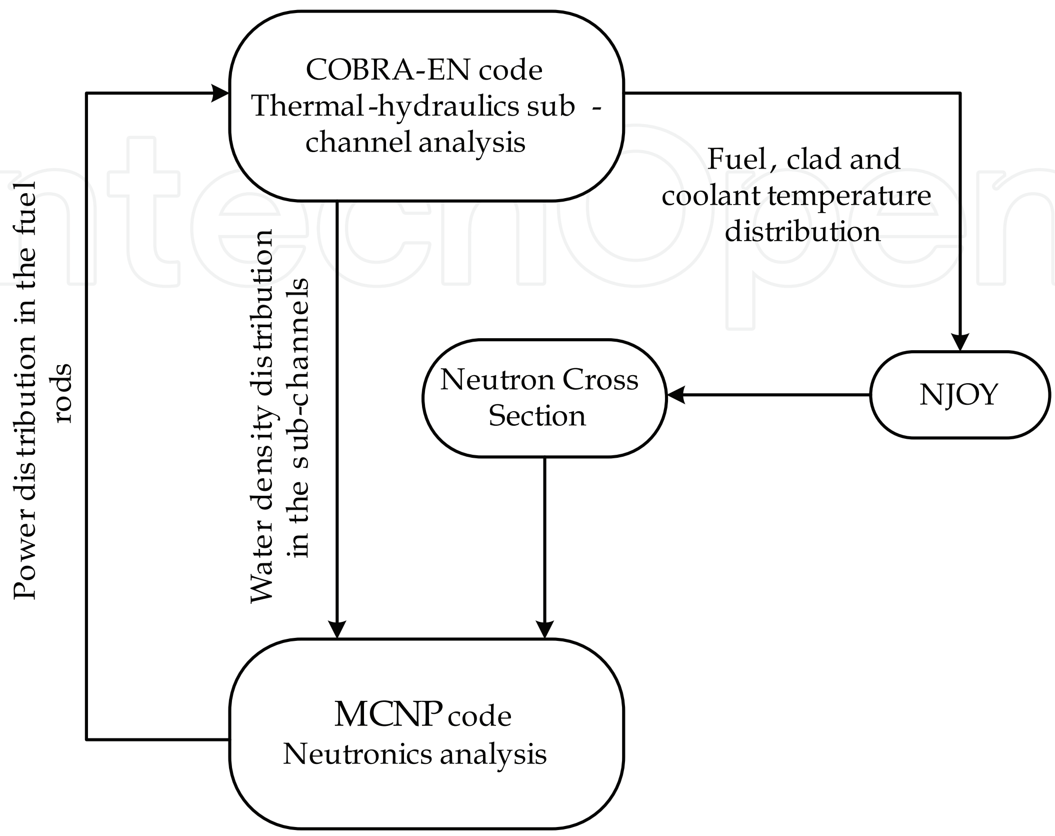

Fig. 5. Coupled MCNP/COBRA-EN for joining neutronic –thermalhydraulics are shown schematically. The cross sections modification are a major concern which are doen using NJOY code

From the literature review, most of the available coupled codes for neutronics/thermal-hydraulics are based on diffusion and system codes resulting in a rather coarse resolution of the core. For a detailed analysis of a VVER-1000 fuel assembly analysis, diffusion codes and system codes are not giving enough local information. All prior application had been to PWR and BWR transient analysis. To accurately analyze a VVER fuel assembly a more detailed analysis fuel rod wise and sub-channel wise is required to predict a hot spot and the temperature distribution around the circumference of a fuel rod. In order to perform such detailed analysis of the VVER fuel assembly, a new coupled code system is required. From the reviewed neutronics and thermal-hydraulics computer codes, the Monte Carlo code and sub-channel codes show to be the best choice of codes to be coupled for detailed fuel assembly analysis. Both have similar spatial resolution. The smallest control volume is in the order of a few cm in both cases. System codes on the other hand would be too coarse for MCNP and CFD codes too fine in resolution.

6. Conclusions

Obviously, due to huge files, it is not possible to present our input files (MCNP and COBRA-EN codes) as our suggested package in this chapter, but reader can consult the

corresponding author to find the MCNP as well as COBRA-EN input files for simulating a VVER-1000 reactors. The MCNP code contains hexagonal core including all core conditions such as all control rod inserted (or withdrawn), boric acid inserted, hot full power condition, etc. Also, reader can find our COBRA-EN code to undrestand how we can simulate thermal hydraulics subchannels of a VVER-1000 reactor. Moreover, as we said previously, temperature cross sections modification are carried out using NJOY code and obviously reader can receive our modification. These so-called data are used as output data for ANN training. If reader are interested, they can consult the corresponding author to get our ANN simulator. Basically, the main objective of the ANN software is to obtain fast estimation tool which allows large explorations of core safety parameters. This software is very useful in reactor core designing and in-core fuel management or loading pattern optimization.
In due course, verification and validation of the procedures are taking into account using available experimental data or other code-to-code benchmarking, and this is an important part of research.

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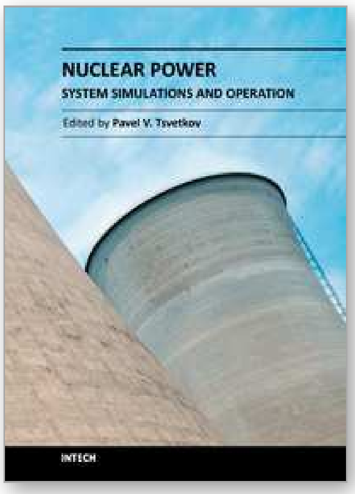

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At the onset of the 21st century, we are searching for reliable and sustainable energy sources that have a potential to support growing economies developing at accelerated growth rates, technology advances improving quality of life and becoming available to larger and larger populations. The quest for robust sustainable energy supplies meeting the above constraints leads us to the nuclear power technology. Todayâ€™s nuclear reactors are safe and highly efficient energy systems that offer electricity and a multitude of co-generation energy products ranging from potable water to heat for industrial applications. Catastrophic earthquake and tsunami events in Japan resulted in the nuclear accident that forced us to rethink our approach to nuclear safety, requirements and facilitated growing interests in designs, which can withstand natural disasters and avoid catastrophic consequences. This book is one in a series of books on nuclear power published by InTech. It consists of ten chapters on system simulations and operational aspects. Our book does not aim at a complete coverage or a broad range. Instead, the included chapters shine light at existing challenges, solutions and approaches. Authors hope to share ideas and findings so that new ideas and directions can potentially be developed focusing on operational characteristics of nuclear power plants. The consistent thread throughout all chapters is the â€œsystem-thinkingâ€ approach synthesizing provided information and ideas. The book targets everyone with interests in system simulations and nuclear power operational aspects as its potential readership groups - students, researchers and practitioners.

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