ABSTRACT
This report deals with the demonstration of an innovative coupled neutronic/thermo-hydraulic tool, for which the models and algorithms were already presented in a companion report [1]. The novelty of the tool resides in its versatility, since many different systems can be investigated and different kinds of calculations can be performed. More precisely, both critical systems and subcritical systems with an external neutron source can be studied, and static and dynamic cases in the frequency domain (i.e. for stationary fluctuations) can be considered. For each situation, the three-dimensional distributions of the static neutron fluxes, all thermo-hydraulic parameters, their respective first-order noise are estimated, as well as the effective multiplication factor of the system. The main advantages of the tool, which is entirely MATLAB based, lie with the robustness of the implemented numerical algorithms, its high portability between different computer platforms and operative systems, and finally its ease of use since no input deck writing is required. The present version of the tool, which is based on two-group diffusion theory, is mostly suited to investigate thermal systems, both Pressurized and Boiling Water Reactors (PWR and BWR, respectively). The tool, for which a complete user’s manual exists [2], is freely available on direct request to the authors of the present report.
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Chapter 1

INTRODUCTION

In a companion report [1], the development of a unique multi-purpose coupled neutronic/thermo-hydraulic tool for research and education was reported. The multi-purpose character of the tool comes from the fact that the tool can consider both critical systems and subcritical systems with an external neutron source, static cases and dynamic cases in the frequency domain (i.e. for stationary fluctuations). For each situation, the three-dimensional distributions of the static neutron fluxes, all thermo-hydraulic parameters and their respective first-order neutron noise can be determined, as well as the effective multiplication factor of the system. The coding was implemented in MATLAB, which makes the pre- and post-processing of data easy, as well as the code highly portable between different operative systems and computer platforms. The code was developed while paying careful attention to data storage requirements and to the robustness of the algorithms. In particular, the numerical algorithms implemented in the neutronic module of the tool take advantage of the sparsity of the matrices, and the MATLAB built-in linear algebra packages LAPACK and UMFPACK are extensively used. In addition, an explicitly-restarted Arnoldi method and a power iteration method using Wielandt’s shift were implemented to solve eigenvalue problems.

This tool uses as input parameters the spatial distributions of reference macroscopic cross-sections, some selected neutronic and thermo-hydraulic parameters extracted from a commercial core simulator. In the present tool, the user can freely define configurations representative of any actual core and most importantly can perturb the system by directly defining perturbations in thermo-hydraulic quantities (core inlet velocity, core inlet temperature or core exit pressure) as well as in the macroscopic cross-sections. Some of the examples of the perturbations which can be modelled with this tool for both PWR and BWR cases will be demonstrated hereafter. Despite the simplicity of the algorithms implemented in the tool, this tool represents a good complement to state-of-the-art coupled neutron kinetics/thermal-hydraulics codes, since the tool can still catch the main physical phenomena and at the same time provide some physical insight in a much simpler and more straightforward manner than the above mentioned codes.

The demonstration of the tool is the main topic covered here. As illustrative examples, the space-frequency distributions of the neutronic/thermo-hydraulic noise induced by two typical perturbations encountered in Light Water Reactors, such as out-of-phase and density wave oscillations are shown. Thereafter, some explanations on the use of the tool are also given.
DEMONSTRATION AND USE OF THE TOOL

2.1 Introduction

The computational tool presented hereafter is delivered with a complete user’s guide [2] explaining the required software/hardware, what the code package contains, the file architecture and required input, the created output, the format of the input and output variables, the variables necessary in the input files, the available variables in the output files, and how to use the code. Some examples are also available within the package.

The main feature of the computational tool is its flexibility and its simplicity in use, since there is no need of writing any input deck. Data input should be provided by the user in several data files describing the three-dimensional distributions of the macroscopic cross-sections throughout the system, its geometry and some thermo-hydraulic parameters. Some additional optional files should also be provided for defining possible external neutron sources and their possible fluctuations, for defining possible sources in the static and dynamic problems, as well as for defining some additional kinetic data necessary for calculating the neutron noise. Prior to using the tool, the user might want to change some default settings and/or fine-tune some parameters related to the numerical techniques implemented in the code. For the latter, the parameters are related to the type of the cross-section model (linear or tabulated), activation of the dynamic calculations, the parameters for the explicitly-restarted Arnoldi method and the power iteration method with Wielandt’s shift technique, the convergence criteria imposed on both thermo-hydraulic and neutronic variables in static and dynamic calculations as well as for the inner (thermo-hydraulic) and outer (coupled) iterations, the initial error for both thermo-hydraulic and neutronic variables in static and dynamic calculations as well as for inner (thermo-hydraulic) and outer (coupled) iterations. These latter parameters might need to be changed in case of convergence problems. Such settings are defined in a separate file (called SETTINGS.m) that the user can modify. Default parameters will be used if the user does not modify any of these settings.

In the following, two examples of the noise calculations, for two different perturbations (an out-phase perturbation and a point-wise perturbation) are discussed for both a PWR and a BWR. The perturbations are imposed on the core inlet temperature in both cases.
2.2 Case of a Pressurized Water Reactor (PWR) heterogeneous system

2.2.1 Static calculations

First, a three-dimensional cylindrical fully heterogeneous PWR system near to criticality is considered. The system is representative of a commercial PWR. All necessary input data were obtained from a commercial core simulator, in the present case SIMULATE-3 [3]. Fig. 2.1 represents the three-dimensional distributions of the static power density, coolant/moderator density, fuel temperature, and coolant/moderator velocity, obtained by CORE SIM. As can be seen in this figure, the fuel temperature closely follows the relative power density. Because of the one-phase nature of the flow, the variation of the coolant/moderator density through the core is mild. Due to mass conservation and decrease of the coolant/moderator density from bottom to top, the coolant/moderator velocity accelerates accordingly.

![Figure 2.1: Three-dimensional distributions of the static neutronic and thermal-hydraulic variables (PWR example, CORE SIM calculations). The horizontal planes gives the radial distributions at $\frac{1}{4}$ elevation from the core bottom, whereas the vertical planes give the axial distributions through the middle of the core.](image)

Due to the heterogeneous nature and coupled character of the system, the proper validation of the developed tool, either against an analytical solution or against measure-
2.2. Case of a Pressurized Water Reactor (PWR) heterogeneous system

ments (due to lack of in-core instrumentation), is not possible. Instead, it was decided to perform a qualitative comparison between the corresponding static solutions: one obtained from the developed tool and another one from the commercial static core simulator SIMULATE-3 (which was used as a reference solution for the CORE SIM tool). The corresponding SIMULATE-3 solution for the power density, coolant/moderator density, fuel temperature and coolant/moderator velocity is given in Fig. 2.2. The numerical solution (i.e. the solution obtained with CORE SIM) was estimated with a node size of $\Delta x = 10.75$ cm, $\Delta y = 10.75$ cm and $\Delta z = 15.24$ cm. The comparison between Figs. 2.1 and 2.2 shows a relatively good agreement between the CORE SIM solution and the reference solution. Some discrepancy close to the radial boundary of the system could nevertheless be observed, due to the better modelling of steep flux gradients in the reference solution than in the CORE SIM solution.

![Figure 2.2: Three-dimensional distributions of the static neutronic and thermal-hydraulic variables (PWR example, reference data). The horizontal planes gives the radial distributions at $\frac{1}{4}$ elevation from the core bottom, whereas the vertical planes give the axial distributions through the middle of the core.](image)

2.2.2 Noise calculations

Fig. 2.3 demonstrates the three-dimensional distributions of the amplitude of the stationary fluctuations at a frequency of 0.5 Hz induced by a perturbation applied on the coolant/moderator temperature at the inlet of the core. This perturbation is defined as
being homogeneous in amplitude, but out-of-phase between the two halves of the core. This figure clearly highlights the corresponding radially asymmetrical response of the neutron flux.

![Diagram of neutron flux fluctuations](image)

**Figure 2.3:** Three-dimensional distributions of the amplitude of the stationary fluctuations of the neutronic and thermal-hydraulic variables (out-of-phase perturbation in the inlet velocity, PWR example). The horizontal planes give the radial distributions at $\frac{1}{4}$ elevation from the core bottom, whereas the vertical planes give the axial distributions through the middle of the core.

As a second illustration, in Fig. 2.3 the three-dimensional distributions of the amplitude of the stationary fluctuations at a frequency of 0.5 Hz induced by a perturbation applied on the coolant/moderator temperature at the inlet of the core are given. The perturbation was placed in the middle of the core (at the radial position (16, 16)).
2.3. Case of a Boiling Water Reactor (BWR) heterogeneous system

2.3.1 Static calculations

A system representing a commercial BWR is discussed hereafter. All necessary input data were again obtained from a commercial core simulator, in the present case POLCA-7 [4]. Fig. 2.5 represents the three-dimensional distributions of the static relative power density, coolant/moderator density, fuel temperature, and coolant/moderator velocity obtained from CORE SIM. Contrary to the PWR example, the variation of the coolant/moderator density between the core inlet and outlet is very significant, because of vapour production. Correspondingly, the flow accelerates drastically.
Chapter 2. DEMONSTRATION AND USE OF THE TOOL

(a) Power density  
(b) Coolant density  

(c) Fuel temperature  
(d) Coolant velocity

Figure 2.5: Three-dimensional distributions of the static neutronic and thermal-hydraulic variables (BWR example, CORE SIM calculations). The horizontal planes gives the radial distributions at 1/4 elevation from the core bottom, whereas the vertical planes give the axial distributions through the middle of the core.

As pointed out earlier, the heterogeneous nature and coupled character of the considered systems do not allow to perform the proper validation of the developed tool, i.e. neither against analytical solutions nor against measurements (due to lack of in-core instrumentation). Therefore, it was decided to undertake the qualitative comparison between the corresponding static solutions: one obtained from the developed tool and another one from the commercial static core simulator POLCA-7 (which was used as a reference solution for the CORE SIM tool). The corresponding POLCA-7 solution for the power density, coolant/moderator density, fuel temperature and coolant/moderator velocity is given in Fig. 2.6. The numerical solution (i.e. the solution obtained with CORE SIM) was estimated with a node size of $\Delta x = 15.375$ cm, $\Delta y = 15.375$ cm and $\Delta z = 14.72$ cm. From the comparison between Figs. 2.5 and 2.6, a good agreement between the CORE SIM solution and the reference solution can be noticed. Some discrepancy could nevertheless be observed, due to the better modelling of two-phase flows in the reference solution than in the CORE SIM solution.
2.3. Case of a Boiling Water Reactor (BWR) heterogeneous system

(a) Power density  
(b) Coolant density  
(c) Fuel temperature  
(d) Coolant velocity

**Figure 2.6:** Three-dimensional distributions of the static neutronic and thermal-hydraulic variables (BWR example, reference data). The horizontal planes give the radial distributions at \( \frac{1}{4} \) elevation from the core bottom, whereas the vertical planes give the axial distributions through the middle of the core.

2.3.2 Noise calculations

Fig. 2.7 shows the three-dimensional distributions of the amplitude of the stationary fluctuations at a frequency of 0.5 Hz induced by a perturbation applied on the coolant/moderator temperature at the inlet of the core. This perturbation is defined as being homogeneous in amplitude, but out-of-phase between the two halves of the core. Compared to the PWR case where asymmetry was observed only in the power density and fuel temperature noise, in the BWR case, the response of the coolant/moderator velocity is also radially asymmetrical.
Figure 2.7: Three-dimensional distributions of the amplitude of the stationary fluctuations of the neutronic and thermal-hydraulic variables (out-phase perturbation in the inlet velocity, BWR example). The horizontal planes gives the radial distributions at $\frac{1}{4}$ elevation from the core bottom, whereas the vertical planes give the axial distributions through the middle of the core.

Similarly to the PWR case, in Fig. 2.3 the three-dimensional distributions of the amplitude of the stationary fluctuations at a frequency of 0.5 Hz induced by a point-wise perturbation applied on the coolant/moderator temperature at the inlet of the core are given. The perturbation was placed in the middle of the core (at the radial position (16, 16)).
2.4 Use of the tool

The computational tool presented above is delivered with a complete user’s guide [2] explaining:

- the required software/hardware;
- what the code package contains;
- the file architecture and required input;
- the created output;
- the format of the input and output variables;
- the variables necessary in the input files and the available variables in the output file;
- how to use the code.

Figure 2.8: Three-dimensional distributions of the amplitude of the stationary fluctuations of the neutronic and thermal-hydraulic variables (point-wise perturbation in the inlet velocity, BWR example). The horizontal planes give the radial distributions at $\frac{1}{4}$ elevation from the core bottom, whereas the vertical planes give the axial distributions through the middle of the core.
Chapter 2. DEMONSTRATION AND USE OF THE TOOL

Some examples are also available within the package.

The tool, which is freely available on request to the authors of the present report, is distributed under a GNU General Public License (http://www.gnu.org/licenses/gpl.html).

The main features of the computational tool are its flexibility and its simplicity in use, since there is no need of writing any input deck. The input required to run the code is made of the following six files:

- **XS_DATA_REF.mat**: file describing the three-dimensional distributions of the reference (extracted from a commercial core simulator) macroscopic cross-sections throughout the system (this file is compulsory);

- **KIN_DATA_REF.mat**: file describing the size of an elementary node in the $x$, $y$- and $z$-directions (this file is compulsory); this file also contains some additional data necessary for calculating the neutron noise (these data are optional and only required if the neutron noise has to be estimated);

- **TH_VARS_MESH_DATA.mat**: file containing grid points of thermo-hydraulic quantities (coolant/moderator density and fuel temperature) which will be used as interpolation variables in the three-dimensional interpolation of the cross-sections (this file is compulsory for using a tabulated cross-section model);

- **XS_MESH_DATA.mat**: file containing grid points of cross-sections which will be used as interpolated variables in three dimensional interpolation of the cross-sections (this file is compulsory for using a tabulated cross-section model);

- **FLX_DATA_REF.mat**: file describing the three-dimensional distributions of both fast and thermal reference (extracted from a commercial core simulator) neutron fluxes throughout the system (this file is compulsory);

- **TH_PARAM_REF.mat**: file containing the information about the thermo-hydraulic parameters together with the three-dimensional distributions of required reference (extracted from a commercial core simulator) thermo-hydraulic variables throughout the system (this file is compulsory).

Some additional optional files can be provided by the user:

- **DF_DATA.mat**: file describing the three-dimensional distributions of the discontinuity factors throughout the system (this file is optional); if this file is not provided all discontinuity factors are automatically set to unity;

- **S_DATA.mat**: file containing the definition of an external neutron source (this file is optional and only required if the static neutron flux of a subcritical system with external neutron source has to be determined);

- **dS_DATA.mat**: file containing the definition of the cross-section (neutronic) noise source (this file is optional and only required if the neutron noise has to be determined);

- **FUE_TAB.mat**: file containing the fuel tables used for calculating the three-dimensional distributions of fuel density and fuel specific heat (this file is optional and only required if the noise in thermo-hydraulic quantities has to be determined);
2.4. Use of the tool

- **XS_DATA_PERT_RHO_LM.mat**: file describing the three-dimensional distributions of the perturbed macroscopic cross-sections throughout the system (for a perturbation induced in the coolant/moderator density; this file is only compulsory if there is not any separate cross-section model provided and is optional otherwise);

- **XS_DATA_PERT_TFU_LM.mat**: file describing the three-dimensional distributions of the perturbed macroscopic cross-sections throughout the system (for a perturbation induced in the fuel temperature; this file is only compulsory if there is no any separate cross-section model provided and is optional otherwise);

- **dTH_DATA_REF.mat**: file containing the definition of the thermo-hydraulic noise source (this file is optional and only required if the noise has to be determined).

Prior to using the tool, the user might want to change some default settings and/or fine-tune some parameters related to the numerical techniques implemented in the code. For the latter, the parameters are related to the type of the cross-section model (linear or tabulated), activation of the dynamic calculations, the parameters for the explicitly-restarted Arnoldi method and the power iteration method with Wielandt’s shift technique, convergence criteria imposed on both thermo-dyraulic and neutronic variables in static and dynamic calculations as well as for inner (thermo-hydraulic) and outer (coupled) iterations, the initial error for both thermo-dyraulic and neutronic variables in static and dynamic calculations as well as for inner (thermo-hydraulic) and outer (coupled) iterations. These latter parameters might need to be changed in case of convergence problems. Such settings are defined in a separate file (called **SETTINGS.m**) that the user can modify. Default parameters will be used if the user does not modify any of these settings.
CONCLUSIONS

In this report, the demonstration of the multi-purpose coupled neutronic/thermo-hydraulic tool earlier described in [1] was reported.

This tool is actually the continuation of some previous work, earlier meant to develop a computational tool allowing the determination of the so-called open-loop reactor transfer function in the frequency-domain [5, 6]. This earlier versions of the tool allowed calculating the neutron noise induced by perturbations of the macroscopic cross-sections in the frequency domain in a two-dimensional and three-dimensional representation of any nuclear core and in the two-group diffusion approximation, with a spatial discretization based on finite differences. In above-mentioned versions of the tool only open-loop systems were considered. The two-dimensional version of the tool has already been successfully applied to numerous practical problems, such as:

- the unfolding of the noise source from the readings of the neutron detectors (in order to locate unseated fuel assemblies in commercial BWRs) [7];
- the explanation of the space-dependence of the Decay Ratio observed in commercial BWRs [8];
- the development of a new noise estimator for estimating the Moderator Temperature Coefficient (MTC) of reactivity (giving the correct MTC value without calibration) and its experimental verification in a commercial PWR [9];
- the diagnostics and modeling of beam/shell-mode core-barrel vibrations in PWRs [10];
- the investigation of the validity of the point-kinetic approximation in subcritical systems with application to subcriticality monitoring [11];
- the development of a Reduced Order Model for BWR instabilities, including possible unseated fuel assemblies driving self-sustained Density Wave Oscillations [12].

All the applications mentioned above are further described in the corresponding papers, as well as in a review paper [10].
The tool reported in this paper estimates the closed-loop transfer function.
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