TOWARDS AN EFFICIENT MULTIPHYSICS MODEL FOR NUCLEAR REACTOR DYNAMICS

by

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Availability of fast computer resources nowadays has facilitated more in-depth modeling of complex engineering systems which involve strong multiphysics interactions. This multiphysics modeling is an important necessity in nuclear reactor safety studies where efforts are being made worldwide to combine the knowledge from all associated disciplines at one place to accomplish the most realistic simulation of involved phenomenon. On these lines coupled modeling of nuclear reactor neutron kinetics, fuel heat transfer and coolant transport is a regular practice nowadays for transient analysis of reactor core. However optimization between modeling accuracy and computational economy has always been a challenging task to ensure the adequate degree of reliability in such extensive numerical exercises. Complex reactor core modeling involves estimation of evolving 3-D core thermal state, which in turn demands an expensive multichannel based detailed core thermal hydraulics model. A novel approach of power weighted coupling between core neutronics and thermal hydraulics presented in this work aims to reduce the bulk of core thermal calculations in core dynamics modeling to a significant extent without compromising accuracy of computation. Coupled core model has been validated against a series of international benchmarks. Accuracy and computational efficiency of the proposed multiphysics model has been demonstrated by analyzing a reactivity initiated transient.

Key words: multiphysics modeling, TRIKIN, space-time kinetics, core thermal hydraulics, coupled core dynamics, power weighted coupling

INTRODUCTION

The foundation pillar in the peaceful utilization of fission nuclear power has always been the strong emphasis on nuclear safety. Safety has been accomplished through in-depth review of design and operations, incorporation of findings from safety R&D worldwide and improvement in methods of evaluation. In the entire chain of safety process, safety analysis has been a vital link which provides an estimation of the capability of the nuclear systems to control or accommodate departures from normal operation or postulated malfunctions or failures. It is also used to demonstrate that the nuclear plant does not pose unacceptable hazards under the worst accident scenarios. Safety analysis is performed using numerical simulation tools (computer codes) which have evolved gradually in terms of accuracy and complexity over the past five decades. These numerical simulation tools are widely used for safety analysis within the framework of the licensing and safety improvement programs of existing nuclear power plants, better utilization of nuclear fuel, higher operational flexibility, for justification of lifetime extensions, development of new emergency operating procedures, analysis of operational events and development of accident management programs. As a conventional practice, problem specific models addressing limited physical phenomenon were developed and used during design and analysis of present generation nuclear reactors. These codes were based on strong emphasis of single physics phenomenon and they were improved and refined thoroughly in that aspect. Since these individual physical models were developed independently to pursue limited objectives, they had very little or almost no connections, e. g., core physics codes were used extensively for fuel management and criticality calculations, systems codes like RELAP, TRAC, and ATHLET [1] were developed for analyzing thermal hydraulics, leaks, system transients, etc., structure codes were used to assess structural integrity, life management and aging like issues, inventory codes like ORIGEN were developed for estimating core radionuclide inventories for consequence analyses. These types of single physics
models though helped appreciably in design and analysis of present generation reactors; they could not address finer aspects of many interphysics interactions. Thus far, major limitation in modeling of finer multiphysics aspects of reactor core through integrated multiphysics computational simulation was lack of strong computing resources. The recent availability of powerful computers and improved computational techniques has made possible developing more realistic models of complex interacting phenomena in nuclear power plant (NPP) with more precise consideration of reactor multiphysics effects. Such multiphysics modeling of NPP at different level of time and scale provides a basis to undertake a more in-depth evaluation of the safety margins found in previous core simulations for which limited conservative models were used. Insights in the complex physical phenomenon may also provide incentives to more efficiently utilise the nuclear fuel and obtain cost benefits in the operation of the NPP without compromising safety. It can also help in relaxing some operational procedures as well as could provide more effective guidelines for optimization of emergency operating procedures. This multiphysics modeling practice has become an inevitable requirement of new generation large power reactors which are being designed to meet more stringent safety requirement. Comprehensive efforts are now being placed at combining knowledge of all involved diverse physical disciplines in high-performance multipurpose simulation models to improve the reliability of computational simulations to the highest level and avoiding all possible sources of analytical uncertainties.

Nuclear reactor dynamics is a stream of reactor analysis which deals with the transient behavior of nuclear reactor core under the influences of internal as well as external changes. These changes could include reactivity effects and/or changes in thermal states and/or changes in dimensions. Discipline of reactor dynamics is characterized by large number of strongly interacting physical phenomenon with significantly diversified time scales as shown in fig. 1. For a situation to be analyzed, if these phenomena do not have significant interaction with each other, they can be studied in an independent manner like structural damage under irradiation, fuel burn-up analysis, radiolysis, etc. However if time scales of involved phenomenon have appreciable overlaps, they should be treated in a coupled manner. This is mainly the domain of reactor kinetics studies where prompt and delayed neutron build-up and decay, temperature feedbacks, control responses, reactivity effects of fission product poisons and system response, etc. evolve in a coupled manner. In case of new generation large power reactors these aspects have become more important where neutronic decoupling due to large core dimensions, strong and possibly asymmetric reactivity feedback mechanisms, conjugate fuel and coolant heat transfer, cross-flow coolant dynamics, vessels mixing related asymmetric reactivity concerns, global and spatial control responses, spatial xenon and iodine dynamic, etc., demand a comprehensive multiphysics model for more realistic simulation. Consistent with this objective, backed up by strong computing resources, many international initiatives have been taken up during last two decades in nuclear industry. Several detailed 3-D core dynamic computer codes like NESTLE [2], DYN3-D [3], NEM [4], PRACS [5], KIKO3-D [6], and TRIKIN [7], etc. have been developed.

For best estimate analysis of reactor core nuclear transients, these models generally employ the multiphysics modeling approach shown in fig. 2, where neutron kinetics module brings out changes in reactor power and power distribution following a given reactivity actions and/or core thermal state changes. This change in power and/or power distribution leads to further core thermal state changes and so on. Thus, 3-D neutron kinetics module requires fuel temperature and coolant density distribution in the core to update the coefficients of multi group neutron diffusion equation consistent with evolving core thermal state which are obtained from fuel heat transfer and coolant transport modules as shown. The way different modules are integrated together affects significantly the efficiency of computation. In principle different physics modules exchange relevant data at pre-defined time intervals for specified set of spatial meshes in the computing domain. Therefore simulation accuracy increases if data is exchanged more frequently among the modules (large number of time meshes) and at more number of space points in the solution domain. Based on these ideas, two approaches of coupling have been conventionally adopted in coupled core modeling, in which either simple single channel core thermal hydraulic (TH) model is coupled to a full 3-D neutron kinetics module in an averaged manner or detailed multichannel core thermal hydraulic model is coupled to a full 3-D neutron kinetics module in a one to one manner. Later approach being more precise provides excellent computing accuracy at the cost of significant additional computing effort associated with excess core thermal calculations. Thus, the two coupling strategies in present coupled
kinetics codes lie at two extremes. Single channel coupling is simple and time efficient but is moderately accurate. On the other hand multichannel based coupling is quite accurate but computationally intensive. Present work aims to bridge this gap through an improved scheme which enhances the accuracy of single channel based coupled core dynamics computation significantly.

The next section of this paper describes governing equations for different modules and their numerical solution. A new coupling scheme for core multiphysics has been explained in the section Power weighted coupling scheme. Application of models and intercomparison of three coupling schemes are presented in the later sections.

MATHEMATICAL MODELS

3-D neutron kinetics

The model almost universally used in space-dependent dynamics is that of multigroup neutron diffusion theory, with coupling to the equations for the delayed neutron precursors. These equations are

\[
\frac{1}{\nu_g} \frac{\partial \phi_g}{\partial t} = \nabla D_g \nabla \phi_g (r,t) - \sum_{i}^{m} \phi_g (r,t) + \chi_d^P (1-\beta) \sum_{g}^{n_g} \gamma_{2} \phi_g (r,t) + \sum_{g}^{n_g} \sum_{i}^{n_g} \lambda_i C_i (r,t)
\]

(1)

\[
\frac{\partial C_i (r,t)}{\partial t} = \beta_i \sum_{g}^{n_g} \gamma_{2} \phi_g (r,t) - \lambda_i C_i (r,t)
\]

(2)

where \( D_g \) is the neutron diffusion coefficient of group \( g \), \( \Sigma_i \) – the removal cross-section, \( \Sigma_f \) – the fission cross-section, \( \beta \) – the delayed neutron fraction, \( \chi_d^P \) – the fraction of prompt neutron of energy \( E \), \( \nu \) – the average number of neutron released per fission, \( \lambda \) – the fraction of delayed neutron of energy \( E \), and \( \lambda_i \) and \( C_i \) are decay constant and concentration of \( i^{th} \) family delayed neutron precursor, respectively.

Approximation methods for the solution of these space-energy dependent neutron kinetics equations have been of significant interest in reactor physics since the early 1960, when a few numerical experiments [8] demonstrated the limitations of the “point-reactor” model for the analysis of the large reactors. The importance of the spatial variations of neu-
tron flux in the safety analysis of nuclear reactors depends on the fact that the “point-reactor” power predictions are not only inaccurate in many cases, but also underestimate the reactivity insertion, and therefore are non-conservative in a safety sense. However, solution of time-dependent multigroup diffusion equation present following difficulties.

(a) A very high dimensionality for realistic multigroup 3-D reactor problems, which result from complete discretization of all the independent variables namely space, time, and energy.

(b) A considerable degree of “stiffness” because of the wide spread in characteristic times.

(c) The presence of discontinuous coefficients as a result of the highly heterogeneous nature of nuclear reactor cores.

In addition to this, in real dynamics problems, especially those involving safety considerations, the coefficients in this system of partial differential equations depend upon parameters such as temperature, void, etc. which themselves depend on the neutron power level. Thus the solution of multigroup diffusion equation with spatially dependent feedback problem comprises a very large and complex system of coupled non-linear PDE. For a realistic reactor problem it is impossible to have an analytical solution but numerical solutions are attempted to various degrees of sophistication. Many methods like direct methods, finite element methods (FEM), nodal methods, modal methods, factorization methods, finite difference methods (FDM), etc., have been developed during the past four decades to solve spatial kinetics equations. These methods differ in terms of accuracy, algebraic simplicity and computational economy, e.g., FDM are simple and easy to implement but require small mesh sizes and therefore are very expensive computationally. Complete numerical scheme and step by step algorithm adopted in the present model to 3-D solve neutron diffusion equation based on improved quasi-static (IQS) approach for different geometries has been explained in detail [7, 9]. The algorithm has been validated against variety of transient benchmarks for different types of power reactors viz; VVER, PHWR, and PWR.

Core thermal hydraulics

Nuclear reactor core is comprised of many fuel assemblies and each fuel assembly consists of large number of fuel pins. To determine the thermal state of the core, the reactor core is transformed into equivalent heated channels. Mass, momentum, and energy equations of the coolant are solved for these channels. A heated channel is generally taken as a representative coolant sub-channel within a fuel assembly (fig. 3) which is assumed to receive coolant only through its bottom inlet. The fuel and clad heat conduction equations are also solved along with the coolant equations. These equations are generally coupled to coolant equations through heat transfer coefficient. Cross-sectional average coolant quantities are considered so that the problem is simplified as a lumped parameter, one dimensional (axial) problem i.e., azimuthal/radial variations of coolant quantities within the channel are ignored. In the simplest model, entire core is repre-

Figure 3. Subchannel representing equivalent core heated channel
The heat flow across the gap is through conduction, where radial/azimuthal variation within the core is much less. For large reactors, fuel assemblies which have nearly identical power distribution are grouped together. Coolant sub-channels representative of these groups form multichannel TH model of the core. These heated channels may be interconnected along the length if there is possibility of cross-flow among the channels. If this cross-flow is neglected then the multi channel model becomes the extension of single channel model with appropriate boundary conditions at inlet and outlet at all the channels. These possible TH models are explained in fig. 4.

Fuel heat transfer in the radial pin is governed by time dependent heat conduction equation. Time dependent radial temperature distribution in the fuel pin is governed by conduction equation in cylindrical geometry

\[ \frac{1}{r} \frac{\partial}{\partial r} \left[ r k(T) \frac{\partial T}{\partial r} \right] + q''(T) = \rho(T)C_p(T) \frac{\partial T}{\partial t} \]  

(3)

where all symbols carry their usual meaning.

The assumptions involved in this equation are:

(a) Axial and azimuthal conduction is negligible.

(b) Volumetric heat generation \( q'' \) is uniformly distributed over the fuel pellet cross-section, gamma heat generation in the gas gap and the cladding is ignored.

(c) Thermal conductivity in the fuel pellet and the cladding depends on temperature, burn up and porosity.

(d) Volumetric heat capacity and density in fuel pellet and cladding are temperature dependent.

(e) Thermal conductance in the gas gap is a function of temperature and burn-up.

Boundary condition which are applied to the heat conduction equation are,

- Adiabatic boundary condition is applied at the inner radius of fuel pin

\[ -k_f(T) \frac{\partial T}{\partial r} \bigg|_{r_i} = 0 \]  

(4)

- The heat flow across the gap is through conduction, convection, and radiation from fuel surface to clad. All these modes of heat transfer are clubbed together in a single parameter known as gap conductance \( h_{\text{gap}} \), i.e.

\[ -k_f(T) \frac{\partial T}{\partial r} \bigg|_{r_i} = h_{\text{gap}}(T_{ci} - T_{in}) \]  

(5)

- The heat flow from the clad outer surface is through coolant forced convection

\[ -k_c(T) \frac{\partial T}{\partial r} \bigg|_{r_o} = h_n(T_{in} - T_n) \]  

(6)

Axial coolant transport is governed by the one dimensional solution of mass, momentum and energy equations for coolant. Properties of coolant are assumed to be constant at every axial mesh i.e., radial or azimuthal variation in the coolant properties is ignored. In all the PWR, there exists a small radial pressure gradient at the core inlet, which vanishes slowly at the core exit and practically there is no radial pressure gradient at the core exit. Thus compared to axial pressure drop, which is driving force for the coolant flow, the radial pressure drop is negligible. This feature of PWR facilitates simplification of coolant modeling, i.e., radial coolant flow can be ignored in the analysis for normal coolant flow condition. Therefore in the existing coolant model, radial coolant motion is ignored and it is assumed that there is no cross flow among the assemblies. This assumption simplifies the coolant problem significantly and the core thermal hydraulics model becomes a problem of multi channels, with channel connected at the inlet and exit plane only. This has been explained in fig. 5.

Solution of mass, momentum, and energy conservation equations in each channel will give the desired coolant properties along the channel. Mass, momentum and energy conservation equations for the single phase fluid in the sub cooled portion of the channel are given in the following:

- Continuity

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (PA_z)}{\partial z} = 0 \]  

(7)

- Momentum

\[ \frac{\partial m}{\partial t} + \frac{\partial (PA_z)}{\partial z} = \frac{P A_z G^2}{\rho g A_z \cos \theta + \frac{f_s G^2}{2 \rho D_w A_z}} \]  

(8)
– Coupled to 3-D neutron kinetics model in a detailed [6]. Multichannel based core TH model has been explained in detail [6]. Multichannel based core TH model has been coupled to 3-D neutron kinetics model in a conventional approach for best analysis of variety of core dynamics scenarios. Computational flow chart of the coupled model has been explained in fig. 6. Complete coupled dynamics model (TRIKIN) has been validated against a series of international benchmarks [10-13] specifically designed for such coupled core dynamics models. For these validations, core TH model based on extensive multichannel simulation was used, which has been found quite expensive computationally. A few improvements in the core dynamics modeling to enhance computing efficiency are presented in the next section.

POWER WEIGHTED COUPLING SCHEME

In case of light water reactors, under normal coolant conditions radial pressure drop among the coolant channels is negligible therefore cross-flow of coolant among various coolant channels can be ignored. This simplifies core TH to one dimensional model, and therefore for most of the cases reactor core thermal modeling is based on equivalent fuel pin simulation where only radial conduction of heat in the fuel pin and axial coolant transport are considered. A very elementary approach to model core TH is to simulate reactor core by single average channel which is used for reactivity feedbacks in all fuel assemblies. Though this single channel simulation minimizes TH computational bulk significantly, averaging of all channels renders following disadvantage.

– Due to average channel based reactivity feedback applied to high power fuel assemblies, power overshoots in these fuel assemblies are under attenuated due to lower feedback temperatures considered.

– Similarly low power fuel assemblies unnecessary get higher magnitude of fuel and coolant temperature correction.

– Though overall effect of these two opposite errors leads to reasonably accurate total core reactivity and temperature calculations, 3-D distribution of power and temperatures are not the most realistic and accurate, i.e. it results in underestimated 3-D peaking in the core, which is neither realistic, nor conservative.

A power reactor core consists of large number of fuel assemblies or coolant channels with different levels of power and different axial power profile, accurate 3-D core thermal state estimation requires as many TH solvers as many coolant channels. In strict sense a core TH model with as many channels as number of fuel assemblies will be the most accurate for this purpose but it will involve high computational bulk. One approach to avoid simulation of all core channels is clubbing of coolant channels of identical power and/or power profile and therefore reducing the number of coolant channels to be analyzed. Though this approach still does not avoid requirement of multichannel core TH simulation, which is a significant computational burden. In summary, the two common approaches to model core TH in coupled 3-D core dynamics model are:

– Core single average channel TH simulation: Computationally economical but not very realistic particularly in 3-D predictions.

– Core multichannel TH simulation: Very accurate, more realistic but computationally expensive.

If one can achieve best estimate results with mere limited/single channel simulations, computing efficiency can be significantly improved. An effort has been made in the present work to develop a new coupling scheme which can serve this purpose. This scheme lies in between single channel and multichannel simulation [14]. Core TH simulation is essentially based on single channel option but reactivity feedbacks are not uniformly applied to all fuel assemblies. Philosophy behind this coupling scheme is very simple and it can be understood from 2-D, one sixth core cartogram of a typical VVER 1000 core, shown in fig. 7. Core map is corresponding to steady state cycle at fresh core.

In an evolving transient, if $\Delta T_f$ and $\Delta T_c$ are rise in fuel and coolant temperature, respectively, obtained from an average single channel simulation, and $\gamma$ is 2-D peaking factor at any fuel assembly at a given axial location, then reactivity feedback at that fuel assembly will be applied based on $\gamma \Delta T_f$ and $\gamma \Delta T_c$. Thus, reactivity feedback on an average pin will be based on $\Delta T_f$ and $\Delta T_c$ and a fuel assembly with higher power compared to average FA will have higher reactivity feedback whereas fuel assembly with lower power compared to average FA will have lower reactivity feedback. Approach essentially assumes that...
Figure 6. Computational flow chart for coupled core dynamics computing in TRIKIN code
 thermo-physical properties like heat capacity, thermal conductivity, gap conductance, etc. of all fuel assemblies are same. It also assumed identical coolant boundary conditions for all heated channels. These assumptions may not always be true. To demonstrate the performance of present coupling scheme, a reactivity initiated transient, Uncontrolled withdrawal of a control rod in VVER-1000 core [15] has been analyzed. Fresh core condition has been considered. Withdrawal of control rod inserts positive reactivity in the core as well as disturbs neutron flux shape. As a conservative measure withdrawal of most effective rod is considered. Problem has been analyzed using three simulations namely:

- 3-D kinetics with single channel thermal hydraulics model with average feedback in all fuel assemblies at every axial layer,
- 3-D kinetics with multi channel TH model. Each fuel assembly is simulated as one heated channel, so total 163 channels have been simulated. This simulation is termed as “best estimate” simulation, and
- 3-D kinetics with single channel TH model with power weighted feedback at all fuel assemblies.

Results of transients with all three simulations are shown in figs. 8, 9, and 10. It can be realized that with single channel and multi channel simulation results differ significantly. However with power weighted feedback option, results tend to come closer to best estimate results, though it take almost half computing time than that of multichannel 3-D feedback option. This demonstrates strength of power weighted coupling scheme to generate best estimate results with reduced thermal hydraulic computing effort for reactivity initiated transients.

LIMITATION

The excellent results obtained from power weighted coupling presented in the previous section are for first cycle fresh core conditions where none of the fuel assembly was irradiated. This situation fairly ensures that thermo-physical properties like heat capacity, thermal conductivity, gap conductance, etc. of all fuel assemblies in the core are identical. Therefore assumption of power proportional temperature rise in the proposed power weight coupling scheme holds good in this case. However it is well known that with irradiation, thermo-physical properties of fuel change
appreciably e.g., thermal conductivity of UO₂ reduces with burn-up [16] and gap conductance of a PWR fuel pin improves with burn-up [17]. Therefore linear and proportional assumption of power weighted coupling scheme may not hold good in a reactor core condition where two fuel assemblies of different burn-up generates same power, i.e., temperatures of two differently irradiated fuel assemblies having same power will be different. This effect has not been considered in the present model. A detailed generation of data bank from pre-calculated fuel and coolant temperature scenarios for different levels of irradiations may be used to implement appropriate correction to assembly power factors (γ) to account burn-up and coolant flow distribution effects. This study is in progress.

SUMMARY

Analysis of reactivity initiated transients at higher power requires accurate estimation of evolving 3-D core thermal state. Multichannel core thermal hydraulic model, being most accurate option for this purpose is computationally very expensive. A novel approach of power weighted coupling between core neutronics and TH presented in this work reduces the bulk of core thermal calculations to a significant extent without compromising accuracy of computation. Proposed coupling scheme involves solution of average coolant channel but employs feedback correction based on the power of respective fuel assemblies. This ensures that fuel assemblies of different power levels get different feedback exactly like multichannel simulation and therefore 3-D core dynamics predictions improve appreciably. However power weighted coupling scheme assume identical coolant flow and uniform thermo-physical properties of different fuel assemblies. This assumption holds good for fresh core for which excellent results for dynamic simulation have been obtained, though this may not be valid for irradiated core condition, as burnup dependence of core state has not been considered in the present model. Extension of present work in regard to these minor improvements is in progress.

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AUTHOR CONTRIBUTIONS

K. Obaidurrahman has played a central role in development of AERB coupled 3-D kinetics code TRIKIN. He has engineered a few notable improvements in the coupled core dynamics modelling of large power reactors. Power weighted coupling presented in this paper is one of them. A. J. Gaikwad is Director of Nuclear Safety Analysis Division. He is leading a team of engineers in nuclear safety analysis and research at Atomic Energy Regulatory Board, India.

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КА ЕФИКАСНОМ МУЛТИФИЗИЧКОМ МОДЕЛУ ДИНАМИКЕ НУКЛЕАРНИХ РЕАКТОРА

Доступност брзих рачунара данас омогућава дубље моделовање сложених инжењерских система који укључују јаке мултифизичке интеракције. Ово мултифизичко моделовање веома је потребно у студијама сигурности и нуклерних реактора, у којима се чине напори широм света да се на једном месту комбинују знања из свих повезаних дисциплина да би се оствариле најреалније симулације укључених феномена. У том працву, спрегнуто моделовање кинетике неутрона у нуклеарном реактору, преноса топлоте горива и транспорта хладиоца, представља данас уобичајену практику у анализи прелазних стања реакторског језгра. Међутим, оптимизација између тачности моделовања и економије прорачуна увек је била изазован задача, са циљем да се обезбеди адекватан степен пузданости у тако обимним нумеричким поступцима. Сложено моделовање реакторског језгра подразумева процену развијања термичког стања тродимензионалног језгра, што за узва р тражи скуп детаљни термохи драулички модел вишеканалног језгра. Нови приступ спрезања пондерисане снаге између физике неутрона и термохи драулике језгра, представљен у овом раду, има за циљ да у значајној мери смањи обим термичких прорачуна при моделовању динамике језгра без угрожавања тачности израчунавања. Модел спрегнутог језгра потврђен је на низу међународних стандардних узора. Тачност и ефикасност рачунања предложеног мултифизичког модела приказане су анализом прелазних стања иницираних реакционарној.

Кључне речи: мултифизичко моделовање, TRIKIN, пространо-временска кинетика, термохи драулика језгра, спрезање динамика језгра, пондерисане снаге