INL/EXT-14-33102

Developing Fully Coupled Subchannel Model in RELAP-7

Hongbin Zhang
Ling Zou
Haihua Zhao
Richard Martineau

September 2014

U.S. Department of Energy
Office of Nuclear Energy

INL/EXT-14-33102

Developing Fully Coupled Subchannel Model in RELAP-7

Hongbin Zhang
Ling Zou
Haihua Zhao
Richard Martineau

September 2014

Idaho National Laboratory
Originating Organization NS&T
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Contents

Figures

Tables

Summary

The traditional approach of using a system safety analysis code such as RELAP-5 to analyze a reactor core would normally use one or a few flow channels along with heat structures to represent a number of fuel assemblies in a region of a reactor core or even the entire core. This kind of homogenized analysis approach would render large uncertainties for certain applications with which more detailed analyses of fuel rod bundles are required such as the minimum DNBR (Departure from Nucleate Boiling Ratio) analysis in a hot channel. Instead, the subchannel codes such as COBRA, VIPER etc. are widely used for the hot channel analyses. The subchannel method preserves the geometry of a fuel rod bundle and the resulting equations contain the geometric features of the rod bundle.

In the traditional safety analysis approach, the system thermal hydraulics analysis and the hot channel analysis are performed separately by independent codes and the results from one code are passed to another code as the boundary conditions. Efforts have been made to couple the system analysis codes and subchannel analysis codes together to remove the inconsistent assumptions and models used between different codes associated with the data transfer approach. However, the operator-splitting approach was normally used to carry out the coupling.

In the RELAP-7 code development, we have launched an effort to develop the subchannel analysis capability in a fully coupled manner with the reactor system analysis capability. The fully coupled analysis capability would eliminate errors associated with using the operator-splitting approach. Other advantages of such an approach include: 1). Consistent models, assumptions and equation sets between the subchannel module and the system analysis module are used, 2). Consistent numerical solvers are used, 3). Consistent closure models are used. All these would make it easier to perform verification, validation and uncertainty quantification. In addition, users only need to maintain one code rather two separate codes. This would reduce the costs of code maintenance for the users. This document summarizes the single phase flow subchannel model implemented into the RELAP-7 code.

1 Introduction

The traditional approach of using a system safety analysis code such as RELAP-5 [1] to analyze a reactor core would normally use one or a few flow channels along with heat structures to represent a number of fuel assemblies in a region of a reactor core or even the entire core. This kind of homogenized analysis approach, as illustrated in Figure 1, would render large uncertainties for certain applications with which more detailed analyses of fuel rod bundles are required such as the minimum DNBR (Departure from Nucleate Boiling Ratio) analysis in a hot channel. The fully 3-D computational fluid dynamics (CFD) codes are not generally used for engineering analyses of the hot channel due to their prohibitive computational expenses. Instead, a variety of averaging methods are applied to the navier-stokes equations so that a more convinent system of equations is obtained. Consequently, the subchannel analysis method [2] has been developed for such purpose and the subchannel codes such as COBRA [3] etc. are widely used for hot channel analyses. The subchannel method preserves the geometry of a fuel rod bundle and the resulting equations contain the geometric features of the rod bundle. Additional to the primary fluids flow in the axial flow direction, the subchannel method also considers the transverse mass flows in the description of the flow field in a rod array. The axial coolant flow is parallel to the rod surfaces. The flow is denoted as positive for vertical up flow in the rod array. The transverse flows are carried out by the velocity components normal to the primary flow direction and are responsible for distribution of the coolant between the subchannels. It is postulated that two mechanisms cause the lateral flows [4]. The first one is the lateral pressure gradients between the adjacent subchannels. This results in the diversion cross flow with net mass exchange between the involved subchannels. The second mechanism is the turbulent mixing that results from the eddy transport in the axial flow between adjacent subchannels. Turbulent mixing results in no net change of mass between the subchannels for single phase flow. However, the turbulent eddies carry with them momentum and energy whcih are exchanged to the involved subchannels. For two phase flow, turbulent mixing will result in net change of mass between the adjacent subchannels due to the disparate densities of the liquid and vapor phases. The transverse crossflows are generally small compared to the axial mass flow rate in the absence of major changes in flow channel geometry such as that due to flow blockage by debris during normal operations or fuel rod deformation under severe accident conditions. Geometry variations and non-uniform changes in fluid density can establish transverse pressure gradients between sub channels. Geometry variations include fuel rod bowing and swelling and the design features such as mixing vane spacer grids introduce variations in the subchannel flow area or the axial pressure gradient. The fluid density is most greatly affected by the presence of boiling. The

resulting difference will effect the crossflow between subchannels. The diversion crossflow rate is determined by the lateral momentum balance equation. Unlike the diversion crossflow, the turbulent mixing is not obtained from the basic fluid flow equations. An empirical description is used instead.

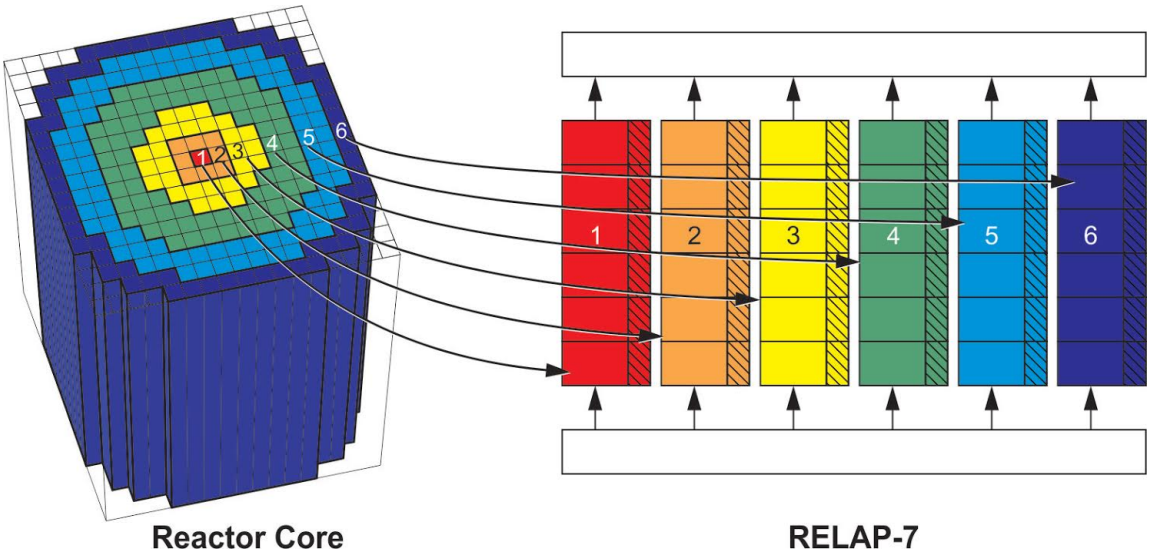

Figure 1. Illustration of a reactor core analysis using a system analysis code

In the traditional safety analysis approach, the system thermal hydraulics analysis and the hot channel analysis are performed separately by independent codes and the results on one code are passed to another code as boundary conditions. Efforts have been made to couple the system analysis codes and subchannel analysis codes together to remove the inconsistent assumptions and models used between different codes associated with the data transfer approach. The MARS code developed at KAERI exemplifies such efforts [5]. The MARS code coupled the RELAP-5 code for 1-D system analysis and the COBRA-TF code for the 3-D reactor vessel thermal hydraulic analysis and subchannel analysis. However, the operator-splitting approach was used to carry out the coupling within the MARS code. In the RELAP-7 code development [6], we have launched an effort to develop the subchannel analysis capability in a fully coupled manner with the reactor system analysis capability. The fully coupled analysis capability would eliminate the errors associated with using the operator-splitting approach. Other advantages of such an approach include: 1).

Consistent models, assumptions and equation sets between the subchannel module and the system analysis module are used, 2). Consistent numerical solvers are used, 3). Consistent closure models are used. All these would make it easier to perform verification, validation and uncertainty quantification. In addition, users only need to maintain one code rather two separate codes. This would reduce the costs of code maintenance for the users.

In this document, the subchannel analysis capability for single-phase flow implemented in a fully coupled manner within the RELAP-7 code is discussed. The implementation of two-phase flow subchannel model into RELAP-7 is left to future work. The RELAP-7 code is the next generation reactor system safety analysis code being developed at the Idaho National Laboratory. RELAP-7 will become the main reactor systems toolkit for the Risk-Informed Safety Margin Characterization Pathway of the U.S. DOE Light Water Reactor Sustainability Program and the next generation tool in the RELAP reactor safety/systems analysis application series. The code is being developed based on INL's modern scientific software development framework - MOOSE (the Multi-Physics Object-Oriented Simulation Environment) [7]. There are over 20 MOOSE based modeling and simulation tools being developed. These include the fuel performance analysis code BISON and neutron kinetics code RattleSnake. MOOSE allows the easy coupling of RELAP-7/BISON/RattleSnake and provides the nuclear power plant safety analysis tool kit.

2 Conservation Equations of the Single Phase Flow Subchannel Model

The conservation equations of the single phase flow subchannel model are presented in this section. Four fluid flow equations are described. These include: 1). The conservation of mass in the axial direction, 2). The conservation of momentum in the axial direction, 3). The conservation of energy in the axial direction, 4). The conservation of momentum in the lateral flow direction. Figure 2 provides a schematic illustration of the subchannel model.

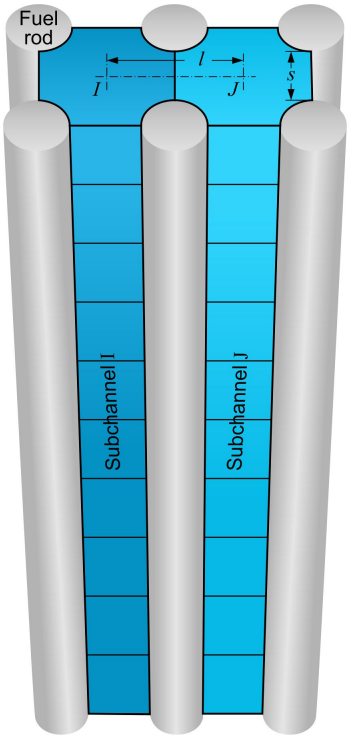

Figure 2. Illustration of the subchannel model

The conservation of mass for the subchannel i is the following:

$$\frac{\partial(\rho A)_i}{\partial t} + \frac{\partial(\rho u A)_i}{\partial x} + \sum_{j \in K(i)} w_{i,j} = 0 \tag{1}$$

where i is the index of subchannel i. A_i is the flow area for subchannel i. ρ and u denote the fluid density and velocity respectively. j is the index of subchannel j which is adjacent to subchannel i. $K(i)$ is the set of lateral interfaces (gaps) on the boundary of subchannel i. $w_{i,j} = \rho u_l s_k$ is the mass flow rate per unit length in the lateral direction across the gap k between sub channels i and j. u_l is the fluid velocity in the lateral direction and s_k is the width of gap k.

The conservation of axial momentum for subchannel i is the following:

$$\frac{\partial(\rho u A)_i}{\partial t} + \frac{\partial((\rho u A)_i u_i)}{\partial x} + \frac{\partial(PA)_i}{\partial x} + (\rho A)_i g + \frac{1}{2}\frac{f_i}{D_{h,i}}(\rho u A)_i |u_i| + \sum_{j \in K(i)} w_{i,j} u^* + \sum_{j \in K(i)} w^t_{i,j}(u_i - u_j) = 0 \tag{2}$$

where P_i is the pressure in subchannel i and f_i is the wall friction coefficient. $D_{h,i}$ is the subchannel hydraulic diameter. K'_i is the form loss coefficient. u^* is the lateral donor axial velocity at gap face k. If the flow is into the subchannel i from the subchannel j, then $u^* = u_j$, and conversely, $u^* = u_i$. $w^t_{i,j}$ is the turbulent mixing mass flow rate per unit length in the lateral direction at gap face k. $w^t_{i,j}$ is the fluctuating crossflow which is related to the eddy diffusivity ϵ_t, by $w^t_{i,j} = \epsilon_t \rho_i \frac{s_k}{l_k}$. In RELAP-7 implementation, $w^t_{i,j}$ is calculated as:

$$w^t_{i,j} = \beta s_k \bar{G} \tag{3}$$

where β is the turbulent mixing parameter and $\bar{G}$ is the average mass flux between the adjacent subchannels i and j, i.e. $\bar{G} = \frac{1}{2}((\rho u)_i + (\rho u)_j)$.

The conservation of lateral momentum for the cross flow between subchannels i and j is the following:

$$\frac{\partial w_{i,j}}{\partial t} + \frac{\partial w_{i,j}\bar{u}}{\partial x} - \frac{s_k}{l_k}(P_i - P_j) + \frac{1}{2}\frac{s_k}{l_k} K_G \frac{|w_{i,j}|}{\bar{\rho} s_k^2} w_{i,j} = 0 \tag{4}$$

where $\bar{u} = \frac{1}{2}(u_i + u_j)$ and $\bar{\rho} = \frac{1}{2}(\rho_i + \rho_j)$. s_k is the width of lateral gap k. l_k is the distance between centroids of subchannels i and j. K_G is the lateral loss coefficient which accounts for the friction and form pressure loss caused by area change.

The conservation of energy for subchannel i is the following:

$$\frac{\partial(\rho EA)_i}{\partial t} + \frac{\partial((\rho HA)_i u_i)}{\partial x} + \sum_{j\in K(i)} w_{i,j} H^* + \sum_{j\in K(i)} w^t_{i,j}(H_i - H_j) + (\rho A)_i u_i g + \sum_{r\in M(i)} \phi_{i,r} P_H h_{w,r}(T_i - T_{w,r}) = 0 \tag{5}$$

where E is the fluid total energy and $H = E + \frac{P}{\rho}$ is the total enthalpy. H^* is the donor total enthalpy. P_H is the total heated perimeter and $\phi_{i,r}$ is the perimeter fraction associated with the subchannel i. $M(i)$ is the set of fuel rods that surround the subchannel i. $h_{w,r}$ is the convective heat transfer coefficient. T_i is the fluids temperature in subchannel i and $T_{w,r}$ is the fuel rod wall temperature which is obtained from the solution of the heat conduction in fuel rods described in the following:

$$\rho_s C_p \frac{\partial T_s}{\partial t} - \nabla \cdot (k \nabla T_s) - q''' = 0 \tag{6}$$

where ρ_s, C_p and k are the density, specific heat capacity, and thermal conductivity of the solid materials respectively. T_s is the temperature distribution whthin the fuel rods and q''' is the heat generation rate per unit volume.

3 Specialized Forms of the Conservation Equations of the Single Phase Flow Subchannel Model for RELAP-7 Implementation

Recall that the mass flow rate per unit length in the lateral direction $w_{i,j} = \rho u_l s_k$ and if we define the mass flux in the lateral direction as $G_{i,j} = \rho u_l$ then

$$w_{i,j} = G_{i,j} s_k \tag{7}$$

The turbulent mixing mass flow rate is calculated as

$$w^t_{i,j} = \beta s_k \bar{G}, \tag{8}$$

and β is the turbulent mixing coefficient. In RELAP-7 implementation, the turbulent mixing flow rate is calculated using the correlation provided by Rogers and Tahir [8],

$$w^t_{i,j} = 0.005 \mu Re_i^{0.9} (\frac{s_k}{d})^{0.106} \tag{9}$$

where μ is the liquid viscosity, Re_i is the axial Reybolds number in the ith subchannel, and d is the fuel rod diameter. In this implementation, it is assumed that the rod geometry is square only and the flow is limited to turbulent flow only. Hence the turbulent mixing coefficient β is the following:

$$\beta = 0.005 \mu Re_i^{0.9} (\frac{s_k}{d})^{0.106} / (s_k \bar{G}) \tag{10}$$

The mass conservation equation can be written as the following:

$$\frac{\partial (\rho A)_i}{\partial t} + \frac{\partial (\rho u A)_i}{\partial x} + \sum_{j \in K(i)} G_{i,j} s_k = 0 \tag{11}$$

The axial momentum equation becomes the following:

$$\begin{aligned} \frac{\partial (\rho u A)_i}{\partial t} + \frac{\partial ((\rho u A)_i u_i)}{\partial x} + \frac{\partial (P A)_i}{\partial x} + (\rho A)_i g + \frac{1}{2} \frac{f_i}{D_{h,i}} (\rho u A)_i |u_i| \\ + \sum_{j \in K(i)} G_{i,j} s_k u^* + \sum_{j \in K(i)} \beta s_k \bar{G} (u_i - u_j) = 0 \end{aligned} \tag{12}$$

The energy equation becomes the following:

$$\begin{aligned}\frac{\partial(\rho EA)_i}{\partial t}+\frac{\partial((\rho HA)_i u_i)}{\partial x}+\sum_{j\in K(i)} G_{i,j}s_k H^*+\sum_{j\in K(i)}\beta s_k\bar{G}(H_i-H_j)\\ +(\rho A)_i u_i g+\sum_{r\in M(i)}\phi_{i,r}P_H h_w a_w(T_i-T_{w,r})A_i=0\end{aligned} \tag{13}$$

The conduction term in the fluids has been ignored.

The lateral momentum equation becomes the following:

$$A_{lat}\frac{\partial G_{i,j}}{\partial t}+A_{lat}\frac{\partial G_{i,j}\bar{u}}{\partial x}-\frac{A_{lat}}{l_k}(P_i-P_j)+\frac{1}{2}\frac{A_{lat}}{l_k}K_G\frac{G_{i,j}|G_{i,j}|}{\bar{\rho}}=0 \tag{14}$$

where $\bar{u}=0.5(u_i+u_j)$, $\bar{\rho}=0.5(\rho_i+\rho_j)$ and $A_{lat}=s_k\Delta x$ is the lateral cross flow area.

In RELAP-7, the conservation equations of mass, axial momentum and energy are solved using CFEM method, however the lateral momentum equation will be solved using the finite difference method. Writing the above equation in the finite difference form yields the following:

$$\begin{aligned}A_{lat}\frac{G_{i,j}^{n+1,m}-G_{i,j}^{n,m}}{\Delta t}+A_{lat}\frac{\bar{u}^{n+1,m}G_{i,j}^{n+1,m}-\bar{u}^{n+1,m-1}G_{i,j}^{n+1,m-1}}{\Delta x}\\ -\frac{A_{lat}}{l_k}(P_i^{n+1,m}-P_j^{n+1,m})+\frac{1}{2}\frac{A_{lat}}{l_k}K_G\frac{G_{i,j}^{n+1,m}|G_{i,j}^{n+1,m}|}{\bar{\rho}^{n+1,m}}=0\end{aligned} \tag{15}$$

where n indicates the time step, m is the spatial element index for subchannel i.

4 Numerical Methods

The RELAP-7 code solves coupled multi-physics problems using the Jacobian-Free Newton Krylov (JFNK) approach via the MOOSE framework. The JFNK method is a fully-coupled, multi-level method for solving large nonlinear equation systems. In general, it consists of at least two levels: the outer Newton loop for the nonlinear solve and the inner Krylov loop for the linear systems of equations associated to Newton iteration. The JFNK method has become an increasingly popular option for solving large nonlinear equation systems arising from multi-physics problems over the last 20 years.

In what follows, we give a brief description of the JFNK method as it applies to the subchannel model in RELAP-7. The field equations (11), (12), (13) and the conduction equation (6) are discretized using the continuous finite element method (FEM). These FEM discretized equations as well as the finite differenced lateral momentum equation (15) form a system of implicitly discretized nonlinear equations

$$\vec{F}(\vec{u}) = \vec{0} \tag{16}$$

where $\vec{F}$ represents the nonlinear equation system and $\vec{u}$ is the solution vector. Newton's method requires an initial guess, $\vec{u}^0$, to start the iteration process. For the transient problems of interest here, the solution at a previous time step is generally used as the initial guess for the method. At the k^{th} iteration, we define the residual vector

$$\vec{r}^k \equiv \vec{F}(\vec{u}^k) \tag{17}$$

Clearly if $\vec{u}^k$ satisfies (16) *exactly*, the k^{th} residual will be zero. To update the solution vector, the following equation is solved for the update vector, $\delta\vec{u}^{k+1}$:

$$J(\vec{u}^k)\delta\vec{u}^{k+1} = -\vec{r}^k \tag{18}$$

where $J(\vec{u}^k)$ is the Jacobian matrix evaluated at $\vec{u}^k$. In index notation, we have

$$J_{ij} \equiv \frac{\partial F_i}{\partial u_j} \tag{19}$$

After $\delta\vec{u}^{k+1}$ is obtained, the $(k+1)^{st}$ solution iterate is computed by

$$\vec{u}^{k+1} = \vec{u}^k + \delta\vec{u}^{k+1} \tag{20}$$

The Newton iteration is terminated when one of the following conditions is met:

1. The residual vector norm, $|\vec{r}^k|$, is sufficiently small.

2. The relative residual vector norm $\frac{|\vec{r}^k|}{|\vec{r}^0|}$ is sufficiently small.

3. The step size norm, $|\delta\vec{u}^{k+1}|$ is sufficiently small.

Note that (18) represents a large linear system of equations. In the JFNK method, we need not explicitly form the matrix J: only its action on a vector (via matrix-vector product) is required. Effective preconditioning is generally required for Krylov subspace methods to be efficient, i.e., for the method to converge in a reasonable number of iterations. A preconditioned version of equation (18) can be expressed as (using right preconditioning as an example),

$$J^k P^{-1} \left(P\delta\vec{u}^{k+1} \right) = -\vec{r}^k \tag{21}$$

where P is the preconditioning matrix. In our current approach, an analytical Jacobian matrix is computed according to (19), and passed to the underlying numerical solver library as the matrix P for preconditioning purposes. Appendix A includes the Jacobian terms for the source terms in the subchannel model.

5 Benchmark Results

The subchannel model in RELAP-7 has been used to simulat the GE nine-rod bundle experiment [9] for the single phase flow test cases. Four tests were made at room temperature and at 1000 psi (6.895 MPa) for single phase flow. The mass fluxes at the exit of one corner, one side and one center subchannel were measured. Figure 3 provides a schematic illustration of the GE nine-rod bundle eperiment.

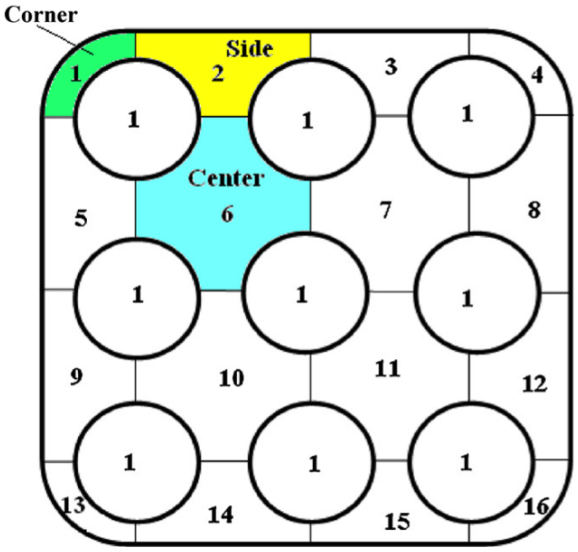

Figure 3. Illustration of the GE nine-rod bundle experiment

Two of the four single phase test cases, 1C and 1D as labelled in Ref. [9], were simulated with the RELAP-7 code. Tables 1 and 2 show the comparisons of the measured versus the calculated mass fluxes for these two test cases respectively. The results have shown that the subchannel model in the RELAP-7 code provided reasonable prediction of the mass fluxes for these two test cases respectively. However, a relatively large discrepancy between the measured mass flux and the RELAP-7 calculated mass flux is observed at the corner subchannel. Since the RELAP-7 code does not have the model to account for the spacer grid loss yet, the wall friction coefficients provided in Ref. [9] were used in the RELAP-7 calculations to match the pressure drop for the rod bundle. It is expected that the difference between the measured versus the predicted mass fluxes will decrease once the appropriate spacer grid loss model is implemented.

Table 1. Measured versus RELAP-7 Predicted Mass Fluxes for Test Case 1C

Test Case 1C	Corner ($kg/m^2 \cdot s$)	Side ($kg/m^2 \cdot s$)	Center ($kg/m^2 \cdot s$)
Measured	950.72	1273.50	1559.66
Predicted	1007.26	1276.24	1540.56
Percent Difference	5.95	0.22	-1.22

Table 2. Measured versus RELAP-7 Predicted Mass Fluxes for Test Case 1D

Test Case 1D	Corner ($kg/m^2 \cdot s$)	Side ($kg/m^2 \cdot s$)	Center ($kg/m^2 \cdot s$)
Measured	1485.07	1954.33	2292.03
Predicted	1513.96	1922.26	2324.11
Percent Difference	1.95	-1.64	1.40

6 Summary and Future Work

The single phase flow subchannel model has been implemented into the next generation reactor system safety analysis code RELAP-7. Numerical benchmark results have shown that the subchannel model in RELAP-7 gave reasonable results. The future work includes extending the fully coupled subchannel analysis capability in the RELAP-7 code to two-phase flow models.

A Residuals and Jacobians of the Source Terms

Following are the residuals and their associated Jacobian terms resulted from the source terms present in the mass, momentum and energy equations of the subchannel model in RELAP-7. The residuals for the neighbor nodes are the opposite of those for the target nodes. To facilitate the derivation of the Jacobian tersm, we define $U_0 = \rho A$, $U_1 = \rho u A$, $U_2 = \rho u E A$ and $U_3 = G_{i,j}$. It is noted that in the RELAP-7 code implementation, $U_3 = G_{i,j}$ is vector with $j = 1, ..., K(i)$.

A.1 Conservation of Mass

The following is the source term in the conservation of mass residual:

$$Sos = G_{i,j} s_k = U_3 s_k \tag{22}$$

Its Jacobian is the following:

$$\frac{\partial Sos}{\partial U_3} = \frac{\partial Sos}{\partial G_{i,j}} = s_k \tag{23}$$

A.2 Conservation of Axial Momentum

Lateral Convection Term

$$Sos = G_{i,j} s_k u^* = (\rho u_l) s_k u^* = U_3 s_k u^* \tag{24}$$

The Jacobian terms are the following:

if $G_{i,j} > 0$ then $u^* = u_i = \frac{U_{1,i}}{U_{0,i}}$ and the residual term becomes:

$$Sos = G_{i,j} s_k u_i = U_3 s_k \frac{U_{1,i}}{U_{0,i}} \tag{25}$$

The Jacobian terms are the following:

$$\frac{\partial Sos}{\partial U_{0,i}} = \frac{\partial Sos}{\partial (\rho A)_i} = -U_3 s_k \frac{U_{1,i}}{U_{0,i}^2} = -G_{i,j} s_k \frac{(\rho u A)_i}{(\rho A)_i^2} \tag{26}$$

$$\frac{\partial Sos}{\partial U_{1,i}} = \frac{\partial Sos}{\partial (\rho u A)_i} = U_3 s_k \frac{1}{U_{0,i}} = G_{i,j} s_k \frac{1}{(\rho A)_i} \tag{27}$$

$$\frac{\partial Sos}{\partial U_3} = \frac{\partial Sos}{\partial G_{i,j}} = s_k \frac{U_{1,i}}{U_{0,i}} = s_k \frac{(\rho u A)_i}{(\rho A)_i} \tag{28}$$

Conversely, if $G_{i,j} < 0$ then then $u^* = u_j = \frac{U_{1,j}}{U_{0,j}}$ and the residual term becomes:

$$Sos = G_{i,j} s_k u_j = U_3 s_k \frac{U_{1,j}}{U_{0,j}} \tag{29}$$

The Jacobian terms are the following:

$$\frac{\partial Sos}{\partial U_{0,j}} = \frac{\partial Sos}{\partial (\rho A)_j} = -U_3 s_k \frac{U_{1,j}}{U_{0,j}^2} = -G_{i,j} s_k \frac{(\rho u A)_j}{(\rho A)_j^2} \tag{30}$$

$$\frac{\partial Sos}{\partial U_{1,j}} = \frac{\partial Sos}{\partial (\rho u A)_j} = U_3 s_k \frac{1}{U_{0,j}} = G_{i,j} s_k \frac{1}{(\rho A)_j} \tag{31}$$

$$\frac{\partial Sos}{\partial U_3} = \frac{\partial Sos}{\partial G_{i,j}} = s_k \frac{U_{1,j}}{U_{0,j}} = s_k \frac{(\rho u A)_j}{(\rho A)_j} \tag{32}$$

Turbulent Momentum Exchange Term

$$Sos = \beta s_k \bar{G}(u_i - u_j) = w_{ij}^t (u_i - u_j) = w_{i,j}^t (\frac{U_{1,i}}{U_{0,i}} - \frac{U_{1,j}}{U_{0,j}}) \tag{33}$$

The Jacobian terms are the following:

$$\frac{\partial Sos}{\partial U_{0,i}} = \frac{\partial Sos}{\partial (\rho A)_i} = -w_{i,j}^t \frac{U_{1,i}}{U_{0,i}^2} = -w_{ij}^t \frac{(\rho u A)_i}{(\rho A)_i^2} \tag{34}$$

$$\frac{\partial Sos}{\partial U_{1,i}} = \frac{\partial Sos}{\partial (\rho u A)_i} = w_{ij}^t \frac{1}{(\rho A)_i} \tag{35}$$

$$\frac{\partial Sos}{\partial U_{0,j}} = \frac{\partial Sos}{\partial (\rho A)_j} = w_{ij}^t \frac{(\rho u A)_j}{(\rho A)_j^2} \tag{36}$$

$$\frac{\partial Sos}{\partial U_{1,j}} = \frac{\partial Sos}{\partial (\rho u A)_j} = -w_{ij}^t \frac{1}{(\rho A)_j} \tag{37}$$

A.3 Conservation of Lateral Momentum

The following constraints make up the entire residuals for the conservation of lateral momentum equation:

Time Varying Term

$$A_{lat}\frac{G_{i,j}^{n+1,m}-G_{i,j}^{n,m}}{\Delta t}=0 \tag{38}$$

Lateral Momentum Spatial Gradient Term

The spatial gradient term is the following:

$$Sos=A_{lat}\frac{\bar{u}^{n+1,m}G_{i,j}^{n+1,m}-\bar{u}^{n+1,m-1}G_{i,j}^{n+1,m-1}}{\Delta x} \tag{39}$$

where n is the index for time, m is the axial element index and $\bar{u}$ is the average velocity between subchannels i and j. The above equation can also be written as the following:

$$Sos=A_{lat}\frac{(u_i^{n+1,m}+u_j^{n+1,m})G_{i,j}^{n+1,m}-(u_i^{n+1,m-1}+u_j^{n+1,m-1})G_{i,j}^{n+1,m-1}}{2\Delta x} \tag{40}$$

or

$$Sos=A_{lat}\frac{(\frac{U_{1,i}^{n+1,m}}{U_{0,i}^{n+1,m}}+\frac{U_{1,j}^{n+1,m}}{U_{0,j}^{n+1,m}})U_3^{n+1,m}-(\frac{U_{1,i}^{n+1,m-1}}{U_{0,i}^{n+1,m-1}}+\frac{U_{1,j}^{n+1,m-1}}{U_{0,j}^{n+1,m-1}})U_3^{n+1,m-1}}{\Delta x} \tag{41}$$

This spatial gradient term has additional Jacobians, as it is affected by the previous node's density and axial mass flux.

$$\frac{\partial Sos}{\partial U_{0,i}^{n+1,m}}=\frac{\partial Sos}{\partial(\rho A)_i^{n+1,m}}=-\frac{1}{2\Delta x}\frac{(\rho uA)_i^{n+1,m}}{((\rho A)_i^{n+1,m})^2}G_{i,j}^{n+1,m}A_{lat} \tag{42}$$

$$\frac{\partial Sos}{\partial U_{1,i}^{n+1,m}}=\frac{\partial Sos}{\partial(\rho uA)_i^{n+1,m}}=\frac{1}{2\Delta x}\frac{1}{(\rho A)_i^{n+1,m}}G_{i,j}^{n+1,m}A_{lat} \tag{43}$$

$$\frac{\partial Sos}{\partial U_{0,j}^{n+1,m}}=\frac{\partial Sos}{\partial(\rho A)_j^{n+1,m}}=-\frac{1}{2\Delta x}\frac{(\rho uA)_j^{n+1,m}}{((\rho A)_j^{n+1,m})^2}G_{i,j}^{n+1,m}A_{lat} \tag{44}$$

$$\frac{\partial Sos}{\partial U_{1,j}^{n+1,m}} = \frac{\partial Sos}{\partial (\rho u A)_j^{n+1,m}} = \frac{1}{2\Delta x} \frac{1}{(\rho A)_j^{n+1,m}} G_{i,j}^{n+1,m} A_{lat} \tag{45}$$

$$\frac{\partial Sos}{\partial U_3^{n+1,m}} = \frac{\partial Sos}{\partial G_{i,j}^{n+1,m}} = \frac{1}{2\Delta x} \left(\frac{(\rho u A)_i^{n+1,m}}{(\rho A)_i^{n+1,m}} + \frac{(\rho u A)_j^{n+1,m}}{(\rho A)_j^{n+1,m}} \right) A_{lat} \tag{46}$$

The Jacobians with respect to the previous node are the following:

$$\frac{\partial Sos}{\partial U_{0,i}^{n+1,m-1}} = \frac{\partial Sos}{\partial (\rho A)_i^{n+1,m-1}} = \frac{1}{2\Delta x} \frac{(\rho u A)_i^{n+1,m-1}}{((\rho A)_i^{n+1,m-1})^2} G_{i,j}^{n+1,m-1} A_{lat} \tag{47}$$

$$\frac{\partial Sos}{\partial U_{1,i}^{n+1,m-1}} = \frac{\partial Sos}{\partial (\rho u A)_i^{n+1,m-1}} = -\frac{1}{2\Delta x} \frac{1}{(\rho A)_i^{n+1,m-1}} G_{i,j}^{n+1,m-1} A_{lat} \tag{48}$$

$$\frac{\partial Sos}{\partial U_{0,j}^{n+1,m-1}} = \frac{\partial Sos}{\partial (\rho A)_j^{n+1,m-1}} = \frac{1}{2\Delta x} \frac{(\rho u A)_j^{n+1,m-1}}{((\rho A)_j^{n+1,m-1})^2} G_{i,j}^{n+1,m-1} A_{lat} \tag{49}$$

$$\frac{\partial Sos}{\partial U_{1,j}^{n+1,m-1}} = \frac{\partial Sos}{\partial (\rho u A)_j^{n+1,m-1}} = -\frac{1}{2\Delta x} \frac{1}{(\rho A)_j^{n+1,m-1}} G_{i,j}^{n+1,m-1} A_{lat} \tag{50}$$

$$\frac{\partial Sos}{\partial U_3^{n+1,m-1}} = \frac{\partial Sos}{\partial G_{i,j}^{n+1,m-1}} = -\frac{1}{2\Delta x} \left(\frac{(\rho u A)_i^{n+1,m-1}}{(\rho A)_i^{n+1,m-1}} + \frac{(\rho u A)_j^{n+1,m-1}}{(\rho A)_j^{n+1,m-1}} \right) A_{lat} \tag{51}$$

Pressure Gradient per Unit Length

$$Sos = -\frac{A_{lat}}{l_k}(P_i - P_j) \tag{52}$$

The Jacobian terms are the following:

$$\frac{\partial Sos}{\partial (\rho A)_i} = \frac{A_{Lat}}{l_k} \frac{\partial P_i}{\partial (\rho A)_i} = \frac{A_{lat}}{l_k} \frac{1}{A_i} \frac{\partial P_i}{\partial \rho_i} \tag{53}$$

$$\frac{\partial Sos}{\partial(\rho uA)_i} = \frac{A_{lat}}{l_k}\frac{1}{A_i}\frac{\partial P_i}{\partial \rho u_i} \tag{54}$$

$$\frac{\partial Sos}{\partial(\rho EA)_i} = \frac{A_{lat}}{l_k}\frac{1}{A_i}\frac{\partial P_i}{\partial \rho E_i} \tag{55}$$

$$\frac{\partial Sos}{\partial(\rho A)_j} = -\frac{A_{lat}}{l_k}\frac{1}{A_j}\frac{\partial P_j}{\partial \rho_j} \tag{56}$$

$$\frac{\partial Sos}{\partial(\rho uA)_j} = -\frac{A_{lat}}{l_k}\frac{1}{A_j}\frac{\partial P_j}{\partial \rho u_j} \tag{57}$$

$$\frac{\partial Sos}{\partial(\rho EA)_j} = -\frac{A_{lat}}{l_k}\frac{1}{A_j}\frac{\partial P_j}{\partial \rho E_j} \tag{58}$$

Lateral Form Loss per Unit Length

$$Sos = \frac{1}{2}\frac{A_{lat}}{l_k}K_G\frac{G_{i,j}|G_{i,j}|}{\bar{\rho}^m} = \frac{A_{lat}}{l_k}K_G\frac{G_{i,j}|G_{i,j}|}{\rho_i + \rho_j} = \frac{A_{lat}}{l_k}K_G\frac{G_{i,j}|G_{i,j}|}{(\rho A)_i/A_i + (\rho A)_j/A_j} \tag{59}$$

The Jacobian terms are the following:

$$\frac{\partial Sos}{\partial(\rho A)_i} = -\frac{A_{lat}}{l_k}K_G\frac{G_{i,j}|G_{i,j}|}{(\rho_i + \rho_j)^2}\frac{1}{A_i} \tag{60}$$

$$\frac{\partial Sos}{\partial(\rho A)_j} = -\frac{A_{lat}}{l_k}K_G\frac{G_{i,j}|G_{i,j}|}{(\rho_i + \rho_j)^2}\frac{1}{A_j} \tag{61}$$

$$\frac{\partial Sos}{\partial G_{i,j}} = \frac{A_{lat}}{l_k}K_G\frac{2|G_{i,j}|}{\rho_i + \rho_j} \tag{62}$$

A.4 Conservation of Energy

The following are the source terms in the conservation of energy residuals:

Lateral Convection

$$Sos = G_{i,j} s_k H^* \tag{63}$$

In finding these Jacobians, it is important to consider that the total enthalpy is defined as $H = E + P/\rho = \rho EA/\rho A + PA/\rho A$. Hence

$$Sos = G_{i,j} s_k H^* = G_{i,j} s_k (\frac{\rho EA}{\rho A} + \frac{PA}{\rho A})^* = U_3 s_k (\frac{U_2}{U_0} + \frac{PA}{U_0})^* \tag{64}$$

The Jacobian terms are the following:

If $G_{i,j} > 0$ then

$$\frac{\partial Sos}{\partial U_{0,i}} = \frac{\partial Sos}{\partial (\rho A)_i} = G_{i,j} s_k \left(-\frac{(\rho EA)_i}{(\rho A)_i^2} + \frac{(\rho A)_i \frac{\partial P_i}{\partial \rho_i} - (PA)_i}{(\rho A)_i^2} \right) \tag{65}$$

$$\frac{\partial Sos}{\partial U_{1,i}} = \frac{\partial Sos}{\partial (\rho uA)_i} = G_{i,j} s_k \left(\frac{\partial P_i}{\partial (\rho u)_i} \frac{1}{(\rho A)_i} \right) \tag{66}$$

$$\frac{\partial Sos}{\partial U_{2,i}} = \frac{\partial Sos}{\partial (\rho EA)_i} = G_{i,j} s_k \left(\frac{1}{(\rho A)_i} + \frac{\partial P_i}{\partial (\rho E)_i} \frac{1}{(\rho A)_i} \right) \tag{67}$$

$$\frac{\partial Sos}{\partial U_{3,i}} = \frac{\partial Sos}{\partial G_{i,j}} = s_k \left(\frac{(\rho EA)_i}{(\rho A)_i} + \frac{(PA)_i}{(\rho A)_i} \right) \tag{68}$$

If $G_{i,j} < 0$ then

$$\frac{\partial Sos}{\partial U_{0,j}} = \frac{\partial Sos}{\partial (\rho A)_j} = G_{i,j} s_k \left(-\frac{(\rho EA)_j}{(\rho A)_j^2} + \frac{(\rho A)_j \frac{\partial P_j}{\partial \rho_j} - (PA)_j}{(\rho A)_j^2} \right) \tag{69}$$

$$\frac{\partial Sos}{\partial U_{1,j}} = \frac{\partial Sos}{\partial (\rho uA)_j} = G_{i,j} s_k \left(\frac{\partial P_j}{\partial (\rho u)_j} \frac{1}{(\rho A)_j} \right) \tag{70}$$

$$\frac{\partial Sos}{\partial U_{2,j}} = \frac{\partial Sos}{\partial (\rho EA)_j} = G_{i,j} s_k \left(\frac{1}{(\rho A)_j} + \frac{\partial P_j}{\partial (\rho E)_j} \frac{1}{(\rho A)_j} \right) \tag{71}$$

$$\frac{\partial Sos}{\partial U_{3,j}} = \frac{\partial Sos}{\partial G_{i,j}} = s_k \left(\frac{(\rho EA)_j}{(\rho A)_j} + \frac{(PA)_j}{(\rho A)_j} \right) \tag{72}$$

Turbulent Energy Exchange Term

$$Sos = w_{i,j}^t (H_i - H_j) = \beta s_k \bar{G} (H_i - H_j) = w_{ij}^t (H_i - H_j) \tag{73}$$

Since $H = E + P/\rho = \frac{\rho EA}{\rho A} + \frac{PA}{\rho A}$, the turbulent energy exchange term can be written as

$$Sos = w_{i,j}^t (\frac{(\rho EA)_i}{(\rho A)_i} + \frac{(PA)_i}{(\rho A)_i} - \frac{(\rho EA)_j}{(\rho A)_j} - \frac{(PA)_j}{(\rho A)_j}) \tag{74}$$

or

$$Sos = w_{i,j}^t (\frac{U_{2,i}}{U_{0,i}} + \frac{(PA)_i}{U_{0,i}} - \frac{U_{2,j}}{U_{0,j}} - \frac{(PA)_j}{U_{0,j}}) \tag{75}$$

the Jacobian terms are the following:

$$\frac{\partial Sos}{\partial U_{0,i}} = \frac{\partial Sos}{\partial (\rho A)_i} = w_{ij}^t (-\frac{(\rho EA)_i}{(\rho A)_i^2} + \frac{(\rho A)_i \frac{\partial P_i}{\partial \rho_i} - (PA)_i}{(\rho A)_i^2}) \tag{76}$$

$$\frac{\partial Sos}{\partial U_{1,i}} = \frac{\partial Sos}{\partial (\rho uA)_i} = w_{ij}^t \frac{\partial P_i}{\partial (\rho u)_i} \frac{1}{(\rho A)_i} \tag{77}$$

$$\frac{\partial Sos}{\partial U_{2,i}} = \frac{\partial Sos}{\partial (\rho EA)_i} = w_{ij}^t (\frac{1}{(\rho A)_i} + \frac{\partial P_i}{\partial (\rho E)_i} \frac{1}{(\rho A)_i}) \tag{78}$$

$$\frac{\partial Sos}{\partial U_{0,j}} = \frac{\partial Sos}{\partial (\rho A)_j} = -w_{ij}^t (-\frac{(\rho EA)_j}{(\rho A)_j^2} + \frac{(\rho A)_j \frac{\partial P_j}{\partial \rho_j} - (PA)_j}{(\rho A)_j^2}) \tag{79}$$

$$\frac{\partial Sos}{\partial U_{1,j}} = \frac{\partial Sos}{\partial (\rho uA)_j} = -w_{ij}^t \frac{\partial P_j}{\partial (\rho u)_j} \frac{1}{(\rho A)_j} \tag{80}$$

$$\frac{\partial Sos}{\partial U_{2,j}} = \frac{\partial Sos}{\partial (\rho EA)_j} = -w_{ij}^t (\frac{1}{(\rho A)_j} + \frac{\partial P_j}{\partial (\rho E)_j} \frac{1}{(\rho A)_j}) \tag{81}$$

B Nomenclature

ρ	density	
ρE	energy density	
ρu	axial mass flux	
$G_{i,j}$	lateral mass flux	
E	specific energy	
u	axial velocity	
u_l	lateral velocity	
$_m$	index of axial elements	
$_i$	index of subchannel	
$_j$	index of adjacent subchannel	
$_k$	index of lateral interface between subchannels $_i$ and $_j$	
K	the set of gaps on the boundary of subchannel $_i$	
$\vec{n}$	unit direction vector	
H	specific total enthalpy	
H^*	lateral donor specific total enthalpy	$h^* = \begin{cases} H_i & \text{if } G_{i,j} \geq 0 \\ H_j & \text{if } G_{i,j} < 0 \end{cases}$
u^*	lateral donor axial velocity	$u^* = \begin{cases} u_i & \text{if } G_{i,j} \geq 0 \\ u_j & \text{if } G_{i,j} < 0 \end{cases}$
w^t	turbulent lateral mass flow rate	$0.005\mu Re_i^{0.9}(\frac{s_k}{d})^{0.106}$
$\bar{\rho}$	average density	$\bar{\rho_i} = \frac{1}{2}(\rho_i + \rho_j)$
T	Temperature	
P	Pressure	
Δx	length of axial interval	
s_k	width of lateral interface	
d	diameter of fuel pins	
l_k	distance between centroids of adjacent subchannels	
A_{lat}	interface area between laterally neighboring subchannels	$A = \Delta x * s_k$
A_i	cross sectional area of ith subchannel	

D_h	hydraulic diameter
μ	dynamic viscosity
k	thermal conductivity
f	friction loss coefficient

References

[1] INL, "RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods, Vol. 1, revision 2.4," Tech. Rep. INEEL-EXT-98-00834, Idaho National Laboratory, June 2005.

[2] J. E. Kelly, "Development of a two-fluid, two-phase model for light water reactor subchannel analysis," Tech. Rep. PhD Dissertation, Massachusetts Institute of Technology, August 1980.

[3] M. Thurgood, "COBRA/TRAC - A Thermal Hydraulics Code for Transient Analysis of Nuclear Reactor Vessels and Primary Coolant Systems - Users Manual," Tech. Rep. NUREG/CR-3046, USNRC, 1983.

[4] AREVA, "COBRA-FLX: A Core Thermal-Hydraulic Analysis Code," Tech. Rep. ANP-10311NP, Marh 2010.

[5] J.-J. Jeong, "Simulation of a main steam line break accident using a coupled system thermal-hydraulics, three-dimensional reactor kinetics, and hot channel analysis code," *Annals of Nuclear Energy*, vol. 33, pp. 820–828, 2006.

[6] "RELAP-7 Simulation Resolving an SBO Scenario on a Simplified Geometry of a BWR," Tech. Rep. INL/EXT-13-29887, Idaho National Laboratory, August 2013.

[7] D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandié, "MOOSE: A parallel computational framework for coupled systems of nonlinear equations," *Nuclear Engineering and Design*, vol. 239, pp. 1768–1778, Oct. 2009. `http://dx.doi.org/10.1016/j.nucengdes.2009.05.021`.

[8] J. Rogers and A. Tahir, "Turbulent interchange mixing in rod bundles and the role of secondary flows," *ASME Paper 75-HT-31*, 1975.

[9] R. Lahey, "Two-phase flow and heat transfer in multirod geometries: Subchannel and pressure drop measurements in a nine-rod bundle for diabatic and adiabatic conditions," Tech. Rep. GEAP-13049, 1970.