CTF RESIDUAL FORMULATION OF SOLID LIQUID COUPLING

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ABSTRACT

Nuclear engineering codes are being used to simulate more challenging problems and at higher fidelities than they were initially developed for. In order to expand the capabilities of these codes, state of the art numerical methods and computer science need to be implemented. One of the key players in this effort is the Consortium for Advanced Simulation of Light Water Reactors (CASL) through development of the Virtual Environment for Reactor Applications (VERA). The sub-channel thermal hydraulic code used in VERA, COBRA-TF (Coolant-Boiling in Rod Arrays - Three Fluids), is partially developed at the Pennsylvania State University by the Reactor Dynamics and Fuel Management Research Group (RDFMG). The RDFMG version COBRA-TF is referred to as CTF.

In an effort to help meet the objectives of CASL, a version of CTF has been developed that solves the residual formulation of the one-dimensional single-phase conservation equations. The formulation of the base equations as residuals allows the code to be run semi-implicitly or fully implicitly while clearly defining the original conservation equations. This paper outlines work to integrate one dimensional solid conduction equations into the residual formulation. This allows the coupling between the solid and liquid equations to be either explicit or implicit. A simple test problem consisting of a single liquid channel and fuel pin is used to compare the different numerical models available from the new residual formulation to an analytical solution. The methods are compared both for steady state and transient conditions to quantify the accuracy of each method. The ability to choose appropriate numerical methods allows for greater fidelity and decreases computational expenses. The comparison to an analytical solution helps to verify that the code is working properly.

KEYWORDS
CTF, Thermal Hydraulic, Residual, Jacobian, Solid Liquid Coupling

1. INTRODUCTION

For the past several decades, the primary focus in nuclear engineering within the United States has been on light water reactors (LWR). Commercially, all nuclear reactors are either boiling water reactors (BWR) or pressurized water reactors (PWR). Correct computation of the thermal hydraulics within the reactor core leads to efficient design and accuracy in the safety analysis. A popular subchannel code for modeling the hydrodynamics within the reactor core is CTF, which is a subchannel thermal-hydraulics code developed from COBRA-TF []. This FORTRAN based code solves 8 conservation equations for liquid, entrained droplet, and vapor phases, plus one conservation equation for non-condensable gases. A residual formulation of the code has been created that is able to solve the 1-D single-phase fluid solution. While other residual formulations have been formed for other versions of CTF [], none have been integrated into the CASL version of CTF. This paper outlines the initial work in coupling the liquid and solid solutions for the residual formulation. Explicit and implicit coupling between the solid and liquid solutions are considered for transient and steady state problems. The steady state calculations are compared to the analytical solution for accuracy.

2. CTF

The thermal hydraulics of a LWR core is an important part of nuclear reactor design. CTF has the ability to solve for the temperature and pressure of water within the rod structure of a LWR reactor core. Currently, the conservation equations analytically reduce into a pressure matrix in a semi-implicit method with rod temperatures solved for explicitly. The residual formulation of the code currently solves the 1-D axial single-phase liquid and 1-D radial solid energy conservation. This residual formulation allows for greater flexibility in the selection of the numerical methods as well as easy parameter exposure work.

2.1. 1-D Single Phase Liquid Conservation Equations

For the single-phase formulation of the Euler equations, the unknown variables are pressure P, velocity u, enthalpy h, and density ρ. Density is considered a function of pressure and enthalpy according to the equation of state as dictated by the steam tables. To solve for the remaining three variables, three conservation equations are needed. The conservation of mass given in equation 1 is the most basic with the rate of change in density equal to the advection from the upwinded cell. The conservation of momentum in equation 2 balances the time rate of change of momentum, the advection of momentum from adjacent cells, the gradient of pressure, and body forces. Frictional losses due to grid spacers and other affects are assumed to be zero for the scope of this work in order focus on the solid liquid coupling. The conservation of energy equation 3 contains two temporal terms; the time rate of change of the enthalpy, and the time rate of change of the pressure. These temporal terms are balanced against the advection of the enthalpy. The amount of heat entering the channel q_{rod} is calculated as $h_f(T_w - T_l)$, where h_f is the heat transfer coefficient from the single phase Dittus-Boelter [] correlation, T_w is the wall temperature, and T_l is the bulk liquid temperature of the cell.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \tag{1}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\bar{\rho}}\frac{\partial P}{\partial x} + g = 0 \tag{2}$$

$$\rho\frac{\partial h}{\partial t} + h\frac{\partial \rho}{t} - \frac{\partial P}{\partial t} + \rho u\frac{\partial h}{\partial x} + h\frac{\partial \rho u}{\partial x} - \frac{q_{rod}}{\forall_{liq}} = 0 \tag{3}$$

2.1.1. CTF fluid meshing

The finite volume structure in CTF in Figure 1 is for a one-dimensional channel in the axial direction with n number of cells. The first and last cells at 0 and n + 1 are ghost cells and act as the boundary conditions for the problem. Pressure, enthalpy, and density are averaged over the cell volume and are located at the center of the cell. Mass flow rate and velocity are located at the faces in between cells. The cells are represented with an index i, and the faces with indexes of i+$1/2$ or i-$1/2$. This project focuses on this 1D configuration and does not take into account adjacent subchannels.

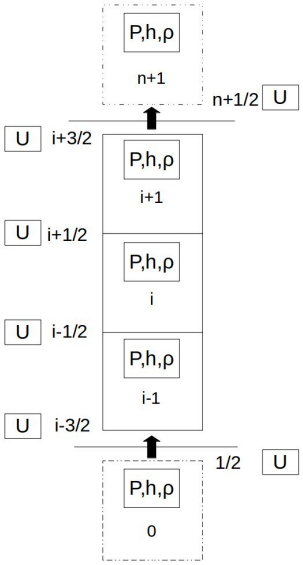

Figure 1. CTF Fluid Volume Meshing

2.1.2. Fluid finite difference equations

The finite difference formulation of the conservation of mass in equation 4 uses a first order accurate forward differencing method for the temporal derivative and the spatial derivatives. The densities evaluated at momentum indexes such as $i + \frac{1}{2}$ represent the density in the adjacent cell to the momentum surface at $i + \frac{1}{2}$ in direction opposite the direction of velocity at the momentum position. In this way, the density is always grabbed from "upwind" from the momentum surface and never "downwind". This is necessary because velocity is not affected by changes "downwind". For the scope of this project, velocity is always positive, so at momentum cell $i + \frac{1}{2}$ the density would be evaluated at cell i. The iterator k, is the iteration level of the solution. If semi-implicit then there is only one iteration and k is equal to n. If implicit, then multiple iterations of k are taken until k reaches $n + 1$. The finite difference formulation of

the conservation of momentum in equation 5 is first order accurate for the temporal and spatial derivatives.

$$\frac{\rho_i^{n+1}-\rho_i^n}{\Delta t}+\frac{\rho^k_{i+\frac{1}{2}}u^{n+1}_{i+\frac{1}{2}}-\rho^k_{i-\frac{1}{2}}u^{n+1}_{i-\frac{1}{2}}}{\Delta x}=0 \tag{4}$$

$$\frac{u^{n+1}_{i+\frac{1}{2}}-u^n_{i+\frac{1}{2}}}{\nabla t}+u^k_{i+\frac{1}{2}}\frac{u^k_{i+\frac{1}{2}}-u^k_{i-\frac{1}{2}}}{\Delta x}+\frac{1}{\overline{\rho}^k_{i+\frac{1}{2}}}\frac{P^{n+1}_{i+1}-P^{n+1}_i}{\Delta x}+g=0 \tag{5}$$

$$\rho_i^k\frac{h_i^{n+1}-h_i^n}{\Delta t}+h_i^k\frac{\rho_i^{n+1}-\rho_i^n}{\Delta t}-\frac{P_i^{n+1}-P_i^n}{\Delta t}+\rho_i^k u^{n+1}_{i+\frac{1}{2}}\frac{h_i^{n+1}-h^{n+1}_{i-1}}{\Delta x}+h_i^k\frac{\rho^k_{i+\frac{1}{2}}u^{n+1}_{i+\frac{1}{2}}-\rho^k_{i-\frac{1}{2}}u^{n+1}_{i-\frac{1}{2}}}{\Delta x}-\frac{q_{rod}}{\forall_{liq}}=0 \tag{6}$$

2.2. 1-D Radial Solid Conduction Equation

The conduction equation for a 1D radial system is given in equation 7.

$$\rho c_p\frac{\partial T}{\partial t}-\frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right)+q'''=0 \tag{7}$$

2.2.1. CTF rod meshing

Rods are meshed differently than fluid cells in CTF as shown by **Error! Reference source not found.**. On the left of the figure, the axial meshing of the rods in grey are shown next to the

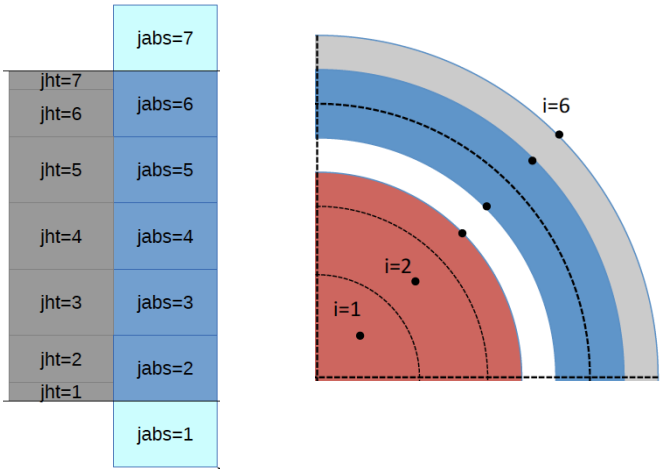

Figure 2. Axial (left) and Radial (right) Rod Meshing

2.2.2. Solid finite difference equations

$$\rho c_p \frac{T_i^{n+1} - T_i^n}{\Delta t} - \frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right) + q''' = 0 \tag{9}$$

2.3. Residual Formulation and Jacobian Construction

A residual is simply the difference between the value at some future iteration k + 1 and the value at the current iteration k. Currently in CTF, the future iteration is taken to be the next time step n+1 and the current iteration is the current time n. The residual can be expressed for desired variables or conservation equations. For example, the residual for density, ρ_i, is the difference between iterates levels k+1 and k, $\rho_i^{k+1} - \rho_i^k$. The residuals for the equations are determined by substituting the residuals into the discretized equations, which should effectively change all n+1 into k. Each cell will have three fluid residual variables and three residual equations. For the entire solution, we will then have a residual variable array δX, and a residual function array F(X) which defines a linear system $J\delta X$=F(X). The Jacobian matrix is defined as the derivative of each response of the function F_j with respect to each variable X_i. The derivative can be calculated numerically as shown by equation (4) where ϵ is a small numerical value.

$$J_{i,j} = \frac{\delta F_j(X_i)}{\delta X_i} \approx \frac{F_j(X_i+\epsilon) - F_j(X_i)}{\epsilon} \tag{9}$$

To build the Jacobian matrix, an object oriented class was created that contains three arrays; an array that points to the residual functions, an array that points to the position within a target variable array, and an array that has the index that the function is to be evaluated at. These lists can be appended in any order, but they have to be appended simultaneously such that variables and functions correspond with each other. The residual function and residual variable arrays can be iterated in nested loops to numerically build the Jacobian matrix where each column represents an index of a residual variable and each row represents a residual function. The explicitly coupled solid liquid Jacobian matrix can be seen on the left in **Error! Reference source not found.**, where blue values represent negative entries and red values positive entries. The black lines represent artificial boundaries between the liquid Jacobian matrix in the top left corner and the solid Jacobian matrix in the top right corner.

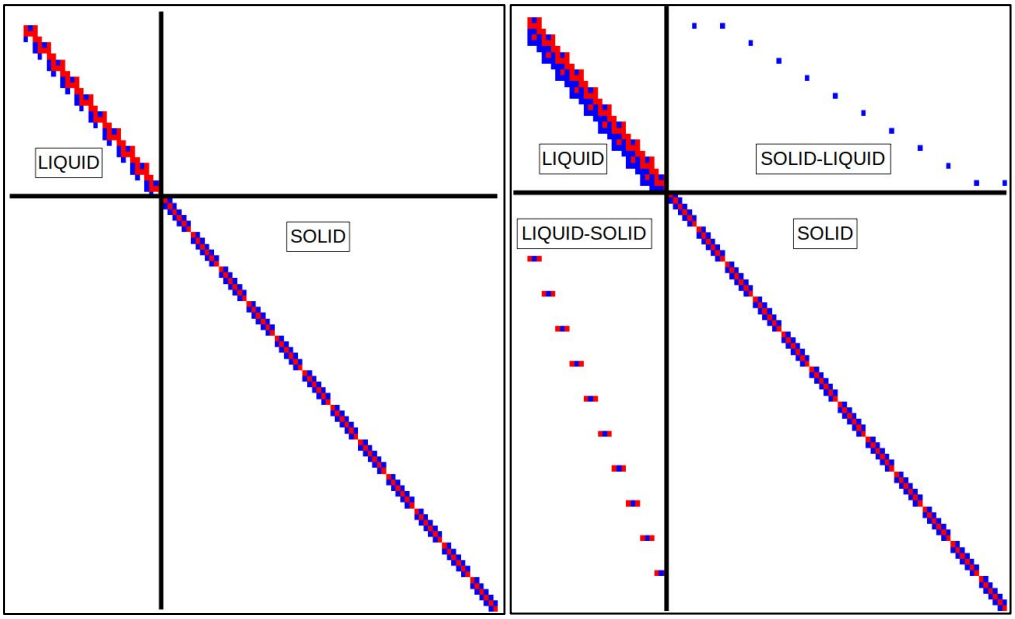

Figure 3. Explicitly (left) and Implicitly Coupled (right) Liquid Solid Jacobian Matrix

The fluid Jacobian matrix contains 3 conservation equations for every axial level. The liquid function residuals are appended in the order of mass conservation, energy conservation, and momentum conservation for each axial level. These correspond the pressure, enthalpy, and velocity at each axial level. The liquid Jacobian matrix can be evaluated as either semi-implicit or fully implicit. The solid Jacobian matrix contains 1 energy conservation equation for each node in the rod. Since axial and azimuthal conduction are not computed, each radial level is computed separately from the rest. This can be seen by the lack of cross terms in the Jacobian matrix at each axial level. The Jacobian matrix on the right is an implicit coupling between the implicit liquid Jacobian matrix and the implicit solid matrix. The cross terms in the top right corner represent the effect of the wall temperature on the energy equation in the liquid Jacobian matrix. The terms on the bottom left represent the effects of pressure, enthalpy, and velocity on the energy equation in the solid Jacobian matrix. The implicit matrix is unconditionally stable given, allowing for time steps greater than the material Courant limits.

3. TEST PROBLEM

3.1. Problem Description

The test problem is a heating rod with uniform heat generation. The heater rod is assumed to have constant material properties according to that of Inconel 600. The mass flow rate, reference pressure, and inlet temperature approximate normal PWR operating conditions. However, the heat generation rate is much less than normal PWR operating conditions to ensure that the problem remains well within the single-phase regime.

Table 1. Test Problem Parameters

Variable	Symbol	Value	Units
Mass Flow Rate	$\dot{m}$	0.300	Kg/sec
Reference Pressure	P_{ref}	16.50	MPa
Liquid Inlet Temperature	T_{inlet}	290.0	$^{\circ}C$
Heat Generation Rate	q'''	56.43167	W/cm^3

Channel Height	L	3.658	m
Rod Radius	R_{rod}	0.450	cm
Rod Pitch	P	12.60	cm
Rod Specific Heat Capacity	C_p	0.431	kJ/kg-K
Rod Cold Density	ρ_{rod}	8470.57	kg/m^3
Thermal Conductivity	k_{rod}	14.83	W/m-k
Number of Axial Nodes	N_{axial}	20	-
Number of Radial Nodes	N_{radial}	10	-

3.2. Steady State Analytical Solution

With uniform heat generation, the original conduction equation can be integrated to obtain equation **Error! Reference source not found.**. The heat at the outer surface of the rod, $T_s(z)$, will depend on the fluid temperature and the heat transfer coefficient. In order to isolate the conduction, the equation is represented as the difference between the temperatures at any radial position, $\Delta T(r)$. Since the right hand side of the equation is now independent of z, the analytical solution for the temperature difference will be the same throughout the interior nodes.

$$T(r,z) - T_s(z) = \frac{q''' R_{rod}^2}{4\, k_{rod}} \left(1 - \frac{r^2}{R_{rod}^2}\right) = \Delta T(r) \tag{10}$$

3.3. Steady State Results

3.4. Transient Results

4. CONCLUSIONS

Present your summary and conclusions here.

NOMENCLATURE

Symbol	Variable
P	Pressure
h	Enthalpy
u	Velocity
ρ	Density
T	Temperature
t	Time
x	Channel Axial Direction
r	Rod Radial Direction
c_p	Specific Heat
k	Thermal Conductivity
q	Heat Rate
q'''	Heat Generation Rate
h_f	Heat Transfer Coefficient

ACKNOWLEDGMENTS

REFERENCES

APPENDIX A