IMPLEMENTATION OF STRONG IMPLICIT PROCEDURE FOR THE ENERGY EQUATIONS IN SUBCHANNEL CODE ATHAS

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ABSTRACT

The poor computational efficiency is one of the main defects of the early developed subchannel codes. With the increased requirement of LWR subchannel pin-by-pin analysis and coupled local neutronics evaluations, it is necessary to improve the computational efficiency of subchannel codes. ATHAS is a subchannel code using the drift flux five equations model and the full implicit algorithm. An exhaustive analysis of the CPU times by code for different stages in the solution process revealed that more than 80 percent of the total CPU time is used for solving energy equations in ATHAS. The energy equations in ATHAS is solved by Gauss-elimination method and it is found that solving the algebraic equations of energy equations accounts for large proportion of the CPU times. In order to improve the computational efficiency, a SIP (strong implicit procedure) method is implemented in the ATHAS code. As a result, the energy matrix will be decomposed into the product of upper triangular matrix and lower triangular matrix as well as an additional nonzero small matrix. Based on the upper triangular matrix and lower triangular matrix, energy equations will be solved iteratively. A whole fuel assembly problem, which has 324 channels, has been calculated in this paper. The calculation results showed that for a 324 channels problem, 77 percent of the total CPU time can be saved by implementing the SIP method into ATHAS code.

KEYWORDS
SIP method; ATHAS; computational efficiency; energy equations

1. INTRODUCTION

Nowadays there are many numerical analysis codes for the reactor core thermal hydraulic reserch, and these codes can be roughly classified into three categories. The first one is the reacter system analysis code, which based on single channel model and considered hot channel factor. Another one is the subchannel analysis code, which considered transverse mixing between subchannels. The last one is the CFD code, which based on finite volume method and has been widely used in industry. The system code is too coarse for the simulation of the reactor core, while the CFD code needs enormous calculation ability that the current computer can not satisfy this requirement. Therefore, the subchannel code still plays an important role in numerical simulation for the reactor core.

The size of channel is allowed to vary in a large scope for a subchannel code. For a fuel assembly problem, the channel surrounded by four fuel rod is usually chosen as a subchannel. For the whole reactor problem, each fuel assembly is usually chosen as a subchannel. In addition, for the reactor core problem or the fuel assembly problem in PWR, it is usually assumed that the core or component is symmetrical, so the number of channels divided into are mostly less than 50, so that the computational efficiency of the subchannel code is acceptable. However, the actual fuel assembly and the reactor core are not symmetrical, due to the existence of the grid spacers as well as the core burnup differences in different

places. Therefore, the original symmetric assumption is not accurate. Based on the above reasons, the LWR subchannel pin-by-pin analysis is advocated. In pin-by-pin analysis, the symmetrical assumption is no longer used, and the channel surrounded by four fuel rod is usually chosen as a subchannel. However, this model leads to the significant increasement of the number of channels, as a result, the computational efficiency of the subchannel code will decrease obviously.

A large number of subchannel codes have been developed since the mid of the last century, and the characteristics of these codes is sumed up in table I. However, most of the codes can not be obtained due to some business reasons. ATHAS code is a subchannel code, which is independently researched and developped by NUSOL team in Xi'an Jiaotong University. As a result, this paper mainly presents the comparision between the original ATHAS code and the improved ATHAS code.

Table I. Features of different subchannel codes

Code	Developed method	Physic model	Numerical method
COBRA-IIIC[1]	Subchannel method	Homogeneous flow model	Step-by-step method
COBRA-IV[2]	Subchannel method	Homogeneous flow model	ICE method
WOSUB[3]	Subchannel method	Drift flow model	Implicit method
ATHAS[4]	Subchannel method	Drift flow model	ICE method
FLICA-4[5]	Subchannel method	Drift flow model	Riemann method
VIPRE-02[6]	Subchannel method	Two fluid model	Implicit method
COMMIX-2[7]	Distributed resistance method	Two fluid model	ICE method
THERMIT-2[8]	Distributed resistance method	Two fluid model	ICE method
COBRA-TF[9]	Subchannel method	Two fluid three field model	Stability two step method

ATHAS code is a subchannel code, which is used to simulate channel flow and phase distribution in the reactor core or bundles as well as simulate various geometries and flow direction. ATHAS code originated from COBRA-IV code, and a number of improvements have been carried out on ATHAS codes. However, the poor computational efficiency is still a major defect of ATHAS code. It is studied that more than 80 percent of the total CPU time of ATHAS code is used to solve energy equations. On the other hand, the energy equations in ATHAS code are solved using Gauss-elimination method, which has very poor computational efficiency. In view of the above reasons, SIP method is implemented to solve the energy equation of the ATHAS code, which can enormously improve the computational efficiency of the code.

2. ALGORITHM MODEL OF SIP METHOD

SIP(strong implicit procedure) method is actually an incomplete LU decomposition method, which was proposed by Stone[10] in 1968. It's a new iterative method, which has been developed for solving the large sets of algebraic equations that arise in the approximate solution of multidimensional partial differential equations by implicit numerical techniques.

Set the matrix form of the discrete equations as follow,

$$A\phi = b \tag{1}$$

And the incomplete LU decomposition means establishing a matrix M. Matrix M can be decomposited into matrix L and matrix U.

$$LU = A + N = M \tag{2}$$

Matrix N is a matrix which should meet the condition that the product of matrix N and vector φ is close to zero. Matrix N equals to that matrix M minus matrix A.

For a two dimensional flow and heat transfer problem, the coefficient matrix A of the discrete equations is a five diagonal matrix. According to Stone's idea, for a five diagonal matrix, matrix L and matrix U are both sparse three diagonal matrix and the diagonal position possessed by non-zero elements of them is the same as the matrix A. Just as shown in Figure 1, the full line of the matrix M represents the position of the matrix A's non-zero elements, and the dotted line of the matrix M represents the extra non-zero elements obtained by the matrix multiplication rule.

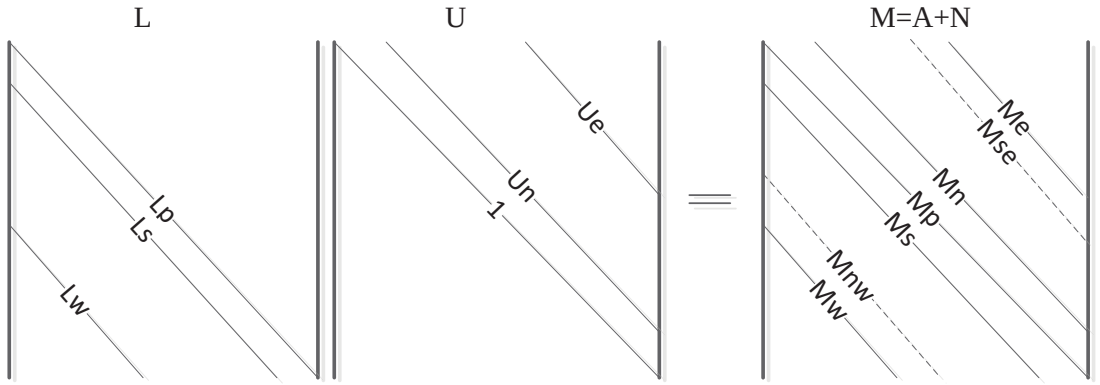

Figure 1. Schematic Diagram of Incomplete Decomposition of the Coefficient Matrix

According to the matrix multiplication rule, the relation of the matrix M to the matrix L and U is as follow,

$$\begin{aligned}
M_w^l &= L_w^l \cdot 1 \\
M_{nw}^l &= L_w^l U_n^{l-M_j} \\
M_s^l &= L_s^l \cdot 1 \\
M_p^l &= L_w^l U_e^{l-M_j} + L_s^l U_n^{l-1} + L_p^l \\
M_n^l &= L_p^l U_n^l \\
M_{se}^l &= L_s^l U_e^{l-1} \\
M_e^l &= L_p^l U_e^l
\end{aligned} \tag{3}$$

As shown in Figure 2, l reprensents the serial number of the nodes, and M_i and M_j represent the number of the nodes in i direction and j direction, respectively.

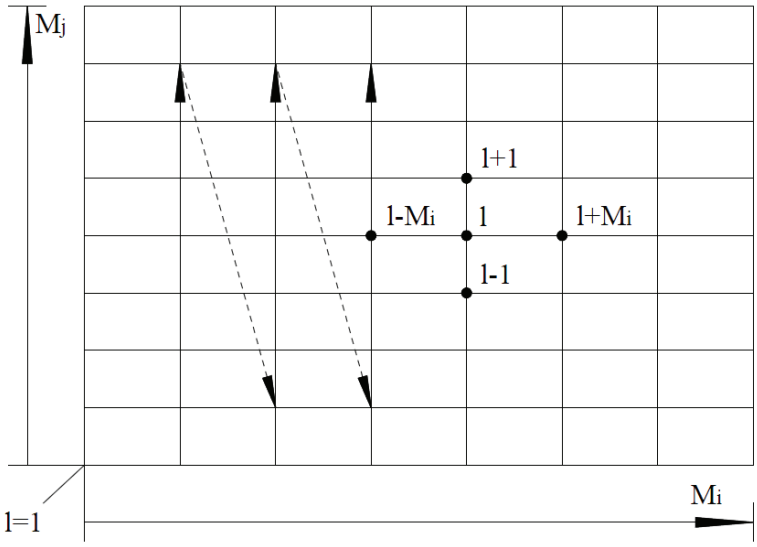

Figure 2. The Type of One Dimensional Numbering

Stone's another idea is that the matrix N is a nonzero seven digonal matrix, so set the elements in the seven digonal line as N_w, N_{sw}, N_s, N_p, N_w, N_{se} as well as N_e, respectively. And the matrix N should meet follow equation,

$$N_p\phi_p + N_n\phi_n + N_s\phi_s + N_e\phi_e + N_w\phi_w + N_{nw}\phi_{nw} + N_{se}\phi_{se} \approx 0 \tag{4}$$

Besides, N_{nw} and N_{se} should be equal to M_{nw} and M_{se}, respectively. As a result, the equation (4) can be also written as the follow form,

$$M_{nw}\left(\phi_{nw} - \phi_{nw}^*\right) + M_{se}\left(\phi_{se} - \phi_{se}^*\right) \approx 0 \tag{5}$$

Stone's third important idea is that ϕ_{nw}^* can be obtained by the adjacent points of the nw point and ϕ_{se}^* can be obtained by the adjacent points of the se point.

$$\begin{aligned} \phi_{nw}^* &= \alpha\left(\phi_w + \phi_n - \phi_p\right) \\ \phi_{se}^* &= \alpha\left(\phi_s + \phi_e - \phi_p\right) \end{aligned} \tag{6}$$

The matrix N can be obtained by putting equation (5) and (6) into equation(4). And then the matrix L and U can be obtained by equation (2).

$$
\begin{aligned}
L_w^l &= A_w^l / \left(1+\alpha U_n^{l-M_j}\right) \\
L_s^l &= A_s^l / \left(1+\alpha U_e^{l-1}\right) \\
L_p^l &= A_p^l + \alpha\left(L_w^l U_n^{l-M_j} + L_s^l U_s^{l-1}\right) - L_w^l U_e^{l-M_j} - L_s^l U_n^{l-1} \\
U_n^l &= \left(A_n^l - \alpha L_w^l U_n^{l-M_j}\right) / L_p^l \\
U_e^l &= \left(A_e^l - \alpha L_s^l U_e^{l-1}\right) / L_p^l
\end{aligned}
\tag{7}
$$

After the matrix L and U defined, the iterative method is derived by adding $N\phi$ to both sides .

$$
\left(A+N\right)\phi^{n+1} = \left(A+N\right)\phi^n + \left(b - A\phi^n\right) \tag{8}
$$

The matrix A+N can be easily decomposed, so the equation (8) can be written as follow.

$$
LU\left(\phi^{n+1} - \phi^n\right) = \left(b - A\phi^n\right) \tag{9}
$$

3. IMPLEMENTING SIP INTO ATHAS CODE

The momentum conversation equations, mass conversation equations and energy conversation equations are solved in sequence, as shown in Figure 3. It is found that more than 80 percent CPU time of the total calculation time is used for solving energy equations. In other words, the computing speed of solving energy equations determines the computional efficiency of the entire code. For the energy equations solving process, three important parameters are calculated. They are respectively liquid enthalpy, vapor enthalpy and mixing enthalpy. ATHAS code applies Newton iterative method to construct a matrix, which consists of the energy differential algebraic equations. The energy equations matrix is solved by Newton elemination method, which badly affect the computional efficiency of the whole code.

On the other hand, when the heat balance model is used, liquid enthalpy and vapor enthalpy is set as its own saturation value. Therefore, after the energy equation matrix is solved, follow correction will be done for liquid enthalpy and vapor enthalpy.

$$
h_{liq} = \min\left(h_{l,sat}, h\right) \tag{10}
$$

$$
h_{vap} = \max\left(h_{v,sat}, h\right) \tag{11}
$$

In this case, liquid enthalpy and vapor enthalpy doesn't need to be solved. It is completely enough to solve mixing enthalpy conservation equation. Therefore, some simplification has been done to ATHAS code in order to avoid calculating the liquid enthalpy and vapor enthalpy. Besides, it is not reasonable to reserve liquid enthalpy term and vapor enthalpy term in mixing enthalpy conservation equation. As a result, original mixing enthalpy conversation equation is changed as follow.

$$\Delta x A \rho \frac{\partial h}{\partial t} + \Delta x \frac{\partial F h}{\partial x} - \Delta x h \frac{\partial F}{\partial x} + \sum_k [Wh]_k$$
$$-h \sum_k (W)_k - \sum_k \left(W' \Delta h\right)_k - \Psi_{i,n} q_{wn} \quad = \quad 0 \tag{12}$$

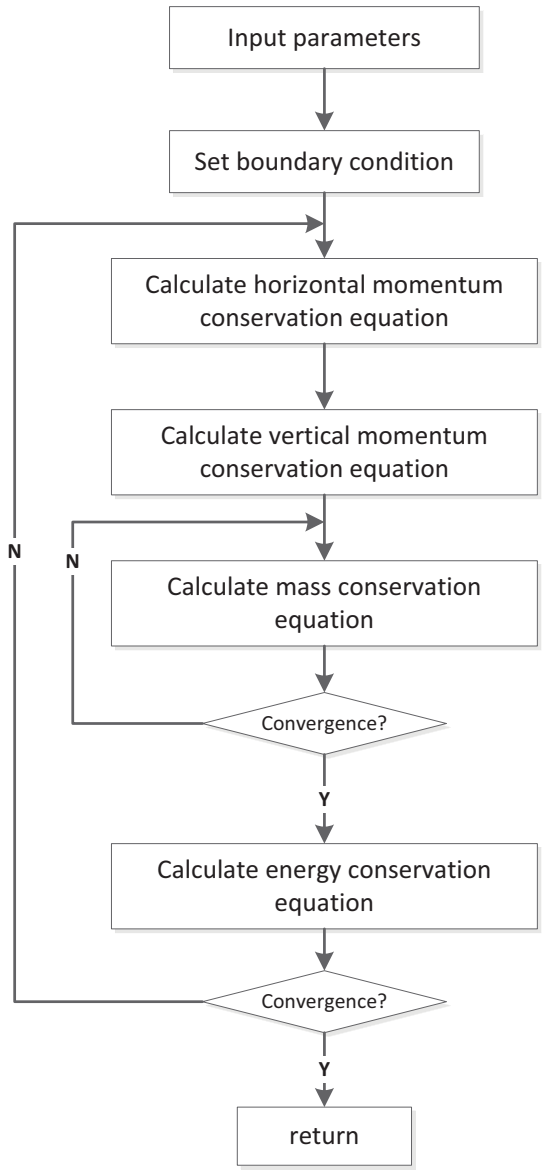

Figure 3. Calculation Flow Chart of ATHAS Code

Subchannel serial number can be defined optionally. However, in order to be convenient to implement SIP method into ATHAS code, the subchannel serial number should be in order. Therefore, the subchannel serial number starts from the southwest, as shown in Figure 4. And then the serial number increases from south to north in sequence.

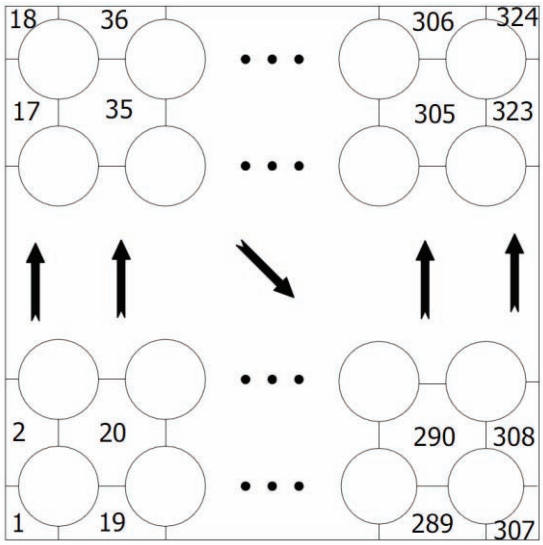

Figure 4. Subchannel Serial Number of ATHAS Code

ATHAS code applies the Newton iterative method to set energy equation matrix. One differncial equation will be set up at each point.

$$\frac{\partial E_l}{\partial h_l}\delta h_l + \frac{\partial E_l}{\partial h_{l-1}}\delta h_{l-1} + \frac{\partial E_l}{\partial h_{l+1}}\delta h_{l+1} + \frac{\partial E_l}{\partial h_{l-M_j}}\delta h_{l-M_j} + \frac{\partial E_l}{\partial h_{l-M_j}}\delta h_{l-M_j} = -E_l \tag{13}$$

For a whole fuel assembly problem, there exist 324 channels. As a result, 324 equations that are all in the same form as equation (13) will be set up to form a 324 order matrix. For each enthalpy correctness in any point, it always associates with the enthalpy correctness in the four neighbor points. Therefore, the energy equations matrix is a five diagonal matrix, as shown in equation (14). For a diagonal matrix, SIP method is very easy to implement.

$$\begin{bmatrix} \frac{\partial E_1}{\partial h_1} & \frac{\partial E_1}{\partial h_2} & 0 & \cdots & 0 & \frac{\partial E_1}{\partial h_{19}} & 0 & \cdots & 0 \\ \frac{\partial E_2}{\partial h_1} & \frac{\partial E_2}{\partial h_2} & \frac{\partial E_2}{\partial h_3} & & & & \ddots & & \\ 0 & \frac{\partial E_3}{\partial h_2} & \ddots & \ddots & & & & & \\ \vdots & & \ddots & & & & & & \vdots \\ \frac{\partial E_{19}}{\partial h_1} & & & & & & & & \\ \vdots & \ddots & & & & & & & \\ 0 & & & & \cdots & & & \frac{\partial E_{324}}{\partial h_{323}} & \frac{\partial E_{324}}{\partial h_{324}} \end{bmatrix} \begin{bmatrix} \delta h_1 \\ \delta h_2 \\ \vdots \\ \delta h_{323} \\ \delta h_{324} \end{bmatrix} = - \begin{bmatrix} E_1 \\ E_2 \\ \vdots \\ E_{323} \\ E_{324} \end{bmatrix} \tag{14}$$

4. RESULT

The heat balance model is applied and some certain simplification has been done to ATHAS code . And the SIP mehod is applied to solving the simplified energy equations matrix. In order to vertify the correctness of the improved ATHAS code, a full fuel assembly problem, which has 324 channels, has been calculated in this paper. As shown in Figure 5 and Figure 6, for a fuel assembly problem, the results of mass flux and flow equilibrium quality in each channel, which are calculated respectively by the original ATHAS code and the improved ATHAS code, are the same. In other words, the improved ATHAS code has the same accuracy as the original ATHAS code.

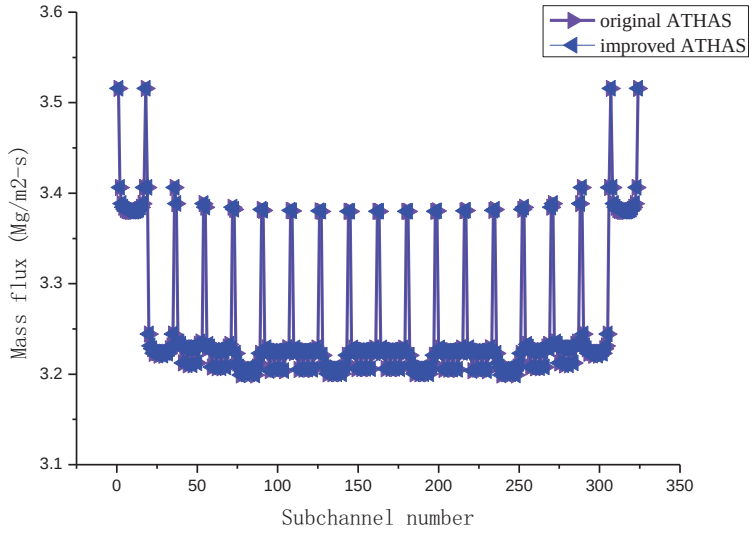

Figure 5. Mass Flux .vs. Channel Number

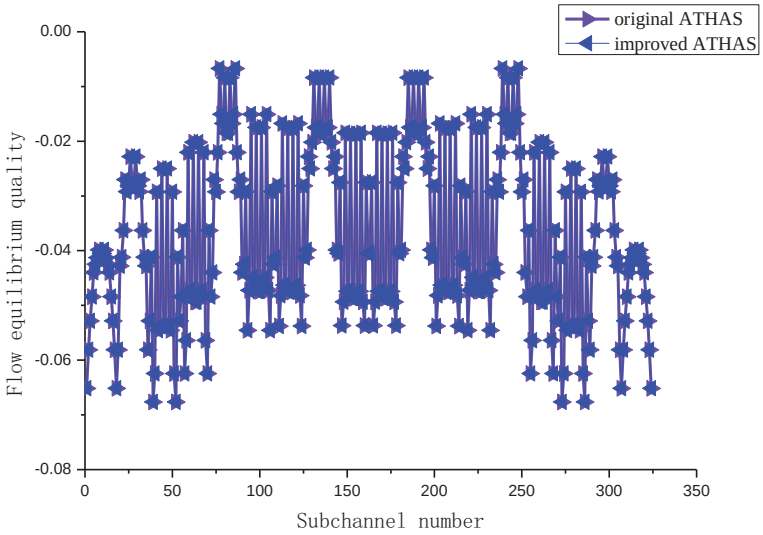

Figure 6. Flow Equilibrium Quality .vs. Channel Number

On the other hand, the computational efficiency of ATHAS code is improved greatly, as shown in table II. For a steady state calculation problem of the PWR fuel assembly, the original ATHAS code needs 706s to achieve convergence, in which solving of energy equation matrix cost 557s. And for the simplified ATHAS code, which applies the strong implicit procedure mehod, only needs 1.6 s to solve the energy equation matix. And the new ATHAS code only needs 163s to achieve convergence condition. In other words, For a steady state calculation condition of PWR fuel assembly, which has 324hannels, the improved ATHAS code saves 77% of the time compared with the original ATHAS code.

Table II. Comparison of the CPU time

Code	Calculation time of the entire code	Calculation time of the energy equation matrix
Original ATHAS	706s	557s
Improved ATHAS	163s	1.6s

When the number of channels increases, the consuming time for energy equation matrix almost rises exponentially. For the whole reactor core problem, the number of channels will be near 50000. Therefore, original ATHAS code will cost much more time and the computional efficiency of the original ATHAS code can hardly meet user's requirement. And when the strong implicit procedure mehod is applied to solving the energy equation matrix, the consumption time for energy equation matrix can be negligible compared with the rest of the calculation time of the whole code. Therefore, the computional efficiency of the whole code will be greatly improved.

5. CONCLUSIONS

The poor computational efficiency is a main defect of the ATHAS code and it's found that the energy equation matrix cost the most of the CPU time. Therefore, some simplification has been done to the energy equation of the ATHAS code at first. After that, the SIP method is accomplished in this paper and implemented into the ATHAS code to improve the solving efficiency of energy equations. For a 324 channels fuel assembly problem, the original ATHAS code needs 706s to achieve convergence, in which the matrix solving of energy equation cost 557s. And the simplified ATHAS code, which applys the strong implicit procedure mehod, just needs 1.6 s to solve the energ equation matix. And the new ATHAS code only needs 163s to achieve convergence condition. In other words, for a 324 channels fuel assembly, the improved ATHAS code saves 77% of the time compared with the original ATHAS code.

NOMENCLATURE

A	Subchannel flow area
x	Axial distance
Δx	Axial space increment
h	Mixture enthalpy
$h_{l,sat}$	Saturation enthalpy of liquid
$h_{v,sat}$	Saturation enthalpy of vapor

h_{liq}	Enthalpy of liquid
h_{vap}	Enthalpy of vapor
F	Axial mass flow rate
W	Cross-flow rate
W'	Inter-subchannel turbulent mixing rate
$\psi_{i,n}$	Fraction of power from rod *n* to subchannel *I*
q_{wn}	Heat transfer rate, wall to interface
E_l	Mixture energy equation residual in the node l
h_l	Mixture enthalpy in the node l

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