Boron Transport Model in the SPACE code

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1. Introduction

Generally in PWR, the boron concentration is controlled to preserve the core criticality. In normal operations, it is important to maintain the boron concentration equally distributed inside the primary coolant. On the other hand, in an accidental condition, such as SLB(steam line break), highly borated water is injected by the emergency core cooling system(ECCS) to maintain the core subcritical. In case of SB-LOCA(small break loss of coolant accident) reflux condensation phase, accumulation of the condensed water in the crossover legs may generate deborated water slugs. When the system reaches to natural circulation with the ECCS or the reactor coolant pumps restart, the deborated water slugs in the crossover legs may flow towards the core, resulting in positive reactivity insertion. Therefore, from a safety point of view, the simulation capability of the boron transport phenomena is important in the system thermal hydraulic codes. In this paper, the boron transport models used in SPACE[1], and their application test results are presented.

2. Governing Equations

The boron transport equations are described separately from the main governing equations which are coupled with each other, as in most of the other system codes such as RELAP5[2] and TRACE[3]. The following assumptions are adopted to develop the boron transport model.

1) Boron concentration does not affect the properties of continuous liquid (liquid hereafter) or dispersed liquid (droplet hereafter).
2) Boron is transported by the droplet field as well as the liquid field
3) Transport velocity of boron is the same as the liquid or the droplet velocity that carries it
4) Boron precipitation and dilution are based on boron solubility limit

Since the liquid field carries boron in the form of a solute, its mass conservation equation is used to derive the liquid boron transport equation.

Liquid mass conservation equation:

$$\varepsilon \frac{\partial}{\partial t}(\alpha_l \rho_l) + \nabla \cdot (\varepsilon \alpha_l \rho_l \mathbf{U}_l) = \varepsilon(-\Gamma_l - S_E + S_D - \Gamma_l^w) \quad (1)$$

Because the evaporation terms do not transfer boron at the liquid/vapor interface, the equation of boron transported by the liquid field is:

$$\frac{\partial(\varepsilon \alpha_l \rho_l \omega_l)}{\partial t} + \nabla \cdot \left(\varepsilon^E \alpha_l \rho_l \omega_l \mathbf{U}_l\right) = -\varepsilon \omega_l S_E + \varepsilon \omega_d S_D \quad (2)$$

Since the droplet field is treated independently from the liquid field in SPACE, the boron transport through the droplet field is also taken into account, as follows.

Droplet mass conservation equation:

$$\varepsilon \frac{\partial}{\partial t}(\alpha_d \rho_d) + \nabla \cdot (\varepsilon \alpha_d \rho_d \mathbf{U}_d) = \varepsilon(-\Gamma_d + S_E - S_D - \Gamma_d^w) \quad (3)$$

Because the evaporation terms do not transfer boron at the drop/vapor interface, the equation of boron transported by the droplet field is:

$$\frac{\partial(\varepsilon \alpha_d \rho_d \omega_d)}{\partial t} + \nabla \cdot \left(\varepsilon^E \alpha_d \rho_d \omega_d \mathbf{U}_d\right) = -\varepsilon \omega_d S_D + \varepsilon \omega_l S_E \quad (4)$$

3. Numerical Solution Methodology

The SPACE code provides two different numerical schemes to solve the boron transport equations, which can be selected by users according to the analysis purpose. In this section, described are the two different numerical schemes available in SPACE: first order upwind scheme and second order Godunov scheme.

3.1 First Order Upwind Scheme

As the default numerical solution scheme of boron transport equations in SPACE, Euler explicit scheme in time and upwind scheme in space are applied to the governing equations (2) and (4). Then, the discretized equation of boron concentration in the liquid field can be written as:

$$\varepsilon V_P \frac{\alpha_l^n \rho_l^n \omega_l^n - \alpha_l \rho_l \omega_l}{\Delta t} + \sum_{E \in P} \varepsilon^{E\ d} \alpha_l^{E\ d} \rho_l^{E\ d} \omega_l^E \left(t_P^E U_{ln}^n A^E \right) = \varepsilon V_P \left(-S_E \omega_l + S_D \omega_d \right) \quad (5)$$

Conservation equation of boron concentration in the droplet field can be also written as follows.

$$\varepsilon V_P \frac{\alpha_d^n \rho_d^n \omega_d^n - \alpha_d \rho_d \omega_d}{\Delta t} + \sum_{E \in P} \varepsilon^{E\ d} \alpha_d^{E\ d} \rho_d^{E\ d} \omega_d^E \left(t_P^E U_{dn}^n A^E \right) = \varepsilon V_P \left(S_E \omega_l - S_D \omega_d \right) \quad (6)$$

Rearranging the above discretized equations, the liquid boron concentration equation can be written by:

$$\omega_l^n = \frac{1}{\alpha_l^n \rho_l^n \varepsilon V_P} \left[\begin{array}{l} \varepsilon V_P \left(S_D \omega_d - S_E \omega_l \right) \Delta t + \varepsilon V_P \left(\alpha_l \rho_l \omega_l \right) \\ -\Delta t \sum_{E \in P} \varepsilon^{E\ d} \alpha_l^{E\ d} \rho_l^{E\ d} \omega_l^E \left(t_P^E U_{ln}^n A^E \right) \\ + B_l^{total} \end{array} \right] \quad (7)$$

The droplet boron concentration equation can be written by:

$$\omega_d^n = \frac{1}{\alpha_d^n \rho_d^n \varepsilon V_P} \left[\begin{array}{l} \varepsilon V_P \left(-S_D \omega_d + S_E \omega_l \right) \Delta t + \varepsilon V_P \left(\alpha_d \rho_d \omega_d \right) \\ -\Delta t \sum_{E \in P} \varepsilon^{E\ d} \alpha_d^{E\ d} \rho_d^{E\ d} \omega_d^E \left(t_P^E U_{dn}^n A^E \right) \end{array} \right] \quad (8)$$

By comparing liquid/droplet boron concentration with the boron solubility limit, the precipitation boron masses can be calculated as follows.

$$B_l = \left[\max(0,\ \omega_l^n - B^s) \right] \alpha_l^n \rho_l^n \varepsilon V_P$$
$$B_d = \left[\max(0,\ \omega_d^n - B^s) \right] \alpha_d^n \rho_d^n \varepsilon V_P \quad (9)$$

$$\omega_l^n = B^s \text{ for } B_l > 0$$
$$\omega_d^n = B^s \text{ for } B_d > 0 \quad (10)$$

The total precipitation boron mass is used again as a source term of the conservation equation of boron concentration in the liquid field.

$$B_l^{total} = B_l + B_d \quad (11)$$

The above first order upwind approach is well known to be stable and its robustness has an advantage in obtaining the numerical solution of the general flow equations. However, it introduces numerical diffusion, which can distort the realistic flow phenomena. For an example, when applying the first order upwind scheme to the typical advection equation (12), the truncation error is represented by the equation (13).

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0 \quad (12)$$

$$\varepsilon_t = \frac{\Delta t}{2} \left(\frac{\partial^2 \phi}{\partial^2 t} \right)_i^n - u \frac{\Delta x}{2} \left(\frac{\partial^2 \phi}{\partial^2 x} \right)_i^n + O\left(\Delta t^2, \Delta x^2 \right) \quad (13)$$

Ignoring the second and higher order truncation errors, and rearranging the right hand terms of the equation (13), the truncation error can be expressed by:

$$\varepsilon_t = D_{num} \left(\frac{\partial^2 \phi}{\partial^2 x} \right)_i^n \quad (14)$$

where

$$D_{num} = \frac{u \Delta x}{2} \left(1 - \frac{u \Delta t}{\Delta x} \right) \quad (15)$$

The above truncation error implies that some numerical diffusions are involved in the solution by the first order upwind scheme, while the positive diffusion term makes the numerical scheme stable within the Courant limit represented by:

$$\frac{u \Delta t}{\Delta x} < 1 \quad (16)$$

3.2 Second Order Godunov Scheme

In order to eliminate the numerical diffusion error involved in the first order upwind scheme, a second order accurate Godunov scheme[4] is implemented as an optional model to solve the boron transport equations. Since the velocity is known in both old and new (n) time steps, it can be linearly interpolated to generate approximation based on time centered velocity as:

$$U^* = \frac{1}{2} \left(U^n + U \right). \quad (17)$$

The donor (upstream) cell boron concentration is modified to:

$$ {}^{G}\omega^{E} = {}^{upstream}\omega + \left(1-\frac{U^{*}\Delta t}{\Delta x^{upstream}}\right)\frac{1}{2}\Delta x^{upstream} S^{E} \quad (18) $$

where the cell centered gradient is given as:

$$ S^{E} = (1+\theta\omega)\Phi(r,1)\, gradient^{E} $$
$$ gradient^{E} = \frac{\omega^{downstream} - \omega^{upstream}}{\Delta x^{E}} \quad (19) $$

The cell centered gradient limiter, S^{E}, can be defined in two steps. First, in order to reduce the oscillatory behavior in the second order central differencing scheme, a compressive limiter such as Super Bee limiter is used. Super Bee limiter is slope limiter, which can be obtained by:

$$ \Phi(r,1) = \max\left[0, \min(2r,1), \min(r,2)\right] $$
$$ r = \frac{gradient^{upperface,E}}{gradient^{E}} \quad (20) $$

Second, in order to make sure that the solution is continuous, the following artificial compression term is introduced.

$$ \text{artificial compression} = (1+\theta\omega) \quad (21) $$

where

$$ \theta = \frac{|1-r|}{1+|r|} $$
$$ \omega = \min\left(\frac{U^{*}\Delta t}{\Delta x^{E}}, 1-\frac{U^{*}\Delta t}{\Delta x^{E}}\right) \quad (22) $$

Then, the equations (5) and (6) can be rewritten as:

$$ \varepsilon V_{P}\frac{\alpha_{l}^{n}\rho_{l}^{n}\omega_{l}^{n} - \alpha_{l}\rho_{l}\omega_{l}}{\Delta t} + \sum_{E\in P}\varepsilon^{E\ d}\alpha_{l}^{E\ d}\rho_{l}^{E\ G}\omega_{l}^{E}\left(\iota_{P}^{E}U_{ln}^{*}A^{E}\right) = \varepsilon V_{P}\left(-S_{E}\omega_{l} + S_{D}\omega_{d}\right) \quad (23) $$

$$ \varepsilon V_{P}\frac{\alpha_{d}^{n}\rho_{d}^{n}\omega_{d}^{n} - \alpha_{d}\rho_{d}\omega_{d}}{\Delta t} + \sum_{E\in P}\varepsilon^{E\ d}\alpha_{d}^{E\ d}\rho_{d}^{E\ G}\omega_{d}^{E}\left(\iota_{P}^{E}U_{dn}^{*}A^{E}\right) = \varepsilon V_{P}\left(S_{E}\omega_{l} - S_{D}\omega_{d}\right) \quad (24) $$

where

$$ {}^{G}\omega^{E} = {}^{upstream}\omega + (1+\theta\omega)\Phi(r,1) \cdot \left(1-\frac{U^{*}\Delta t}{\Delta x^{upstream}}\right)\frac{1}{2}\Delta x^{upstream} gradient^{E} \quad (25) $$

The second order accurate Godunov scheme eliminate the numerical diffusion errors, resulting in increasing the accuracy significantly in the boron transport model.

4. Test Results

A test of boron injection in a vertical pipe (see Figure 1) is performed to check the boron transport models of the SPACE code. The vertical pipe which has a length of 20 m and an area of 1.0 m^2 was modeled using 20 cells and 19 faces(junctions). The entire pipe is initially filled with deborated(boron-free) water of 353 °K and 0.4 MPa. An inlet boundary condition is given at the bottom, and an outlet boundary condition is given at the top of the vertical pipe: borated water of 353 °K, 0.4 MPa and 10 % concentration of boric acid(H_3BO_3) is injected at the inlet boundary with velocity of 1 m/s, and the outlet pressure is 0.4 MPa. In this conceptual test problem, the boron solubility limit is ignored to focus on the boric acid concentration transport phenomena. Figure 2 shows boric acid concentration behavior of each cell predicted by the first order upwind scheme. About 30 seconds are taken for every cell to reach 10 % boric acid concentration along the entire pipe, which is much longer than the exact solution, 20 seconds. The difference between the numerical prediction and exact solution is caused mainly by the aforementioned numerical diffusion. Figure 3 shows boric acid concentration behavior of each cell predicted by the second order Godunov scheme without gradient limiter. The numerical diffusion is reduced, but a numerical oscillation appears. Figure 4 shows the result predicted by the second order Godunov scheme with gradient limiter. The numerical diffusion is not only eliminated, but also the numerical oscillation disappears.

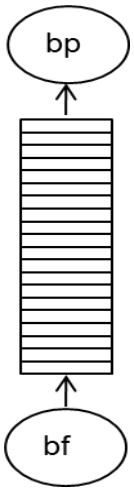

Fig. 1. Test problem

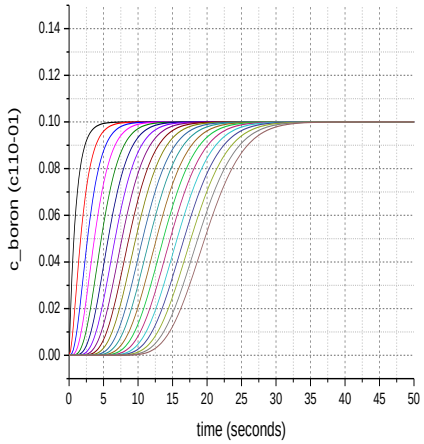

Fig. 2. Boron concentration at each cell (upwind scheme)

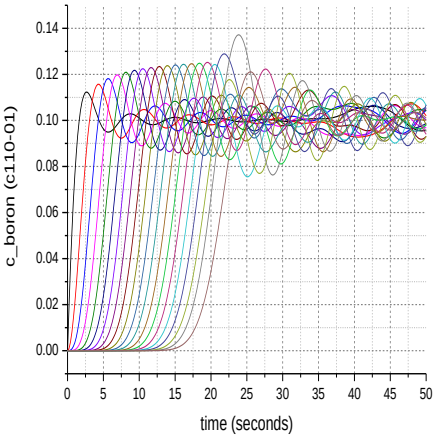

Fig. 3. Boron concentration at each cell (Godunov scheme without gradient limiter)

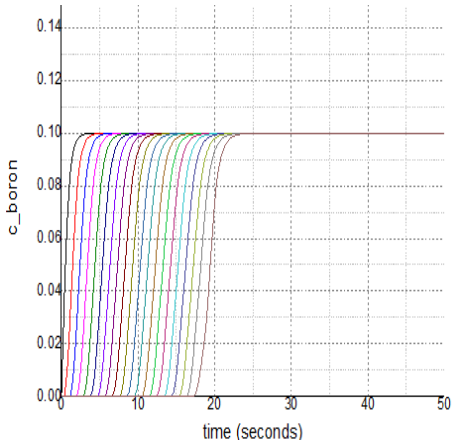

Fig. 4. Boron concentration at each cell (Godunov scheme with gradient limiter)

5. Conclusions

The SPACE code has an advantage of three field representation of two-phase flow model, which allows the liquid and droplet fields to transport boron with individual phasic velocities. The first order upwind and the second order Godunov schemes are implemented to solve the liquid and droplet boron transport equations. A boron injection test in the vertical pipe is performed to check the performance of both the boron transport numerical models. It is concluded that the upwind scheme is stable but includes some numerical diffusion, and the Godunov scheme with gradient limiter can be used to eliminate the numerical diffusion with improved model accuracy.

NOMENCLATURE

A^E	= face area
B_ϕ	= boron precipitation from liquid or droplet field
B^S	= boron solubility limit
D_{num}	= numerical diffusion coefficient
$E \in P$	= every face belonging to the current cell, P
S_E	= entrainment from liquid
S_D	= de-entrainment to liquid
U_n^E	= normal component of velocity vector at face
$U_{\phi n}$	= face-normal velocity of each field
$\mathbf{U}_\phi$	= velocity vector of each field
$\boldsymbol{u}$	= advection velocity
V_P	= volume of the current cell, P
α_ϕ	= volume fraction of each field
ε	= porosity

ϕ = property carried by advection

Γ_ϕ = evaporation from liquid or droplet field

Γ_ϕ^w = near wall evaporation from liquid or droplet field

t_P^E = direction factor of face at a cell, P (1 for outward face, -1 for inward face)

ρ_ϕ = phasic density of each field

ω_ϕ = boron concentration of each field

Subscripts

d = droplet

l = liquid

n = face normal component of velocity vector

ϕ = phase or field indicator

Superscripts

d = face property given by upwind (donor) scheme

E = current face (edge) property

G = face property given by Godunov scheme

n = next time step

$upperface, E$ = upper face (edge) property

$upstream$ = upstream cell property

w = near wall region

REFERENCES

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