DEVELOPMENT OF A COMPUTER PROGRAM FOR REACTOR CORE THERMAL HYDRAULICS:

Finite Differencing in a 3-D Staggered Mesh
Suitable for Irregular Boundary Applications

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I. Introduction

A formulation utilizing a finite difference scheme for the direct numerical simulation of time varying two-phase flow problems in three space dimensions with irregular boundary geometry is presented. The formulation of such problems introduces a complicated set of coupled non-linear partial differential equations for the conservation of mass, momentum, energy, appropriate constitutive equations, and equations of state coupling the two phases. Discretization of the partial differential equations by finite difference procedures allows for numerical solution of the governing equations. The finite difference scheme uses a staggered grid system so often used in hydrodynamics where the velocities are located at the tips of a cell with the pressure, temperature, and density being located at the central mesh point as shown in Figure 1. Although this staggered mesh provides several conservation properties it requires some adjustment when dealing with irregular boundaries.

If the boundaries were curved and the variables were discretized at every mesh point the usual formulation as described in any textbook on numerical solution of partial differential equations could be utilized. However, the staggered mesh requires that only certain boundary intersections of the mesh system be allowed. At this time it is required that in any given direction for a boundary intersection the first internal mesh point always be a pressure point. Because of the usual sensitivity involved in pressure calculations the velocities will be calculated from internal pressure gradients and then extrapolated to the wall. In the last section of this memo the extrapolation procedure is defined. For example, for a no-slip boundary condition, the conditions on velocity on the wall require that all of the components be identically zero. However, in the case of a free-slip wall where the tangential velocity is non-zero and parallel to the streamline, only the normal component is zero. Hence, from a correct calculation of the internal velocities due to internal pressure gradients the velocities or their averages can be extrapolated to the wall and the proper tangential velocity obtained along the wall. Although the requirement for the first internal mesh point to be a pressure point is presently being incorporated, other boundary-mesh cuts will be investigated to determine if this restriction can be alleviated.

ρ, H, p, α = density, enthalpy, pressure, void fraction
 u, v, w = velocity components in x, y, z

Figure 1. Location of Variables and Indices About a Computational Cell (staggered mesh systems)

II. Finite Differencing of the Governing Differential Equations

In order to obtain estimates of the dependent variable distributions at discrete points throughout the domain of interest, partial derivative expressions appearing in the governing differential equations are approximated by finite differences. Location of these discrete points is made via a staggered mesh partitioning of the solution domain. The staggered mesh partitioning consists of four different mesh systems: one mesh system for the field variables (i.e., ρ , P , α , H) and one for each of the three velocity components (u , v , w).

To illustrate the finite difference techniques as applied to a staggered mesh, governing equations 1-5 will be considered. While these equations contain other terms (i.e., O.T.), only the convective terms will be considered here.

$$\frac{\partial(\alpha_l \rho_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l u_l)}{\partial x} + \frac{\partial(\alpha_l \rho_l v_l)}{\partial y} + \frac{\partial(\alpha_l \rho_l w_l)}{\partial z} = 0.T.* \quad (1)$$

$$\frac{\partial(\alpha_l \rho_l u_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l u_l u_l)}{\partial x} + \frac{\partial(\alpha_l \rho_l u_l v_l)}{\partial y} + \frac{\partial(\alpha_l \rho_l u_l w_l)}{\partial z} = -\alpha_l \frac{\partial P}{\partial x} + 0.T. \quad (2)$$

$$\frac{\partial(\alpha_l \rho_l v_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l v_l u_l)}{\partial x} + \frac{\partial(\alpha_l \rho_l v_l v_l)}{\partial y} + \frac{\partial(\alpha_l \rho_l v_l w_l)}{\partial z} = -\alpha_l \frac{\partial P}{\partial y} + 0.T. \quad (3)$$

$$\frac{\partial(\alpha_l \rho_l w_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l w_l u_l)}{\partial x} + \frac{\partial(\alpha_l \rho_l w_l v_l)}{\partial y} + \frac{\partial(\alpha_l \rho_l w_l w_l)}{\partial z} = -\alpha_l \frac{\partial P}{\partial z} + 0.T. \quad (4)$$

$$\begin{aligned} & \frac{\partial(\alpha_l \rho_l H_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l H_l u_l)}{\partial x} + \frac{\partial(\alpha_l \rho_l H_l v_l)}{\partial y} + \frac{\partial(\alpha_l \rho_l H_l w_l)}{\partial z} = \frac{\partial}{\partial t}(\alpha_l P) + \frac{\partial}{\partial x}(\alpha_l P u_l) \\ & + \frac{\partial}{\partial y}(\alpha_l P v_l) + \frac{\partial}{\partial z}(\alpha_l P w_l) - \alpha_l P \left[\frac{\partial u_l}{\partial x} + \frac{\partial v_l}{\partial y} + \frac{\partial w_l}{\partial z} \right] + 0.T. \end{aligned} \quad (5)$$

The finite differencing of these equations will be general enough to accommodate an irregularly shaped domain.

To clarify locations on the staggered mesh, reference is made to field points, u points, v points, and w points. Equations 1 and 5 are at field points while equations 2, 3, and 4 are at u points, v points, and w points, respectively.

*The subscript l refers to "liquid", for illustrative purposes.

Consider equation 1, term by term, evaluated at field point 0 in Figures 2 and 3.

$$\left. \frac{\partial}{\partial t} (\alpha_{\ell} \rho_{\ell}) \right|_0 = \frac{(\alpha_{\ell})_0^{n+1} (\rho_{\ell})_0^{n+1} - (\alpha_{\ell})_0^n (\rho_{\ell})_0^n}{\Delta t} \quad (6)$$

Hereafter, delete ℓ subscript and consider it implied. When superscript n is absent consider it implied.

$$\text{Let } \overline{(\alpha\rho)}_1 = 1/2 [(1 + \text{SGN}(u_1)) \alpha_1 \rho_1 + (1 - \text{SGN}(u_1)) \alpha_0 \rho_0]$$

$$\overline{(\alpha\rho)}_2 = 1/2 [(1 + \text{SGN}(u_2)) \alpha_0 \rho_0 + (1 - \text{SGN}(u_2)) \alpha_2 \rho_2]$$

$$\left. \frac{\partial}{\partial x} (\alpha \rho u) \right|_0 = \frac{u_2 \overline{(\alpha\rho)}_2 - u_1 \overline{(\alpha\rho)}_1}{\Delta x_2 + \Delta x_3} \quad (7)$$

$$\text{Let } \overline{(\alpha\rho)}_3 = 1/2 [(1 + \text{SGN}(v_1)) \alpha_3 \rho_3 + (1 - \text{SGN}(v_1)) \alpha_0 \rho_0]$$

$$\overline{(\alpha\rho)}_4 = 1/2 [(1 + \text{SGN}(v_2)) \alpha_0 \rho_0 + (1 - \text{SGN}(v_2)) \alpha_4 \rho_4]$$

$$\left. \frac{\partial}{\partial y} (\alpha \rho v) \right|_0 = \frac{v_2 \overline{(\alpha\rho)}_4 - v_1 \overline{(\alpha\rho)}_3}{\Delta y_2 + \Delta y_3} \quad (8)$$

$$\text{Let } \overline{(\alpha\rho)}_5 = 1/2 [(1 + \text{SGN}(w_1)) \alpha_5 \rho_5 + (1 - \text{SGN}(w_1)) \alpha_0 \rho_0]$$

$$\overline{(\alpha\rho)}_6 = 1/2 [(1 + \text{SGN}(w_2)) \alpha_0 \rho_0 + (1 - \text{SGN}(w_2)) \alpha_6 \rho_6]$$

$$\left. \frac{\partial}{\partial z} (\alpha \rho w) \right|_0 = \frac{w_2 \overline{(\alpha\rho)}_6 - w_1 \overline{(\alpha\rho)}_5}{\Delta z_2 + \Delta z_3} \quad (9)$$

Consider equation 5 evaluated at field point 0 in Figures 2 and 3.

□ field points

● u points

+ v points

x w points

Figure 2. Grid System Around Field Point '0' in x-y Plane.

Figure 3. Grid System Around Field Point '0' in x - z Plane.

$$\left. \frac{\partial}{\partial t}(\alpha \rho H) \right|_o = \frac{\alpha_o^{n+1} \rho_o^{n+1} H_o^{n+1} - \alpha_o^n \rho_o^n H_o^n}{\Delta t} \quad (10)$$

$$\text{Let } \overline{(\alpha \rho H)}_1 = 1/2 [(1 + \text{SGN}(u_1)) \alpha_1 \rho_1 H_1 + (1 - \text{SGN}(u_1)) \alpha_o \rho_o H_o]$$

$$\overline{(\alpha \rho H)}_2 = 1/2 [(1 + \text{SGN}(u_2)) \alpha_o \rho_o H_o + (1 - \text{SGN}(u_2)) \alpha_2 \rho_2 H_2]$$

$$\left. \frac{\partial}{\partial x}(\alpha \rho H u) \right|_o = \frac{u_2 \overline{(\alpha \rho H)}_2 - u_1 \overline{(\alpha \rho H)}_1}{\Delta x_2 + \Delta x_3} \quad (11)$$

$$\text{Let } \overline{(\alpha \rho H)}_3 = 1/2 [(1 + \text{SGN}(v_1)) \alpha_3 \rho_3 H_3 + (1 - \text{SGN}(v_1)) \alpha_o \rho_o H_o]$$

$$\overline{(\alpha \rho H)}_4 = 1/2 [(1 + \text{SGN}(v_2)) \alpha_o \rho_o H_o + (1 - \text{SGN}(v_2)) \alpha_4 \rho_4 H_4]$$

$$\left. \frac{\partial}{\partial y}(\alpha \rho H v) \right|_o = \frac{v_2 \overline{(\alpha \rho H)}_4 - v_1 \overline{(\alpha \rho H)}_3}{\Delta y_2 + \Delta y_3} \quad (12)$$

$$\text{Let } \overline{(\alpha \rho H)}_5 = 1/2 [(1 + \text{SGN}(w_1)) \alpha_5 \rho_5 H_5 + (1 - \text{SGN}(w_1)) \alpha_o \rho_o H_o]$$

$$\overline{(\alpha \rho H)}_6 = 1/2 [(1 + \text{SGN}(w_2)) \alpha_o \rho_o H_o + (1 - \text{SGN}(w_2)) \alpha_6 \rho_6 H_6]$$

$$\left. \frac{\partial}{\partial z}(\alpha \rho H w) \right|_o = \frac{w_2 \overline{(\alpha \rho H)}_6 - w_1 \overline{(\alpha \rho H)}_5}{\Delta z_2 + \Delta z_3} \quad (13)$$

$$\left. \frac{\partial}{\partial t}(\alpha \rho) \right|_o = \frac{\alpha_o^{n+1} \rho_o^{n+1} - \alpha_o^n \rho_o^n}{\Delta t} \quad (14)$$

$$\text{Let } \overline{(\alpha P)}_1 = 1/2 [(1 + \text{SGN}(u_1)) \alpha_1 P_1 + (1 - \text{SGN}(u_1)) \alpha_o P_o]$$

$$\overline{(\alpha P)}_2 = 1/2 [(1 + \text{SGN}(u_2)) \alpha_o P_o + (1 - \text{SGN}(u_2)) \alpha_2 P_2]$$

$$\left. \frac{\partial}{\partial x}(\alpha P u) \right|_o = \frac{u_2 \overline{(\alpha P)}_2 - u_1 \overline{(\alpha P)}_1}{\Delta x_2 + \Delta x_3} \quad (15)$$

$$\text{Let } \overline{(\alpha P)}_3 = 1/2 [(1 + \text{SGN}(v_1)) \alpha_3 P_3 + (1 - \text{SGN}(v_1)) \alpha_o P_o]$$

$$\overline{(\alpha P)}_4 = 1/2 [(1 + \text{SGN}(v_2)) \alpha_o P_o + (1 - \text{SGN}(v_2)) \alpha_4 P_4]$$

$$\left. \frac{\partial}{\partial y} (\alpha P v) \right|_o = \frac{v_2 \overline{(\alpha P)}_4 - v_1 \overline{(\alpha P)}_3}{\Delta y_2 + \Delta y_3} \quad (16)$$

$$\text{Let } \overline{(\alpha P)}_5 = 1/2 [(1 + \text{SGN}(w_1)) \alpha_5 P_5 + (1 - \text{SGN}(w_1)) \alpha_o P_o]$$

$$\overline{(\alpha P)}_6 = 1/2 [(1 + \text{SGN}(w_2)) \alpha_o P_o + (1 - \text{SGN}(w_2)) \alpha_6 P_6]$$

$$\left. \frac{\partial}{\partial z} (\alpha P w) \right|_o = \frac{w_2 \overline{(\alpha P)}_6 - w_1 \overline{(\alpha P)}_5}{\Delta z_2 + \Delta z_3} \quad (17)$$

$$\alpha P \left. \frac{\partial u}{\partial x} \right|_o = \alpha_o P_o \frac{u_2 - u_1}{\Delta x_2 + \Delta x_3} \quad (18)$$

$$\alpha P \left. \frac{\partial v}{\partial y} \right|_o = \alpha_o P_o \frac{v_2 - v_1}{\Delta y_2 + \Delta y_3} \quad (19)$$

$$\alpha P \left. \frac{\partial w}{\partial z} \right|_o = \alpha_o P_o \frac{w_2 - w_1}{\Delta z_2 + \Delta z_3} \quad (20)$$

Note that in the finite difference expressions from equations 1 and 5 as evaluated at field point 0, only Δx_2 , Δx_3 , Δy_2 , Δy_3 , Δz_2 , and Δz_3 appear. However, other increments Δx_1 , Δx_4 , Δy_1 , Δy_4 , Δz_1 , Δz_4 will appear in the finite difference expressions of diffusive terms which are included in O.T.

Consider equation 2 evaluated at u-point 0 in Figures 4 and 5.

Let

$$\overline{(\alpha \rho)}_o^n = \frac{\Delta x_3 \alpha_3^n \rho_3^n + \Delta x_4 \alpha_4^n \rho_4^n}{\Delta x_3 + \Delta x_4} \quad (21)$$

$$\left. \frac{\partial}{\partial t} (\alpha \rho u) \right|_o = \frac{\overline{(\alpha \rho)}_o^{n+1} u_o^{n+1} - \overline{(\alpha \rho)}_o^n u_o^n}{\Delta t}$$

Figure 4. Grid System Around u-point '0' in x-y Plane.

Figure 5. Grid System Around u -point '0' in x - z Plane.

$$\text{Let } \overline{(\alpha\rho)}_1 = \frac{\Delta x_1^{\alpha_2\rho_2} + \Delta x_2^{\alpha_1\rho_1}}{\Delta x_1 + \Delta x_2}$$

$$\overline{(\alpha\rho)}_2 = \frac{\Delta x_5^{\alpha_4\rho_4} + \Delta x_6^{\alpha_3\rho_3}}{\Delta x_5 + \Delta x_6}$$

$$\overline{u}_1 = \frac{\Delta x_2^{u_0} + \Delta x_3^{u_1}}{\Delta x_2 + \Delta x_3}$$

$$\overline{u}_2 = \frac{\Delta x_4^{u_2} + \Delta x_5^{u_0}}{\Delta x_4 + \Delta x_5}$$

$$\overline{(\alpha\rho u)}_1 = \frac{1}{2} [(1 + \text{SGN}(\overline{u}_1)) \overline{(\alpha\rho)}_1 u_1 + (1 - \text{SGN}(\overline{u}_1)) \overline{(\alpha\rho)}_0 u_0]$$

$$\overline{(\alpha\rho u)}_2 = \frac{1}{2} [(1 + \text{SGN}(\overline{u}_2)) \overline{(\alpha\rho)}_0 u_0 + (1 - \text{SGN}(\overline{u}_2)) \overline{(\alpha\rho)}_2 u_2]$$

$$\frac{\partial}{\partial x} (\alpha\rho u) \Big|_0 = \frac{\overline{u}_2 \overline{(\alpha\rho u)}_2 - \overline{u}_1 \overline{(\alpha\rho u)}_1}{\Delta x_3 + \Delta x_4} \quad (22)$$

$$\text{Let } \overline{(\alpha\rho)}_3 = \frac{\Delta x_7^{\alpha_6\rho_6} + \Delta x_8^{\alpha_5\rho_5}}{\Delta x_7 + \Delta x_8}$$

$$\overline{(\alpha\rho)}_4 = \frac{\Delta x_{13}^{\alpha_8\rho_8} + \Delta x_{14}^{\alpha_7\rho_7}}{\Delta x_{13} + \Delta x_{14}}$$

$$\overline{v}_1 = \frac{\Delta x_9^{v_2} + \Delta x_{10}^{v_1}}{\Delta x_9 + \Delta x_{10}}$$

$$\overline{v}_2 = \frac{\Delta x_{11}^{v_4} + \Delta x_{12}^{v_3}}{\Delta x_{11} + \Delta x_{12}}$$

$$\overline{(\alpha\rho u)}_3 = \frac{1}{2} [(1 + \text{SGN}(\overline{v}_1)) \overline{(\alpha\rho)}_3 u_3 + (1 - \text{SGN}(\overline{v}_1)) \overline{(\alpha\rho)}_0 u_0]$$

$$\overline{(\alpha\rho u)}_4 = \frac{1}{2} [(1 + \text{SGN}(\overline{v}_2)) \overline{(\alpha\rho)}_0 u_0 + (1 - \text{SGN}(\overline{v}_2)) \overline{(\alpha\rho)}_4 u_4]$$

$$\frac{\partial}{\partial y} (\alpha \rho u v) \big|_o = \frac{\bar{v}_2 \overline{(\alpha \rho u)}_4 - \bar{v}_1 \overline{(\alpha \rho u)}_3}{\Delta y_2 + \Delta y_3} \quad (23)$$

$$\text{Let } \overline{(\alpha \rho)}_5 = \frac{\Delta x_{15} \alpha_{10}^o \rho_{10} + \Delta x_{16} \alpha_{9}^o \rho_9}{\Delta x_{15} + \Delta x_{16}}$$

$$\overline{(\alpha \rho)}_6 = \frac{\Delta x_{21} \alpha_{12}^o \rho_{12} + \Delta x_{22} \alpha_{11}^o \rho_{11}}{\Delta x_{21} + \Delta x_{22}}$$

$$\bar{w}_1 = \frac{\Delta x_{17} w_2 + \Delta x_{16} w_1}{\Delta x_{17} + \Delta x_{16}}$$

$$\bar{w}_2 = \frac{\Delta x_{19} w_4 + \Delta x_{20} w_3}{\Delta x_{19} + \Delta x_{20}}$$

$$\overline{(\alpha \rho u)}_5 = \frac{1}{2} [(1 + \text{SGN } (\bar{w}_1)) \overline{(\alpha \rho)}_5 u_5 + (1 - \text{SGN } (\bar{w}_1)) \overline{(\alpha \rho)}_o u_o]$$

$$\overline{(\alpha \rho u)}_6 = \frac{1}{2} [(1 + \text{SGN } (\bar{w}_2)) \overline{(\alpha \rho)}_o u_o + (1 - \text{SGN } (\bar{w}_2)) \overline{(\alpha \rho)}_6 u_6]$$

$$\frac{\partial}{\partial z} (\alpha \rho u w) \big|_o = \frac{\bar{w}_2 \overline{(\alpha \rho u)}_6 - \bar{w}_1 \overline{(\alpha \rho u)}_5}{\Delta z_2 + \Delta z_3} \quad (24)$$

$$\text{Let } \overline{(\alpha)}_o = \frac{\Delta x_3 \alpha_3 + \Delta x_4 \alpha_2}{\Delta x_3 + \Delta x_4}$$

$$(\alpha \frac{\partial P}{\partial x}) \big|_o = \overline{(\alpha)}_o \left[\frac{P_3 - P_2}{\Delta x_3 + \Delta x_4} \right] \quad (25)$$

Consider equation 3 evaluated at v - point o in Figures 6 and 7.

$$\text{Let } \overline{(\alpha \rho)}_o^n = \frac{\Delta y_3 \alpha_{3\rho_3}^n + \Delta y_4 \alpha_{2\rho_2}^n}{\Delta y_3 + \Delta y_4}$$

Figure 6. Grid System Around v-point '0' in x-y Plane.

Figure 7. Grid System Around v-point '0' in y-z Plane.

$$\frac{\partial}{\partial t} (\alpha \rho v) \Big|_0 = \frac{\overline{(\alpha \rho)_0^n + 1} \overline{v_0^n + 1} \overline{(\alpha \rho)_0^n v_0^n}}{\Delta t} \quad (26)$$

$$\text{Let } \overline{(\alpha \rho)}_1 = \frac{\Delta y_1 \alpha_2 \rho_2 + \Delta y_2 \alpha_1 \rho_1}{\Delta y_1 + \Delta y_2}$$

$$\overline{(\alpha \rho)}_2 = \frac{\Delta y_5 \alpha_4 \rho_4 + \Delta y_6 \alpha_3 \rho_3}{\Delta y_5 + \Delta y_6}$$

$$\overline{v}_1 = \frac{\Delta y_2 v_0 + \Delta y_3 v_1}{\Delta y_2 + \Delta y_3}$$

$$\overline{v}_2 = \frac{\Delta y_4 v_2 + \Delta y_5 v_0}{\Delta y_4 + \Delta y_5}$$

$$\overline{(\alpha \rho v)}_1 = \frac{1}{2} [(1 + \text{SGN}(\overline{v}_1)) \overline{(\alpha \rho)}_1 v_1 + (1 - \text{SGN}(\overline{v}_1)) \overline{(\alpha \rho)}_0 v_0]$$

$$\overline{(\alpha \rho v)}_2 = \frac{1}{2} [(1 + \text{SGN}(\overline{v}_2)) \overline{(\alpha \rho)}_0 v_0 + (1 - \text{SGN}(\overline{v}_2)) \overline{(\alpha \rho)}_2 v_2]$$

$$\frac{\partial}{\partial y} (\alpha \rho v v) \Big|_0 = \frac{\overline{v}_2 \overline{(\alpha \rho v)}_2 - \overline{v}_1 \overline{(\alpha \rho v)}_1}{\Delta y_3 + \Delta y_4} \quad (27)$$

$$\text{Let } \overline{(\alpha \rho)}_3 = \frac{\Delta y_7 \alpha_6 \rho_6 + \Delta y_8 \alpha_5 \rho_5}{\Delta y_7 + \Delta y_8}$$

$$\overline{(\alpha \rho)}_4 = \frac{\Delta y_{13} \alpha_8 \rho_8 + \Delta y_{14} \alpha_7 \rho_7}{\Delta y_{13} + \Delta y_{14}}$$

$$\overline{u}_1 = \frac{\Delta y_9 u_2 + \Delta y_{10} u_1}{\Delta y_9 + \Delta y_{10}}$$

$$\overline{u}_2 = \frac{\Delta y_{11} u_4 + \Delta y_{12} u_3}{\Delta y_{11} + \Delta y_{12}}$$

$$\begin{aligned}\overline{(\alpha\rho v)}_3 &= \frac{1}{2} [(1 + \text{SGN}(\overline{u}_1)) \overline{(\alpha\rho)}_3 v_3 + (1 - \text{SGN}(\overline{u}_1)) \overline{(\alpha\rho)}_0 v_0] \\ \overline{(\alpha\rho v)}_4 &= \frac{1}{2} [(1 + \text{SGN}(\overline{u}_2)) \overline{(\alpha\rho)}_0 v_0 + (1 - \text{SGN}(\overline{u}_2)) \overline{(\alpha\rho)}_4 v_4] \\ \frac{\partial}{\partial x} (\alpha\rho v u)|_0 &= \frac{\overline{u}_2 \overline{(\alpha\rho v)}_4 - \overline{u}_1 \overline{(\alpha\rho v)}_3}{\Delta x_2 + \Delta x_3}\end{aligned}\quad (28)$$

$$\text{Let } \overline{(\alpha\rho)}_5 = \frac{\Delta y_{15} \alpha_{10} \rho_{10} + \Delta y_{16} \alpha_9 \rho_9}{\Delta y_{15} + \Delta y_{16}}$$

$$\overline{(\alpha\rho)}_6 = \frac{\Delta y_{21} \alpha_{12} \rho_{12} + \Delta y_{22} \alpha_{11} \rho_{11}}{\Delta y_{21} + \Delta y_{22}}$$

$$\overline{w}_1 = \frac{\Delta y_{17} w_2 + \Delta y_{18} w_1}{\Delta y_{17} + \Delta y_{18}}$$

$$\overline{w}_2 = \frac{\Delta y_{19} w_4 + \Delta y_{20} w_3}{\Delta y_{19} + \Delta y_{20}}$$

$$\overline{(\alpha\rho v)}_5 = \frac{1}{2} [(1 + \text{SGN}(\overline{w}_1)) \overline{(\alpha\rho)}_5 v_5 + (1 - \text{SGN}(\overline{w}_1)) \overline{(\alpha\rho)}_0 v_0]$$

$$\overline{(\alpha\rho v)}_6 = \frac{1}{2} [(1 + \text{SGN}(\overline{w}_2)) \overline{(\alpha\rho)}_0 v_0 + (1 - \text{SGN}(\overline{w}_2)) \overline{(\alpha\rho)}_6 v_6]$$

$$\frac{\partial}{\partial z} (\alpha\rho v w)|_0 = \frac{\overline{w}_2 \overline{(\alpha\rho v)}_6 - \overline{w}_1 \overline{(\alpha\rho v)}_5}{\Delta z_2 + \Delta z_3}\quad (29)$$

$$\text{Let } \overline{(\alpha)}_0 = \frac{\Delta y_3 \alpha_3 + \Delta y_4 \alpha_2}{\Delta y_3 + \Delta y_4}$$

$$\left(\alpha \frac{\partial P}{\partial y}\right)|_0 = \overline{(\alpha)}_0 \left[\frac{P_3 - P_2}{\Delta y_3 + \Delta y_4}\right]\quad (30)$$

Consider equation 4 evaluated at w - point o in Figures 8 and 9.

$$\text{Let } \overline{(\alpha\rho)}_o^n = \frac{\Delta z_3^{\alpha\rho_3^n} + \Delta z_4^{\alpha\rho_2^n}}{\Delta z_3 + \Delta z_4}$$

$$\frac{\partial}{\partial t} (\alpha\rho w) \Big|_o = \frac{\overline{(\alpha\rho)}_o^{n+1} w_o^{n+1} - \overline{(\alpha\rho)}_o^n w_o^n}{\Delta t} \quad (31)$$

$$\text{Let } \overline{(\alpha\rho)}_3 = \frac{\Delta z_7^{\alpha\rho_6} + \Delta z_8^{\alpha\rho_5}}{\Delta z_7 + \Delta z_8}$$

$$\overline{(\alpha\rho)}_4 = \frac{\Delta z_{13}^{\alpha\rho_8} + \Delta z_{14}^{\alpha\rho_7}}{\Delta z_{13} + \Delta z_{14}}$$

$$\overline{u}_1 = \frac{\Delta z_9^{u_2} + \Delta z_{10}^{u_1}}{\Delta z_9 + \Delta z_{10}}$$

$$\overline{u}_2 = \frac{\Delta z_{11}^{u_4} + \Delta z_{12}^{u_3}}{\Delta z_{11} + \Delta z_{12}}$$

$$\overline{(\alpha\rho w)}_3 = \frac{1}{2} [(1 + \text{SGN } (\overline{u}_1)) \overline{(\alpha\rho)}_3 w_3 + (1 - \text{SGN } (\overline{u}_1)) \overline{(\alpha\rho)}_o w_o]$$

$$\overline{(\alpha\rho w)}_4 = \frac{1}{2} [(1 + \text{SGN } (\overline{u}_2)) \overline{(\alpha\rho)}_o w_o + (1 - \text{SGN } (\overline{u}_2)) \overline{(\alpha\rho)}_4 w_4]$$

$$\frac{\partial}{\partial x} (\alpha\rho w u) \Big|_o = \frac{\overline{u}_2 \overline{(\alpha\rho w)}_4 - \overline{u}_1 \overline{(\alpha\rho w)}_3}{\Delta x_2 + \Delta x_3} \quad (32)$$

$$\text{Let } \overline{(\alpha\rho)}_5 = \frac{\Delta z_{15}^{\alpha\rho_{10}} + \Delta z_{16}^{\alpha\rho_9}}{\Delta z_{15} + \Delta z_{16}}$$

$$\overline{(\alpha\rho)}_6 = \frac{\Delta z_{21}^{\alpha\rho_{12}} + \Delta z_{22}^{\alpha\rho_{11}}}{\Delta z_{21} + \Delta z_{22}}$$

Figure 8. Grid System Around w-point '0' in x-z Plane.

Figure 9. Grid System Around w-point '0' in y-z Plane.

$$\bar{v}_1 = \frac{\Delta z_{17} v_2 + \Delta z_{18} v_1}{\Delta z_{17} + \Delta z_{18}}$$

$$\bar{v}_2 = \frac{\Delta z_{19} v_4 + \Delta z_{20} v_3}{\Delta z_{19} + \Delta z_{20}}$$

$$\overline{(\alpha p w)}_5 = \frac{1}{2} [(1 + \text{SGN}(\bar{v}_1)) \overline{(\alpha p)}_5 w_5 + (1 - \text{SGN}(\bar{v}_1)) \overline{(\alpha p)}_0 w_0]$$

$$\overline{(\alpha p w)}_6 = \frac{1}{2} [(1 + \text{SGN}(\bar{v}_2)) \overline{(\alpha p)}_0 w_0 + (1 - \text{SGN}(\bar{v}_2)) \overline{(\alpha p)}_6 w_6]$$

$$\left. \frac{\partial}{\partial y} (\alpha p w w) \right|_0 = \frac{\bar{v}_2 \overline{(\alpha p w)}_6 - \bar{v}_1 \overline{(\alpha p w)}_5}{\Delta y_2 + \Delta y_3} \quad (33)$$

Let $\overline{(\alpha p)}_1 = \frac{\Delta z_1 \alpha_2 p_2 + \Delta z_2 \alpha_1 p_1}{\Delta z_1 + \Delta z_2}$

$$\overline{(\alpha p)}_2 = \frac{\Delta z_5 \alpha_4 p_4 + \Delta z_6 \alpha_3 p_3}{\Delta z_5 + \Delta z_6}$$

$$\bar{w}_1 = \frac{\Delta z_2 w_0 + \Delta z_3 w_1}{\Delta z_2 + \Delta z_3}$$

$$\bar{w}_2 = \frac{\Delta z_4 w_2 + \Delta z_5 w_0}{\Delta z_4 + \Delta z_5}$$

$$\overline{(\alpha p w)}_1 = \frac{1}{2} [(1 + \text{SGN}(\bar{w}_1)) \overline{(\alpha p)}_1 w_1 + (1 - \text{SGN}(\bar{w}_1)) \overline{(\alpha p)}_0 w_0]$$

$$\overline{(\alpha p w)}_2 = \frac{1}{2} [(1 + \text{SGN}(\bar{w}_2)) \overline{(\alpha p)}_0 w_0 + (1 - \text{SGN}(\bar{w}_2)) \overline{(\alpha p)}_2 w_2]$$

$$\left. \frac{\partial}{\partial z} (\alpha p w w) \right|_0 = \frac{\bar{w}_2 \overline{(\alpha p w)}_2 - \bar{w}_1 \overline{(\alpha p w)}_1}{\Delta z_3 + \Delta z_4} \quad (34)$$

$$\text{Let } \overline{(\alpha)}_o = \frac{\Delta z_3 \alpha_3 + \Delta z_4 \alpha_2}{\Delta z_3 + \Delta z_4}$$

$$\left(\alpha \frac{\partial P}{\partial z} \right) \Big|_o = \overline{(\alpha)}_o \left[\frac{P_3 - P_2}{\Delta z_3 + \Delta z_4} \right] \quad (35)$$

III. Extrapolation Procedure for Irregular Boundaries

In problems where the region under consideration has a curved boundary, it is necessary to determine certain variables through the use of irregular cells. A method for determining a variable located on a boundary from internally calculated points is presented. The method uses an interpolation technique which eliminates the need for information from points external to the boundary, which are in fact purely fictitious and inadmissible with respect to the finite difference scheme.

Suppose a general function f is known at point x_0 and x_{+1} and designated by $f_{i,j,k}$ and $f_{i+1,j,k}$ respectively, as shown in Figure 10. If the boundary passes through point x , then $f_{i-1,j,k}$ located at x_{-1} is exterior to the boundary and should not be used in the determination of $f_{i,j,k}$ at point x .

Figure 10 Typical Curved Boundary Intersection with Rectangular Mesh System

As a first approximation to the value $\hat{f}_{i,j,k}$ on the boundary, a linear interpolation involving the information at points x_0 and x_{-1} is made.

$$f_{i,j,k} = \frac{\Delta x_1 (1 - \xi) f_{i,j,k} + (\xi \Delta x_1 + \Delta x_2) f_{i-1,j,k}}{\Delta x_2 + \Delta x_1} = A_1 f_{i,j,k} + A_2 f_{i-1,j,k} \quad (36)$$

where $A_1 = \frac{(1 - \xi) \Delta x_1}{\Delta x_2 + \Delta x_1}$

$$A_2 = \frac{\xi \Delta x_1 + \Delta x_2}{\Delta x_2 + \Delta x_1}$$

It is noted that equation 36 requires information at point x_{-1} for $f_{i-1,j,k}$. A second approximation must be made for $f_{i,j,k}$ which can eliminate $f_{i-1,j,k}$. If a three point Lagrangian interpolation is used for points x_{-1} , x_0 and x_{+1} , elimination of $f_{i-1,j,k}$ can be accomplished. A value for $\hat{f}_{i,j,k}$ can be obtained as follows through Lagrangian interpolation.

$$\hat{f}_{i,j,k} = L_0 f_{i-1,j,k} + L_1 f_{i,j,k} + L_2 f_{i+1,j,k} \quad (37)$$

where L_0 , L_1 and L_2 are the Lagrangian coefficients given by

$$L_0 = \frac{(x-x_0)(x-x_{+1})}{(x_{-1}-x_0)(x_{-1}-x_{+1})} = \frac{(\xi \Delta x_1 + \Delta x_2)(\xi \Delta x_1 + \Delta x_2 + \Delta x_3 + \Delta x_4)}{(\Delta x_1 + \Delta x_2)(\Delta x_1 + \Delta x_2 + \Delta x_3 + \Delta x_4)}$$

$$L_1 = \frac{(x-x_{-1})(x-x_{+1})}{(x_0-x_{-1})(x_0-x_{+1})} = \frac{(\Delta x_1 - \xi \Delta x_1)(\xi \Delta x_1 + \Delta x_2 + \Delta x_3 + \Delta x_4)}{(\Delta x_1 + \Delta x_2)(\Delta x_3 + \Delta x_4)}$$

$$L_2 = \frac{(x-x_{-1})(x-x_0)}{(x_{+1}-x_{-1})(x_{+1}-x_0)} = \frac{(\Delta x_1 - \xi \Delta x_1)(\xi \Delta x_1 + \Delta x_2)}{(\Delta x_1 + \Delta x_2 + \Delta x_3 + \Delta x_4)(\Delta x_3 + \Delta x_4)}$$

Now eliminate $f_{i-1,j,k}$ from equations 36 and 37 and solve for $\hat{f}_{i,j,k}$ on the boundary

$$\hat{f}_{i,j,k} = \left[\frac{1}{1 - \frac{L_0}{A_2}} \right] \left\{ \left[L_1 - L_0 \frac{A_1}{A_2} \right] f_{i,j,k} + L_2 f_{i+1,j,k} \right\} \quad (38)$$

Equation 38 allows for the determination of a variable on the boundary from determined interior field information. For various specific boundary inter-sections this general formulation is developed in Appendix A.

IV. Boundary Conditions

General geometrical configurations require the specification of several types of boundary conditions. The boundary conditions applied at the walls of the computing mesh are typically one of the following: i) inflow, ii) outflow, iii) no-slip and iv) free slip. The boundary conditions are set before and after each iteration. The treatment of specific boundary conditions because of staggered mesh in three dimensions always requires successive interpolation and extrapolation to provide the appropriate variables at the boundary.

The code as being developed will identify each boundary point separately and be named independent of the mesh indices. In addition, its location relative to the mesh layout will also be determined. For each named boundary point the unit vectors for the surface passing through that point will be determined and stored. This is done initially once and for all.

i) Inflow: For every intersection of an inflow surface by a u, v , or w velocity line, a vector velocity as well as density and enthalpy will be prescribed. Hence, if the point, for example, is labeled as point xx , then

$$\begin{aligned}u(xx) &= u_b \\v(xx) &= v_b \\w(xx) &= w_b \\\rho(xx) &= \rho_b \\h(xx) &= h_b\end{aligned}$$

where u_b , v_b , w_b , ρ_b and h_b are specified.

ii) Outflow: On an outflow boundary several boundary conditions can be applied. Selection of the conditions to be used on an outflow boundary requires care. The conditions should be determined in such a way that their choice has minimal effect on the flow region of interest yet be physically meaningful. The idea of using a condition that has the least upstream effect has been used successfully by many investigators and will be used in the present code. The condition is really one of smoothness that is applied to the velocity components. One possible set of conditions may be

$$\begin{aligned}u_{i,j,k} &= u_{i-1,j,k} \\v_{i,j,k} &= v_{i-1,j,k} \\w_{i,j,k} &= w_{i-1,j,k} \\\rho_{i,j,k} &= \rho_{i-1,j,k} \\h_{i,j,k} &= h_{i-1,j,k}\end{aligned}$$

Other plausible conditions, such as the second derivative of the velocity components vanish may be used; however, the above are sufficient for illustrative purposes.

iii) No-Slip: The boundary conditions for a solid wall with viscosity present in the fluid require the sticking condition, i.e., no relative motion between the fluid particles at the wall and the wall. This condition implies that the velocity components at the wall vanish. Since the boundary points are labeled we would have at point xx on the boundary

$$u_b(xx) = 0$$

$$v_b(xx) = 0$$

$$w_b(xx) = 0$$

iv) Free Slip: The free-slip boundary condition for solid walls requires that there be zero normal flow across the wall, i.e., $\underline{V} \cdot \underline{n} = 0$ where $\underline{n}$ is the unit normal to the surface. The unit vectors defining the boundary surface are calculated and stored at the start of the code. Hence, the velocity conditions which are appropriately interpolated and then extrapolated to a boundary point can be used to satisfy the zero normal flux condition as well as determine the tangential component, i.e., the slip velocity along the wall, by using the unit normal and decomposing the velocity.

For the cases (iii) and (iv) the temperature can be specified for either the constant wall temperature condition or the constant heat flux condition, whichever is appropriate for the given problem.

Appendix A

In this appendix the general formulation presented in Section III is applied to several mesh-boundary intersection cases.

Case I: Right Intersection.

First, apply linear interpolation

$$\hat{u}_{i,j} = \frac{\Delta x_0 (1 - \xi) u_{i,j,k} + (\xi \Delta x_0 + \Delta x_1) u_{i-1,j,k}^*}{\Delta x_0 + \Delta x_1} = A_1 u_{i,j,k} + A_2 u_{i-1,j,k}$$

where

$$A_1 = \frac{(1 - \xi) \Delta x_0}{\Delta x_0 + \Delta x_1} \quad (A-1)$$

$$A_2 = \frac{\xi \Delta x_0 + \Delta x_1}{\Delta x_0 + \Delta x_1}$$

Second, use 3 points, to find coefficients

$$\begin{array}{ccccccc} & & \downarrow & & & & \\ & & x & & & & \\ x_n & x_{-1} & & x_0 & x_{+1} & & \\ f_n & u_{i-1,j,k} & & u_{i,j,k} & u_{i+1,j,k} & & \\ & & \uparrow & & & & \\ & & u_{i,j,k} & & & & \end{array}$$

*Note: Take right minus left as
always positive

$$\begin{aligned}
 L_0 &= \frac{(x-x_0)(x-x_{+1})}{(x_1-x_0)(x_{-1}-x_{+1})} = + \frac{(\xi \Delta x_0 + \Delta x_1)(\xi \Delta x_0 + \Delta x_1 + \Delta x_2 + \Delta x_3)}{(\Delta x_0 + \Delta x_1)(\Delta x_0 + \Delta x_1 + \Delta x_2 + \Delta x_3)} \\
 L_1 &= \frac{(x-x_{-1})(x-x_{+1})}{(x_0-x_{-1})(x_0-x_{+1})} = + \frac{(\Delta x_0 - \xi \Delta x_0)(\xi \Delta x_0 + \Delta x_1 + \Delta x_2 + \Delta x_3)}{(\Delta x_0 + \Delta x_1)(\Delta x_2 + \Delta x_3)} \\
 L_2 &= \frac{(x-x_{-1})(x-x_0)}{(x_{+1}-x_{-1})(x_{+1}-x_0)} = - \frac{(\Delta x_0 - \xi \Delta x_0)(\xi \Delta x_0 + \Delta x_1)}{(\Delta x_0 + \Delta x_1 + \Delta x_2 + \Delta x_3)(\Delta x_2 + \Delta x_3)}
 \end{aligned}$$

$$u_{i,j,k}^{\wedge} = L_0 u_{i-1,j,k} + L_1 u_{i,j,k} + L_2 u_{i+1,j,k} \quad (A-2)$$

Now eliminate external point $u_{i-1,j,k}$ and solve for $u_{i,j,k}^{\wedge}$ which is on the boundary.

From equation (A-1), we obtain

$$u_{i-1,j,k} = \frac{1}{A_2} u_{i,j,k}^{\wedge} - \frac{A_1}{A_2} u_{i,j,k} \quad (A-3)$$

Substituting equation (A-3) into (A-2)

$$\begin{aligned}
 u_{i,j,k}^{\wedge} &= L_0 \left[\frac{1}{A_2} u_{i,j,k}^{\wedge} - \frac{A_1}{A_2} u_{i,j,k} \right] + L_1 u_{i,j,k} + L_2 u_{i+1,j,k} \\
 u_{i,j,k}^{\wedge} \left[1 - \frac{L_0}{A_2} \right] &= \left[L_1 - L_0 \frac{A_1}{A_2} \right] u_{i,j,k} + L_2 u_{i+1,j,k} \\
 u_{i,j,k}^{\wedge} &= \frac{1}{\left[1 - \frac{L_0}{A_2} \right]} \left\{ \left[L_1 - L_0 \frac{A_1}{A_2} \right] u_{i,j,k} + L_2 u_{i+1,j,k} \right\} \quad (A-4)
 \end{aligned}$$

Case II: Left Intersection

Apply linear interpolation,

$$\hat{u}_{i,j,k} = A_1 u_{i,j,k} + A_2 u_{i+1,j,k} \quad (A-5)$$

$$A_1 = \frac{(1 - \eta) \Delta x_3}{\Delta x_2 + \Delta x_3}$$

$$A_2 = \frac{\eta \Delta x_3 + \Delta x_2}{\Delta x_2 + \Delta x_3}$$

$$u_{i+1,j,k} = \frac{1}{A_2} \hat{u}_{i,j,k} - \frac{A_1}{A_2} u_{i,j,k} \quad (A-6)$$

Use three points,

$$\begin{aligned}
 L_0 &= \frac{(x-x_0)(x-x_{+1})}{(x_{-1}-x_0)(x_{-1}-x_{+1})} = - \frac{(\eta\Delta x_3 + \Delta x_2)(\Delta x_3 - \eta\Delta x_3)}{(\Delta x_0 + \Delta x_1)(\Delta x_0 + \Delta x_1 + \Delta x_2 + \Delta x_3)} \\
 L_1 &= \frac{(x-x_{-1})(x-x_{+1})}{(x_0-x_{-1})(x_0-x_{+1})} = + \frac{(\eta\Delta x_3 + \Delta x_2 + \Delta x_1 + \Delta x_0)(\Delta x_3 - \eta\Delta x_3)}{(\Delta x_0 + \Delta x_1)(\Delta x_2 + \Delta x_3)} \\
 L_2 &= \frac{(x-x_{-1})(x-x_0)}{(x_{+1}-x_{-1})(x_{+1}-x_0)} = + \frac{(\eta\Delta x_3 + \Delta x_2 + \Delta x_1 + \Delta x_0)(\eta\Delta x_3 + \Delta x_2)}{(\Delta x_0 + \Delta x_1 + \Delta x_2 + \Delta x_3)(\Delta x_1 + \Delta x_6)}
 \end{aligned}$$

$$\therefore \hat{u}_{i,j,k} = L_0 u_{i-1,j,k} + L_1 u_{i,j,k} + L_2 u_{i+1,j,k} \quad (A-7)$$

Substitute equation (A-6) into equation (A-7), we obtain

$$\begin{aligned}
 \hat{u}_{i,j,k} &= L_0 u_{i-1,j,k} + L_1 u_{i,j,k} + L_2 \left[\frac{1}{A_2} \hat{u}_{i,j,k} - \frac{A_1}{A_2} u_{i,j,k} \right] \\
 \hat{u}_{i,j,k} \left[1 - \frac{L_2}{A_2} \right] &= L_0 u_{i-1,j,k} + \left[L_1 - L_2 \frac{A_1}{A_2} \right] u_{i,j,k} \\
 \hat{u}_{i,j,k} &= \frac{1}{\left[1 - \frac{L_2}{A_2} \right]} \left\{ L_0 u_{i-1,j,k} + \left[L_1 - L_2 \frac{A_1}{A_2} \right] u_{i,j,k} \right\} \quad (A-8)
 \end{aligned}$$

Case III: Top Intersection

Apply linear interpolation,

$$v_{i,j,k} = \frac{(\Delta y_3 - \gamma \Delta y_3) v_{i,j-1,k} + (\gamma \Delta y_3 + \Delta y_2) v_{i,j,k}}{\Delta y_2 + \Delta y_3}$$

$$v_{i,j,k} = B_1 v_{i,j-1,k} + B_2 v_{i,j,k} \quad (A-9)$$

$$\text{where } B_1 = \frac{\Delta y_3 (1-\alpha)}{\Delta y_2 + \Delta y_3}$$

$$B_2 = \frac{\alpha \Delta y_3 + \Delta y_2}{\Delta y_2 + \Delta y_3}$$

Use three points,

↓
y

y_n, y_{-1} y_o y_{+1}

f_n, v_{i,j,k} v_{i,j,k} v_{i,j-1,k} v_{i,j-2,k}

$$L_o = \frac{(y-y_o)(y-y_{+1})}{(y_{-1}-y_o)(y_{-1}-y_{+1})} = + \frac{(\alpha \Delta y_3 + \Delta y_2)(\alpha \Delta y_3 + \Delta y_2 + \Delta y_1 + \Delta y_o)}{(\Delta y_3 + \Delta y_2)(\Delta y_3 + \Delta y_2 + \Delta y_1 + \Delta y_o)}$$

$$L_1 = \frac{(y-y_{-1})(y-y_{+1})}{(y_o-y_{-1})(y_o-y_{+1})} = + \frac{(\Delta y_3 - \alpha \Delta y_3)(\alpha \Delta y_3 + \Delta y_2 + \Delta y_1 + \Delta y_o)}{(\Delta y_3 + \Delta y_2)(\Delta y_1 + \Delta y_o)}$$

$$L_2 = \frac{(y-y_{-1})(y-y_o)}{(y_{+1}-y_{-1})(y_{+1}-y_o)} = - \frac{(\Delta y_3 - \alpha \Delta y_3)(\alpha \Delta y_3 + \Delta y_2)}{(\Delta y_3 + \Delta y_2 + \Delta y_1 + \Delta y_o)(\Delta y_1 + \Delta y_o)}$$

$$v_{i,j,k}^{\wedge} = L_0 v_{i,j,k} + L_1 v_{i,j-1,k} + L_2 v_{i,j-2,k} \quad (A-10)$$

Now eliminate external point $v_{i,j,k}$

From equation (A-9)

$$v_{i,j,k} = \frac{1}{B_2} v_{i,j,k}^{\wedge} - \frac{B_1}{B_2} v_{i,j-1,k} \quad (A-11)$$

Substituting equation (A-9) into equation (A-10), we obtain

$$\begin{aligned} v_{i,j,k} &= L_0 \left[\frac{1}{B_2} v_{i,j,k}^{\wedge} - \frac{B_1}{B_2} v_{i,j-1,k} \right] + L_1 v_{i,j-1,k} + L_2 v_{i,j-2,k} \\ \left[1 - \frac{L_0}{B_2} \right] v_{i,j,k}^{\wedge} &= \left[L_1 - L_0 \frac{B_1}{B_2} \right] v_{i,j-1,k} + L_2 v_{i,j-2,k} \\ v_{i,j,k}^{\wedge} &= \frac{1}{\left[1 - \frac{L_0}{B_2} \right]} \left\{ \left[L_1 - L_0 \frac{B_1}{B_2} \right] v_{i,j-1,k} + L_2 v_{i,j-2,k} \right\} \end{aligned} \quad (A-12)$$

$$v_{i,j,k}^{\hat{}} = L_0 v_{i,j,k} + L_1 v_{i,j-1,k} + L_2 v_{i,j-2,k} \quad (A-15)$$

Substituting equation (A-14) into equation (A-15), we obtain

$$v_{i,j,k}^{\hat{}} = L_0 v_{i,j,k} + L_1 v_{i,j-1,k} + L_2 \left[\frac{1}{B_2} v_{i,j,k}^{\hat{}} - \frac{B_1}{B_2} v_{i,j-1,k} \right]$$

$$1 - \frac{L_2}{B_2} v_{i,j,k}^{\hat{}} = L_0 v_{i,j,k} + \left[L_1 - L_2 \frac{B_1}{B_2} \right] v_{i,j-1,k}$$

$$v_{i,j,k}^{\hat{}} = \frac{1}{\left[1 - \frac{L_2}{B_2} \right]} \left\{ L_0 v_{i,j,k} + \left[L_1 - L_2 \frac{B_1}{B_2} \right] v_{i,j-1,k} \right\} \quad (A-16)$$

Case V: Front Intersection

Apply linear interpolation

$$w_{i,j,k-hat} = \frac{(\Delta z_3 - \alpha \Delta z_3) w_{i,j,k-1} + (\alpha \Delta z_3 + \Delta z_2) w_{i,j,k}}{\Delta z_2 + \Delta z_3}$$

$$w_{i,j,k-hat} = C_1 w_{i,j,k-1} + C_2 w_{i,j,k} \quad (A-17)$$

where $C_1 = \frac{\Delta z_3 (1 - \alpha)}{\Delta z_2 + \Delta z_3}$

$$C_2 = \frac{\alpha \Delta z_3 + \Delta z_2}{\Delta z_2 + \Delta z_3}$$

Use three points,

$$L_0 = \frac{(z - z_0)(z - z_{+1})}{(z_{-1} - z_0)(z_{-1} - z_{+1})} = + \frac{(\alpha \Delta z_3 + \Delta z_2)(\alpha \Delta z_3 + \Delta z_3 + \Delta z_1 + \Delta z_0)}{(\Delta z_3 + \Delta z_2)(\Delta z_3 + \Delta z_2 + \Delta z_1 + \Delta z_0)}$$

$$L_1 = \frac{(z - z_{-1})(z - z_{+1})}{(z_0 - z_{-1})(z_0 - z_{+1})} = + \frac{(\Delta z_3 - \alpha \Delta z_2)(\alpha \Delta z_3 + \Delta z_2 + \Delta z_1 + \Delta z_0)}{(\Delta z_3 + \Delta z_2)(\Delta z_1 + \Delta z_0)}$$

$$L_2 = \frac{(z - z_{-1})(z - z_0)}{(z_{+1} - z_{-1})(z_{+1} - z_0)} = - \frac{(\Delta z_3 - \alpha \Delta z_3)(\alpha \Delta z_3 + \Delta z_2)}{(\Delta z_3 + \Delta z_2 + \Delta z_1 + \Delta z_0)(\Delta z_1 + \Delta z_0)}$$

$$w_{i,j,\hat{k}} = L_o w_{i,j,k} + L_1 w_{i,j,k-1} + L_2 w_{i,j,k-2} \quad (A-18)$$

Now eliminate external point $w_{i,j,k}$

From Eq. (A-17)

$$w_{i,j,k} = \frac{1}{C_2} w_{i,j,\hat{k}} - \frac{C_1}{C_2} w_{i,j,k-1} \quad (A-19)$$

Substituting Eq. (A-19) into Eq. (A-18), we obtain

$$w_{i,j,\hat{k}} = L_o \left[\frac{1}{C_2} w_{i,j,\hat{k}} - \frac{C_1}{C_2} w_{i,j,k-1} \right] + L_1 w_{i,j,k-1} + L_2 w_{i,j,k-2}$$

$$w_{i,j,\hat{k}} = \frac{1}{\left[1 - \frac{L_o}{C_2} \right]} \left\{ \left[L_1 - L_o \frac{C_1}{C_2} \right] w_{i,j,k-1} + L_2 w_{i,j,k-2} \right\} \quad (A-20)$$

Case VI: Back Intersection

Apply linear interpolation

$$w_{i,j,k} = C_1 w_{i,j,k-1} + C_2 w_{i,j,k-2} \quad (A-21)$$

$$C_1 = \frac{(1 - \delta) \Delta z_0}{\Delta z_1 + \Delta z_0}$$

$$C_2 = \frac{\delta \Delta z_0 + \Delta z_1}{\Delta z_1 + \Delta z_0}$$

$$w_{i,j,k-2} = \frac{1}{C_2} w_{i,j,k} - \frac{C_1}{C_2} w_{i,j,k-1} \quad (A-22)$$

Use three points,

$$L_0 = \frac{(z - z_0)(z - z_{+1})}{(z_{-1} - z_0)(z_{-1} - z_{+1})} = - \frac{(\delta \Delta z_0 + \Delta z_1)(\Delta z_0 - \delta \Delta z_0)}{(\Delta z_3 + \Delta z_2)(\Delta z_3 + \Delta z_2 + \Delta z_1 + \Delta z_0)}$$

$$L_1 = \frac{(z - z_{-1})(z - z_{+1})}{(z_0 - z_{-1})(z_0 - z_{+1})} = + \frac{(\delta \Delta z_0 + \Delta z_1 + \Delta z_2 + \Delta z_3)(\Delta z_0 - \delta \Delta z_0)}{(\Delta z_3 + \Delta z_2)(\Delta z_1 + \Delta z_0)}$$

$$L_2 = \frac{(z - z_{-1})(z - z_0)}{(z_{+1} - z_{-1})(z_{+1} - z_0)} = + \frac{(\delta \Delta z_0 + \Delta z_1 + \Delta z_2 + \Delta z_3)(\delta \Delta z_0 + \Delta z_1)}{(\Delta z_3 + \Delta z_2 + \Delta z_1 + \Delta z_0)(\Delta z_1 + \Delta z_0)}$$

$$w_{i,k,k} = L_0 w_{i,j,k} + L_1 w_{i,j,k-1} + L_2 w_{i,j,k-2} \quad (A-23)$$

Substituting Eq. (A-22) into Eq. (A-23), we obtain

$$w_{i,j,\hat{k}} = L_0 w_{i,j,k} + L_1 w_{i,j,k-1} + L_2 \left[\frac{1}{C_2} w_{i,j,k} - \frac{C_1}{C_2} w_{i,j,k-1} \right]$$

$$\left[1 - \frac{L_2}{C_2} \right] w_{i,j,\hat{k}} = L_0 w_{i,j,k} + \left[L_1 - L_2 \frac{C_1}{C_2} \right] w_{i,j,k-1}$$

$$w_{i,j,\hat{k}} = \frac{1}{\left[1 - \frac{L_2}{C_2} \right]} \left\{ L_0 w_{i,j,k} + \left[L_1 - L_2 \frac{C_1}{C_2} \right] w_{i,j,k-1} \right\} \quad (A-24)$$