MOMENTUM CONVECTION WITHIN THE STAGGERED GRID FORMULATION

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ABSTRACT

Like many finite volume-based thermal-hydraulic codes used within the nuclear industry, GOTHIC™ uses a staggered grid formulation, where the control volumes for the momentum equations are offset from the control volumes for the mass and energy equations. This scheme is advantageous because it directly couples the pressure and velocity in a numerically stable solution, but it also creates challenges for formulating the convection terms. In particular, the momentum convected by an orthogonal component of the velocity is the most difficult to handle numerically and the formulation can influence results and stability.

The effect of the finite volume formulation for the orthogonal convection terms in momentum equations is most apparent in a situation where the velocity vector is diagonal to the grid lines and there is a strong spatial gradient in the convected momentum. In a multiphase code like GOTHIC, these large gradients are typically due to large gradients in the phase volume fractions. Depending on the treatment of the orthogonal convection terms, these conditions can lead to a numerical momentum source in the phase that is being depleted as it moves across the grid. The momentum source was evident in a case with liquid injection (either continuous or droplets) into a gas filled volume at an angle to the grid. A particular example is drop injection from a spray nozzle. Although the observed momentum source is non-physical, this behavior had minimal impact on the overall results because the volume (and mass) of the accelerating fluid is diminishing with distance from the injection location.

A modified approach for calculating the momentum convected by orthogonal velocity components has been developed and implemented in GOTHIC that offers an improved treatment for this unique scenario. Both first- and second-order accurate schemes are considered. This paper outlines the modified donoring schemes with an emphasis on the attributes that address consistency, stability, and phase appearance. Results from initial testing comparing the original and modified schemes for a simple and more detailed simulation are presented.

GOTHIC™ incorporates technology developed for the electric power industry under the sponsorship of EPRI, the Electric Power Research Institute.

KEYWORDS
GOTHIC, staggered grid, multiphase flow, numerical methods

1. INTRODUCTION

The staggered grid formulation, where the control volumes for the momentum equations is offset from the control volumes for the mass and energy equations, is traditionally used by thermal-hydraulic codes. In this formulation, the velocity and flow rates are determined on the momentum mesh where the momentum equations are solved while the volume properties (volume fractions, pressure, enthalpy, density, *etc*.) are determined in the scalar mesh where the mass and energy equations are solved. This formulation is advantageous because it couples the pressure and velocity solutions, but it also creates challenges for formulating the momentum convection terms.

For a general Cartesian grid there are two distinct momentum transport terms: in-line transport and orthogonal transport. Generically, momentum convection for two-phase flow is expressed mathematically for phase ϕ as:

$$\nabla \cdot \left(\alpha_\phi\, \rho_\phi\, \vec{U}_\phi\, \vec{U}_\phi\right) \tag{1}$$

where α_ϕ is the phasic volume fraction, ρ_ϕ is the phasic density, and $\vec{U}_\phi$ is the phasic velocity vector, which is represented in Cartesian coordinates as:

$$\vec{U} = u\,\hat{\boldsymbol{\imath}} + v\,\hat{\boldsymbol{\jmath}} + w\,\hat{\boldsymbol{k}} \tag{2}$$

Integrating the convection term over a computational volume yields:

$$\int \nabla \cdot \left(\alpha_\phi\, \rho_\phi\, \vec{U}_\phi\, \vec{U}_\phi\right) dV = \underbrace{\int \left(\alpha_\phi\, \rho_\phi\, \vec{U}_\phi\, \vec{U}_\phi\right) \cdot dA}_{\text{By Divergence Theorem}} = \underbrace{\left(\alpha_\phi\, \rho_\phi\, \vec{U}_\phi\, \vec{U}_\phi\right) \cdot A}_{\text{Assuming uniform flux across the face}} = F\psi \tag{3}$$

where: F is the velocity through the face times the area of the face
ψ is the convected quantity (e.g., $\alpha_\phi \rho_\phi U_\phi$ for momentum)

Physically this represents force transmitted across the surfaces of the control volume. Expanding the outer product of the velocity vector yields a second-rank tensor:

$$\vec{U}\,\vec{U} = \begin{bmatrix} u \\ v \\ w \end{bmatrix} \begin{bmatrix} u & v & w \end{bmatrix} = \begin{bmatrix} uu & uv & uw \\ vu & vv & vw \\ wu & wv & ww \end{bmatrix} \tag{4}$$

The convected quantity, ψ, is determined based on the differencing scheme that is applied (e.g., upwind, central difference, *etc*.). Thermal-hydraulic codes applied within the nuclear industry traditionally employ a first order upwind (FOUP) scheme. The FOUP method is very stable, but can result in significant over prediction of the diffusion of the transported quantities. Some codes have introduced second-order accurate schemes, which reduce the numerical diffusion at a small penalty in run time. One example is a bounded second order (BSOUP) scheme, where bounded refers to limits that prevent the overshoot or undershoot issues that are typically associated with second-order accurate schemes.

Regardless of which differencing scheme is selected, the orthogonal transport terms are the most difficult to handle numerically and the selected formulation can influence results and stability. Using the FOUP scheme as an example, the donoring associated with the momentum convection in the transverse direction typically involves quantities associated with the momentum cell, which is highlighted on the schematic given in Figure 1. In the figures and formulations below, the upper case subscripts refer to the continuity cell values and lower case subscripts are used for the momentum cell values (continuity cell face values).

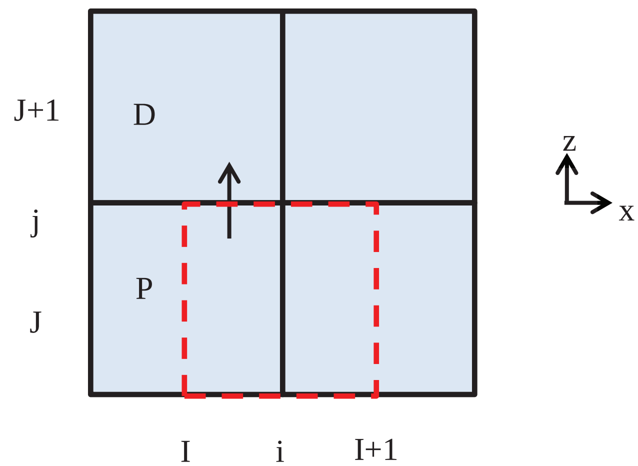

Figure 1. Schematic of the Traditional FOUP Donoring approach.

Assigning characteristic values for the momentum cell typically involves averaging the conditions of the adjacent continuity cells. For the case shown in the schematic (assuming positive flow through the face):

$$\overbrace{\left(U_{\phi,z,j}\, A_{I,j}\right)}^{F}\overbrace{\left[U_{\phi,x,i}\left(\alpha_\phi \rho_\phi\right)_{i,J}\right]}^{\psi} \tag{5}$$

where a volume weighted macroscopic density is applied:

$$\left(\alpha_\phi \rho_\phi\right)_{i,J} = \frac{\left(V\alpha_\phi \rho_\phi\right)_{I,J} + \left(V\alpha_\phi \rho_\phi\right)_{I+1,J}}{V_{I,J} + V_{I+1,J}} \tag{6}$$

Under certain conditions this can be a source of inconsistency between the mass and momentum solutions. Specifically, in the presence of large gradients, this can result in the momentum convected across this interface to be significantly different than the mass convected across this same interface. In a multiphase code these large gradients are typically due to large gradients in the phase volume fractions.

For applications with predominately 1-D flow, the above described issue is not a concern because in-line transport are the dominate momentum convection mechanisms and the orthogonal transport contributions are negligible. Most reactor system conditions are representative of this scenario and therefore the staggered grid formulation poses minimal concerns. However, the effect of the finite volume formulation for the orthogonal convection terms in momentum equations is most apparent in a situation where 1) the velocity vector is diagonal to the grid lines and 2) there is a strong spatial gradient in the convected momentum. One example would be liquid injection (either continuous or droplets) into a gas filled volume at an angle to the grid. This situation can be representative of a containment spray system when using a grid that has a higher resolution than the length scale of the liquid jet. For most applications the momentum effects are secondary to mass and energy contributions of the liquid injection and therefore the liquid injection can be modeled without explicitly representing the angle of injection. However, GOTHIC allows the user to specify the injection angle because the jet/spray trajectory is important for some applications and needs to be captured in the simulation.

Depending on the treatment of the orthogonal convection terms, minor inconsistencies between the mass and momentum solutions that are introduced by the staggered grid formulation can lead to a numerical momentum source in the phase that is being depleted as it moves across the grid. This manifests itself as liquid accelerating just downstream of the injection location, which is shown in Figure 2. It is important to note that although the observed momentum source is non-physical and can be observed on a local scale, this behavior had minimal impact on the overall results because the volume (and mass) of the accelerating fluid is diminishing with distance from the injection location.

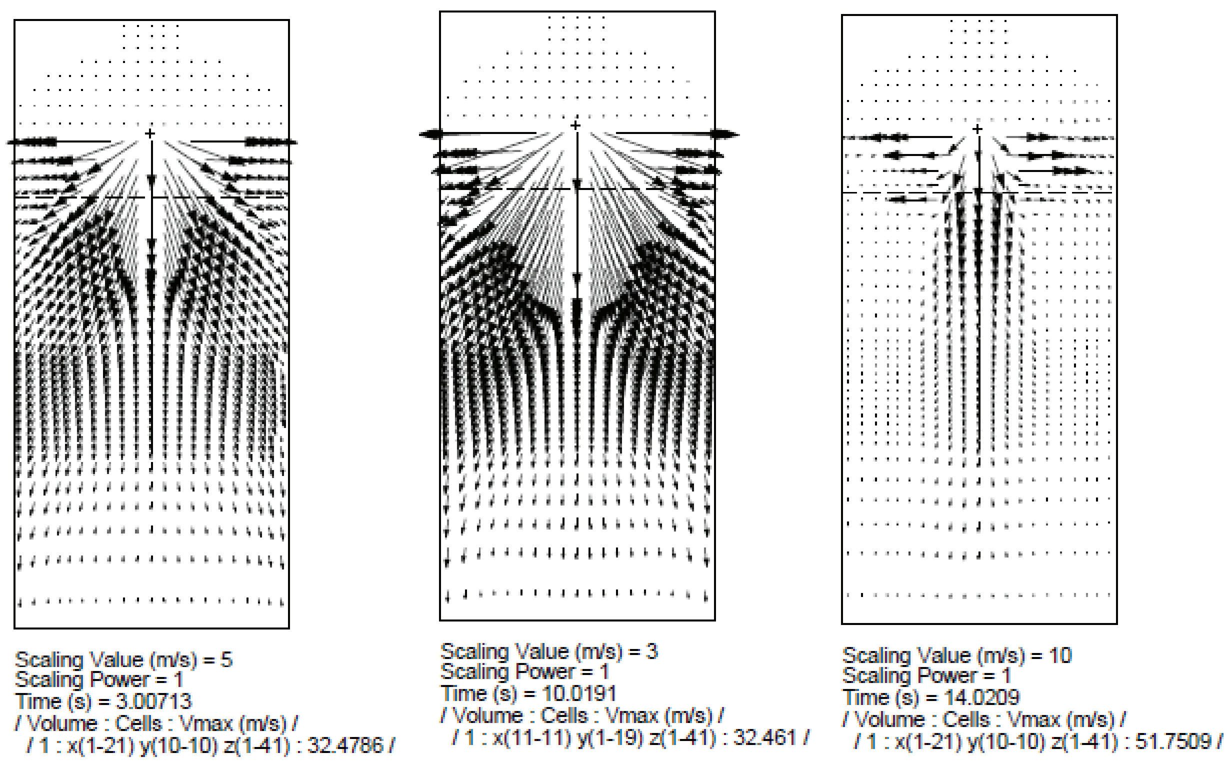

Figure 2. Vector Velocity Profiles predicted for Droplet Injection using BSOUP.

2. APPROACH

Alternative approaches and differencing schemes were examined in an effort to resolve the unique issue outlined in the previous section. Ultimately two additional approaches for calculating the momentum convected by orthogonal velocity components has been implemented into GOTHIC [1]. These include Modified First Order Upwind (MFOUP) and Flux-Limiter Second Order Upwind (FLSOUP) schemes.

2.1. Modified First Order Upwind (MFOUP) Method

In this approach, the continuity cell quantities are convected rather than those associated with the momentum cell. This is depicted in Figure 3. For the case depicted in the schematic with positive flow through the face the momentum convection is now calculated as:

$$\overbrace{\left(U_{\phi,z,j}\;A_{I,j}\right)}^{F}\overbrace{\left[U_{\phi,x,i}\;\left(\alpha_{\phi}\rho_{\phi}\right)_{I,J}\right]}^{\psi} \tag{8}$$

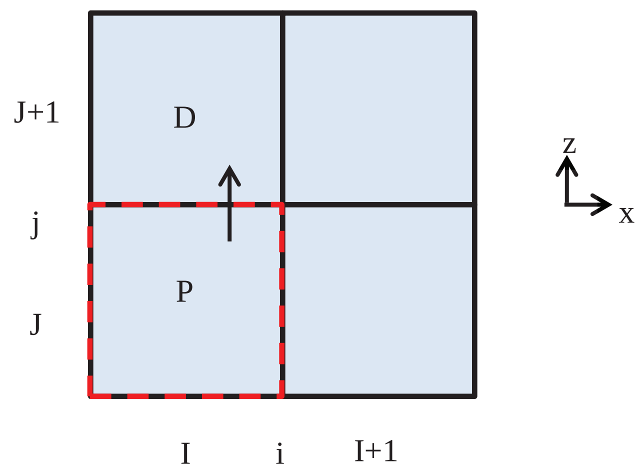

Figure 3. Schematic the of Modified Donoring approach (MFOUP Scheme).

2.1.1. Implementation Details

A new user selectable option has been added to GOTHIC, referred to as MFOUP. This modified approach is applied to all terms where momentum is convected by an orthogonal velocity component. The momentum convected by the inline velocity component and the donoring for all scalar quantities (e.g., density, volume fraction, enthalpy, etc.) still uses the standard FOUP method.

2.2. Flux-Limiter Second Order Upwind (FLSOUP) Method

While the modified donoring approach described in the previous section resolved the issue for a first-order accurate upwind scheme, issues still existed following the implementation of the same approach for the bounded second-order upwind scheme (BSOUP). This is because with the increased stencil, or range of influence, of the second-order scheme, the momentum convection can still be inconsistent with the mass transport in the vicinity of large void fraction gradients.

To address this issue a logical test was implemented on the void fraction to detect phase/field appearance within the range of computational cells considered. If phase/field appearance was detected then the solution would revert back to using the first-order upwind scheme rather than the second-order accurate scheme for that particular location. This approach successfully resolved the acceleration issues for the BSOUP scheme; however, some numerical instabilities were now observed in the predicted velocities (particularly for the case of droplet injection). It was postulated this was caused by potential inconsistencies in the donoring for different quantities associated with the same field (e.g., void fraction, density, and enthalpy). While the indices for the donor, upstream, and downstream cells are established based on a common convected quantity, the test for monotonic behavior or the application of the bounds associated with the solution could effectively yield different donoring between the quantities (e.g., some revert to upwind while others are bounded). It was postulated there may be an increased potential for this in the presence of steep gradients.

This was the motivation for considering a new approach using flux limiter schemes. These types of schemes, which are described in Reference [2] and [3], are intended to reduce numeral diffusion due to strong gradients in convected quantities while preserving the stability of lower order advection schemes. Flux limiter schemes are defined as:

$$Q_e = Q_{e,1st} + \phi(r)\left[Q_{e,2nd} - Q_{e,1st}\right] \tag{9}$$

where: $\phi(r)$ is the flux-limiter function, $Q_{e,1st}$ represents a convected quantity using a first-order accurate scheme, and $Q_{e,2nd}$ is the corresponding convected quantity from a a second-order accurate scheme. In this equation Q represents any quantity of interest that must be donored (e.g., volume fraction, density, enthalpy, momentum, etc.) and subscripts P, U, and D refer to the donor cell, the cell upwind of the donor cell, and the cell downwind of donor cell, respectively (see Figure 4).

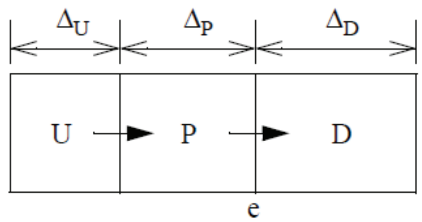

Figure 4. Finite Volume Cells.

Based on this definition, if $\phi(r) = 0$ then the first order accurate scheme is applied and if $\phi(r) = 1$ then the second order accurate scheme is applied. The smoothness parameter, r, which is an input to the flux-limiter function, is defined as:

$$r = \frac{Q_P - Q_D}{Q_U - Q_P}$$

Therefore, the smoothness parameter represents the ratio of successive gradients on the solution mesh.

The general advantages of flux-limiter schemes are:

1) They provide a quantitative estimate of the gradients associated with the cell of interest via the smoothness parameter, r, and therefore can handle strong gradients in a generalized fashion.

2) They provide a "smooth" transition between conditions where second order versus first order upwind schemes are applied, which may be numerically stabilizing.

3) They potentially allow for a single smoothness parameter to be calculated for each location and used for all variables at that location, providing an additional level of consistency in the donoring scheme.

Various limiter functions, $\phi(r)$, have been proposed (e.g., MinMod, SUPERBEE, *etc*.) each with different switching characteristics, which refers the magnitude of the gradient required before the scheme transitions between the higher and lower order accuracy solutions. Unfortunately, no particular limiter has been found to work universally well for all problems and therefore selection is often based on trial and error. However, the selected formulation should be symmetric and numerically stable. Symmetry ensures that the limiter treats positive and negative gradients of the same magnitude equally. Mathematically a symmetric limiter would exhibit the following property [3]:

$$\frac{\phi(r)}{r} = \phi\left(\frac{1}{r}\right) \tag{10}$$

Although several different flux limiters were investigated, ultimately the MinMod limiter [3] was selected because it is symmetric, tends to be robust, and is generally applicable to a wide class of problems. The MinMod limiter is defined as:

$$\phi(r) = max\big(0, min(r, 1)\big) \tag{11}$$

Therefore, a smoothness parameter greater than or equal to one results in the second-order upwind scheme being applied. Meanwhile, a smoothness parameter less than or equal to zero, which would correspond to a negative (non-monotonic) gradient between the upstream, donor, and downstream cells, results in the solution reverting back to the first order upwind solution. For values between 0 and 1 the solution smoothly transitions between the results for the first and second order accurate schemes.

MathCAD was used to perform some parametric studies over the void fraction domain to investigate the similarities/differences between these two schemes and visualize the characteristics. This was done by specifying the volume fraction associated with the donor volume and then varying the volume fraction associated with the upstream and downstream nodes. Therefore, a positive "change" represents an increase in volume fraction relative to the donor node and a negative "change" represents a decrease. A surface plot showing the resulting value for the advected volume fraction over the possible domain is shown in Figure 5. A surface plot showing the corresponding value for the limiter function is shown in Figure 6. A donor volume fraction of 30% was used for the sample results provided here. Therefore the change in volume fraction for the upstream/downstream volumes could range between -30% and +70%.

During the course of this evaluation it was determined that the bounded second order upwind (BSOUP) scheme is mathematically equivalent to a flux limiter scheme with the following definition for the limiter:

$$\phi(r) = max\big(0, min(2r, 1)\big) \tag{12}$$

Although similar to the MinMod limiter, as shown in Figure 7, this function is not symmetric. Meanwhile, Figure 8 shows the difference in advected volume fraction predicted by the two schemes. It can be seen that generally the two provide nearly identical results, except in the region between forward and backward gradients due to one being symmetric (MinMod), while the other is not (BSOUP).

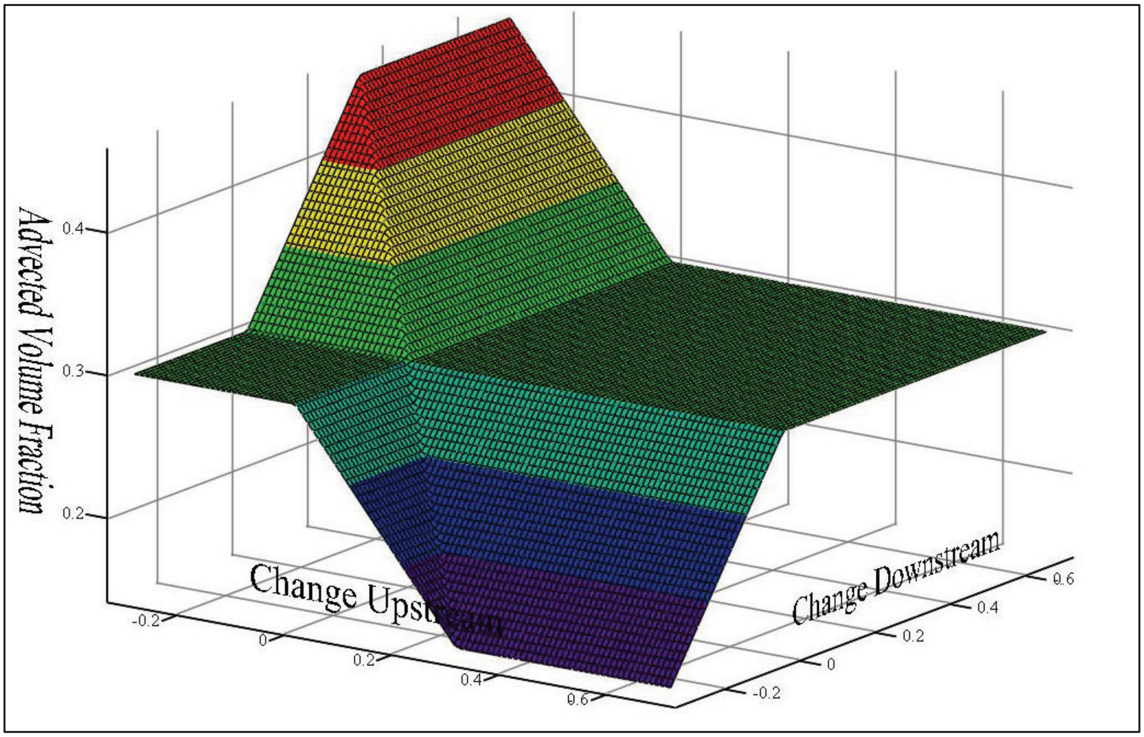

Figure 5. Advected Volume Fraction for MinMod Limiter with a 30%Volume Fraction in the Donor Cell.

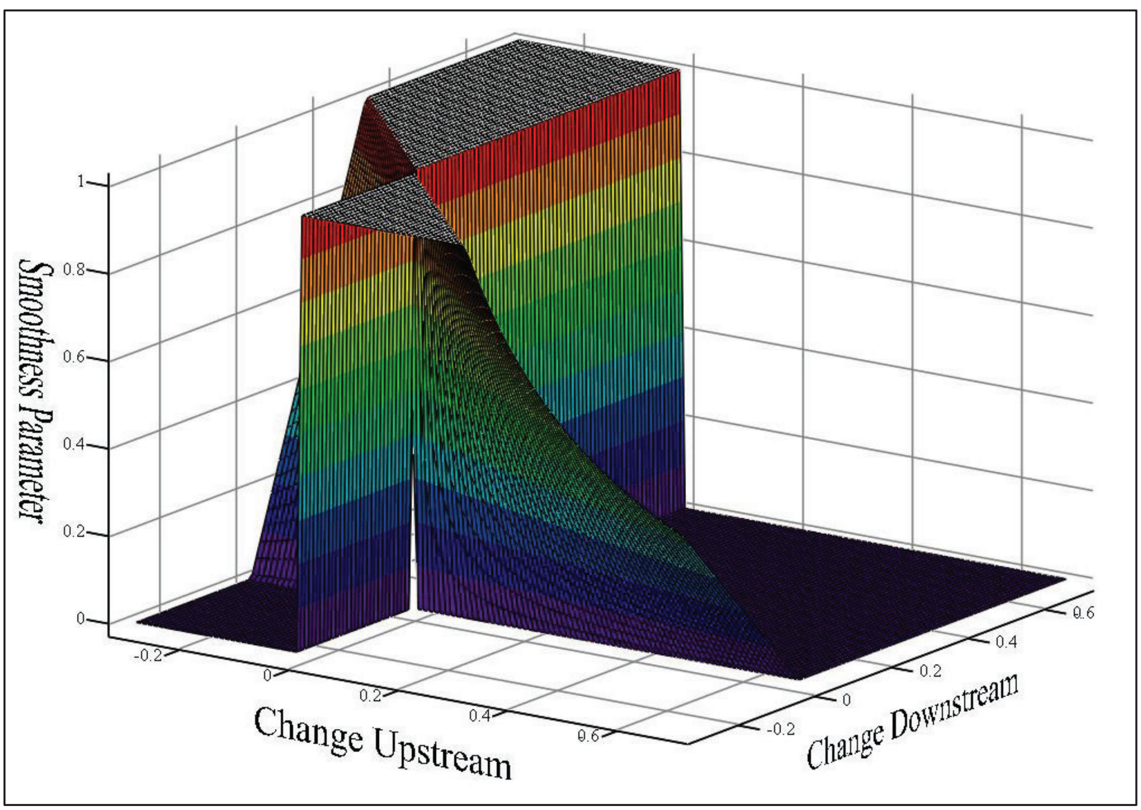

Figure 6. Corresponding Value of the MinMod Limiter.

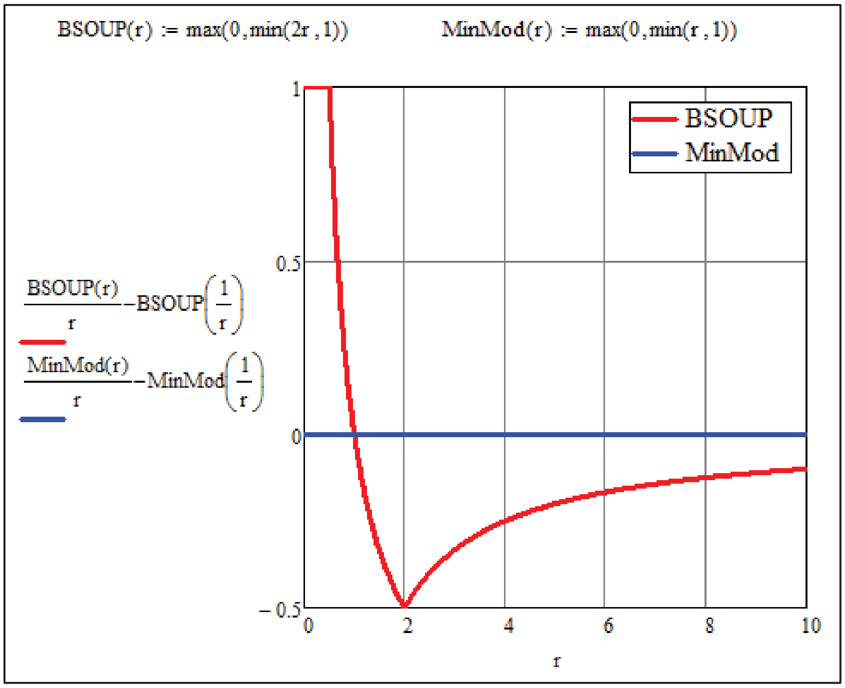

Figure 7. Symmetry Check.

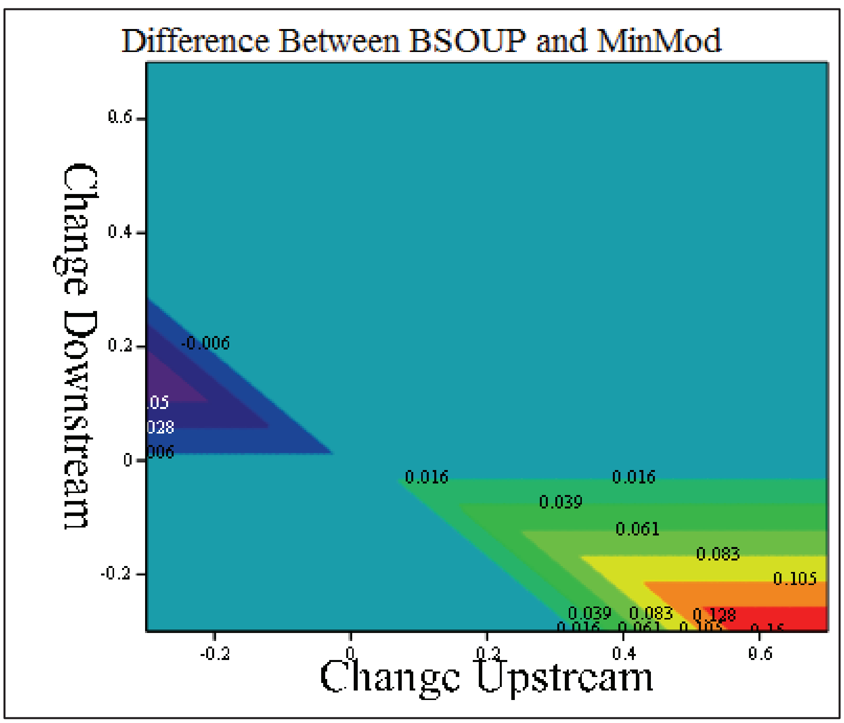

Figure 8: Difference between Advected Volume Fraction for the BSOUP and MinMod Schemes.

2.2.1. Implementation Details

A new user selectable option has been added to GOTHIC, referred to as FLSOUP. This new scheme includes:

1) a flux limiter (MinMod) scheme for calculating all donored quantities
2) the modified donoring approach (similar to the approach applied in the MFOUP method)
3) logic to detect phase/field appearance within cells U, P, and D.

A two-step process is applied that considers the gradient in both volume fraction and the quantity of interest (e.g., density, enthalpy, momentum, etc.). The minimum value for the smoothing parameter, from either the volume fraction or the individual quantity of interest, is used. This approach ensures the largest gradient between the two is captured.

As described previously, applying only Items 2 and 3 to the existing second order accurate scheme in GOTHIC successfully resolved the acceleration issues; however, some numerical instabilities were observed in the predicted velocities (particularly for the case of droplet injection). The logical test on the volume fraction to detect phase/field appearance was needed to ensure the mass and momentum convection are consistent in the vicinity of large volume fraction gradients. If phase/field appearance is detected then the solution reverts back to using the first-order upwind scheme rather than the second-order accurate scheme for that particular location.

3. RESULTS

A simple test case was generated that recreated the localized acceleration downstream of the injection location. This simple case was more computationally efficient than the original model and therefore was used as the test case during the development stage. Once the new differencing schemes (MFOUP and FLSOUP) were working as intended for the simple test problem they were exercised using the more complex problem.

3.1. Simple Test Case

The model used to test the behavior for these different schemes consists of a 2 meter cube that is sub-divided in all three directions (11 sub-volumes in each direction). There is a single flow boundary condition that is applied and connected to cell 896 (row 5, column 5, plane 8). This boundary condition is directed downwards and supplies 3 kg/s of liquid (101.35 kPa, 26.667 C). The flow path connecting the boundary condition to the subdivided volume has a tilt of 30 degrees, a rotation of 180 degrees, and a hydraulic diameter of 0.005 meters. A schematic representation of this test case is provided in Figure 9. The entire subdivided volume is initially filled with steam/air at 101.35 kPa, 26.667 C and 100% relative humidity. Injection in the form of either continuous liquid (droplet fraction = 0) or droplets (droplet fraction = 1 with a droplet diameter of 0.05 cm) was tested.

The primary figure-of-merit is the horizontal/transverse liquid velocity downstream of the injection location. Strip plots showing this velocity for the cell upstream (cell 895) and the 4 cells downstream of the injection location (cells 896 through 899) are provided for each of the four differencing schemes investigated: FOUP, MFOUP, BSOUP, and FLSOUP (with MinMod limiter). These plots can be used to examine velocities relative to one another (checking for acceleration/deceleration) and to ensure a numerically stable solution is obtained. Results are provided for both injection types (droplets on the left and continuous liquid on the right). The results can be summarized as follows:

1) FOUP – reasonable behavior for droplet injection, but small acceleration for liquid injection. Both are numerically stable.

2) MFOUP – acceleration associated with liquid injection eliminated and droplet behavior unchanged. Both still numerically stable.

3) BSOUP – acceleration for both droplet and liquid injection. Large numerical instabilities in predicted liquid velocity, but droplet case is numerically stable

4) FLSOUP – acceleration still exists downstream of the injection location; however, this acceleration is not as large as previously observed for the BSOUP case and the results are numerically stable.

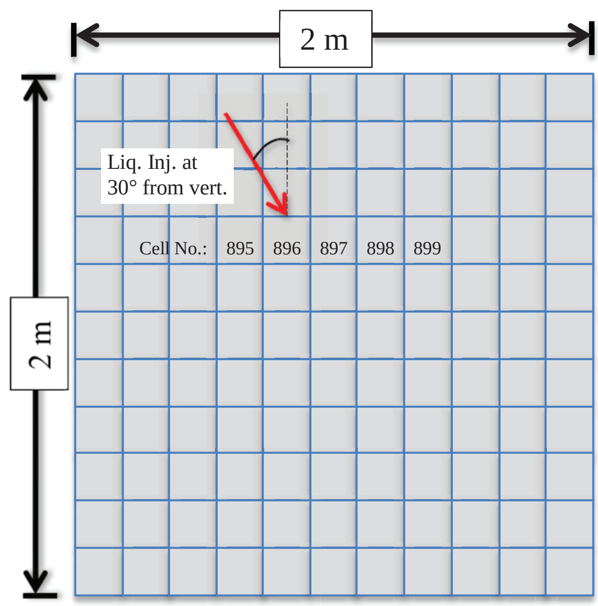

Figure 9: Schematic of Simple Test Case (2-D slice where liquid injection is located).

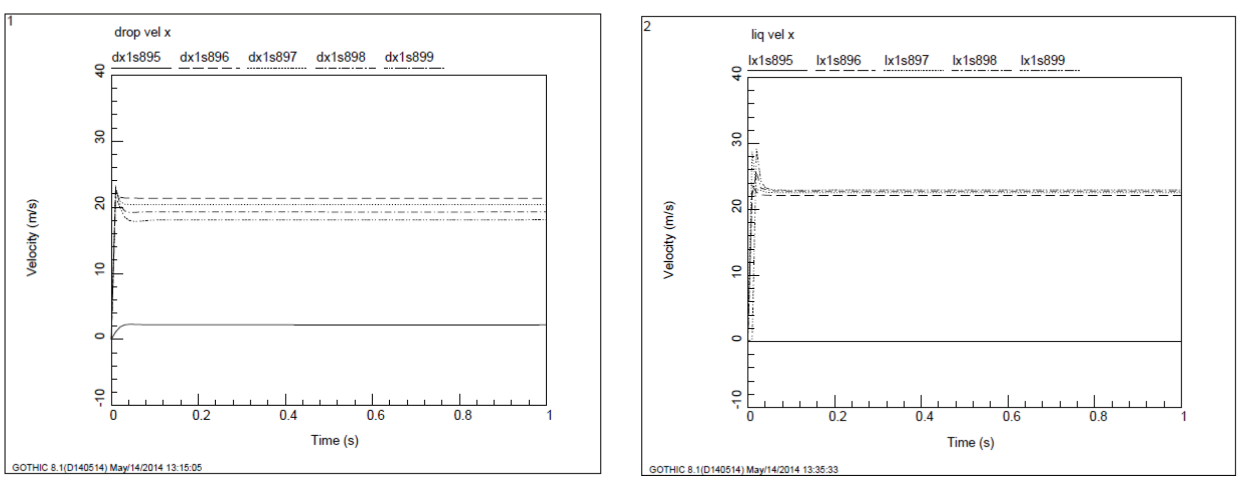

Figure 10: Transverse Velocities predicted using the FOUP scheme.

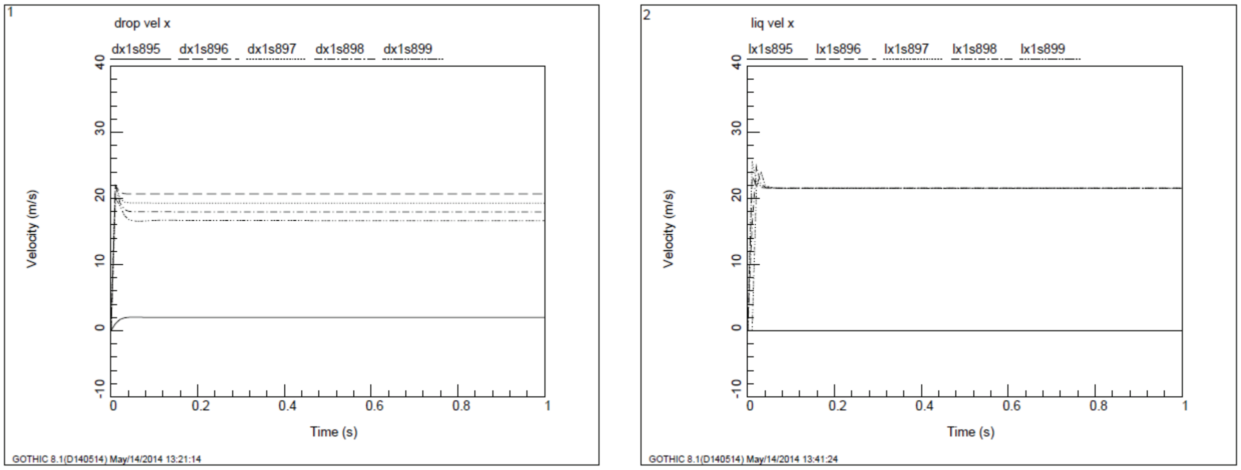

Figure 11: Transverse Velocities predicted using the MFOUP scheme.

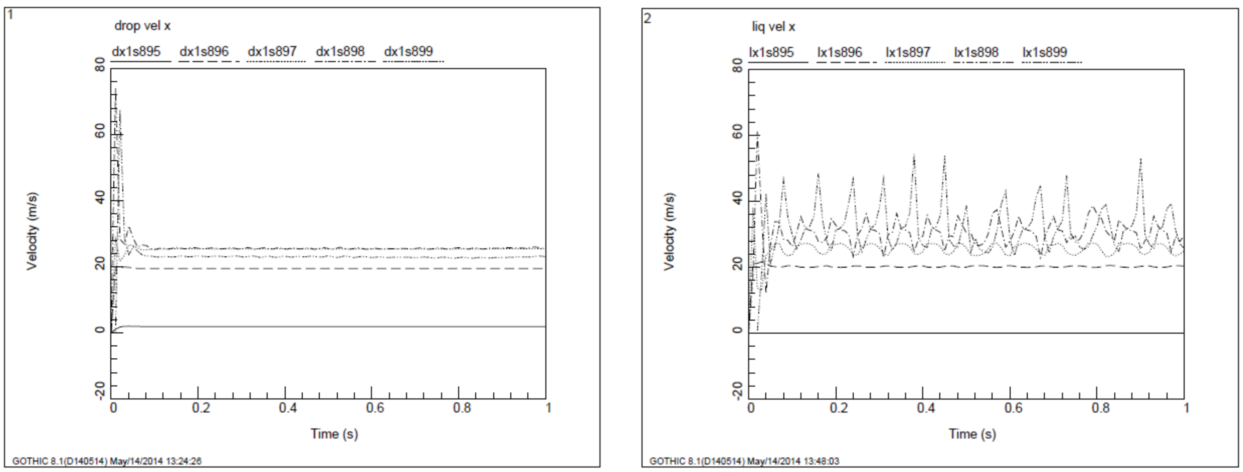

Figure 12: Transverse Velocities predicted using the BSOUP scheme.

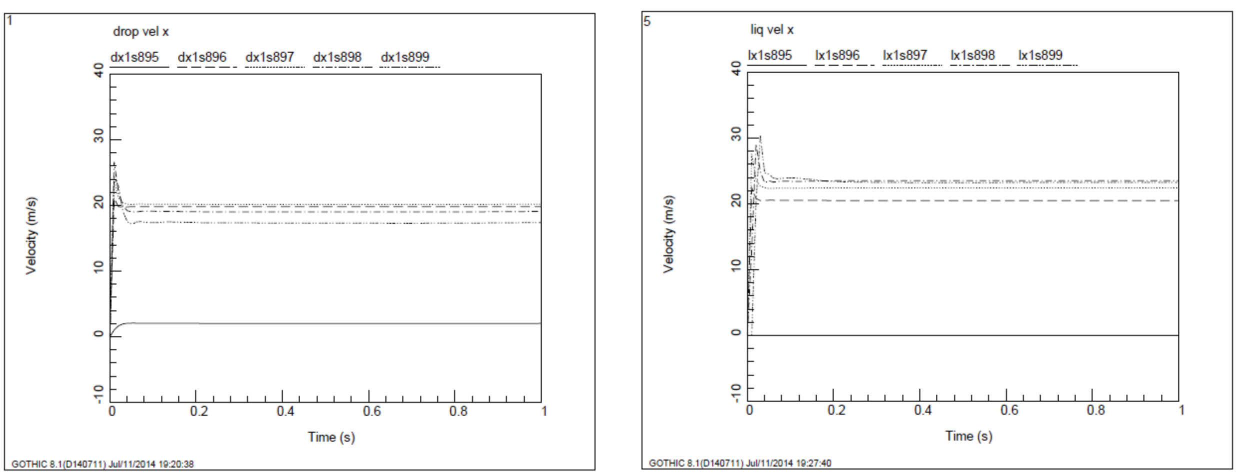

Figure 13: Transverse Velocities predicted using the FLSOUP scheme.

3.2. Detailed Test Case

This test case is representative of a containment spray system where the angle of the sprays is explicitly modeled and a high resolution grid is used to capture the spray distribution. The results obtained using the new MFOUP scheme are shown in Figure 14 for the more complex problem. Qualitatively the predicted results align with expectations. The velocity profiles emanating from the injection location are reasonable and the liquid is decelerating in all directions. Although not shown here, the results using the tradition FOUP scheme are very similar to those obtained using the new MFOUP scheme.

There are significant differences between the results obtained for the BSOUP scheme, which were shown previously in Figure 2, and the results obtained for the new FLSOUP scheme, which are shown in Figure 15. The new FLSOUP routine eliminates the transverse droplet acceleration that is observed in the vicinity of the injection location and therefore better aligns with expected behavior. Additionally, qualitatively, the predicted behavior using the FLSOUP scheme better aligns with the behavior observed for the first order accurate scheme.

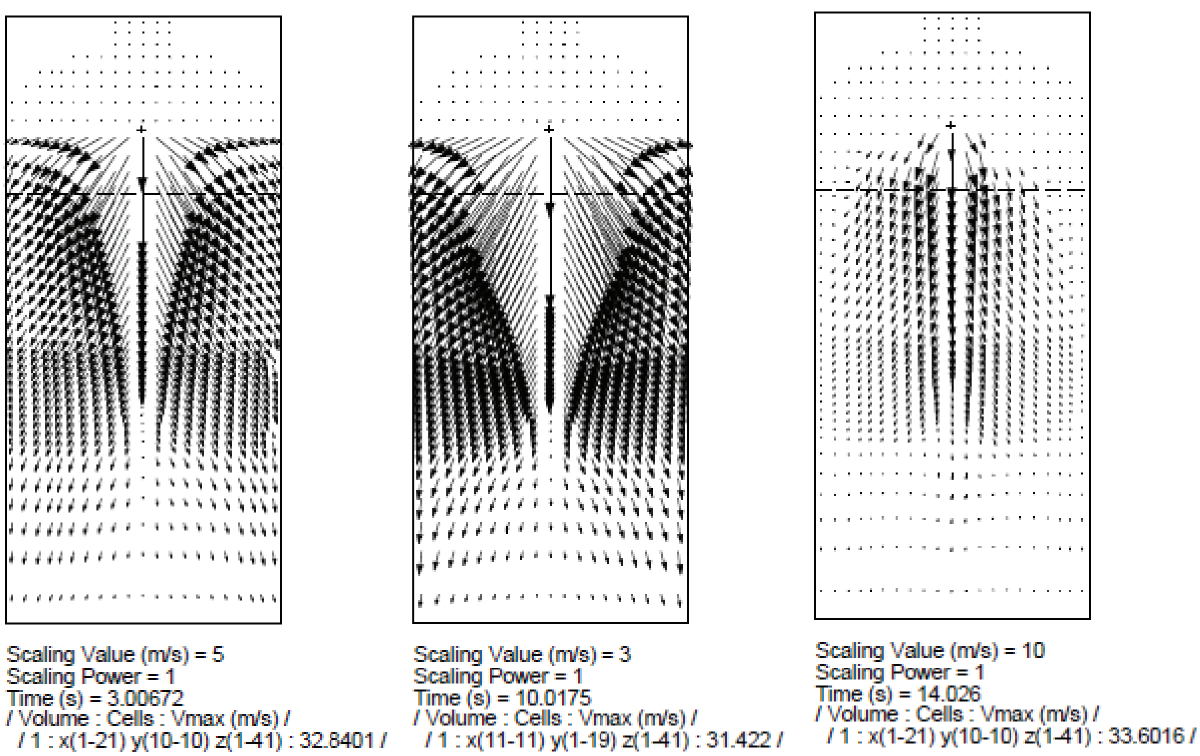

Figure 14. Vector Velocity Profiles predicted for Droplet Injection using MFOUP.

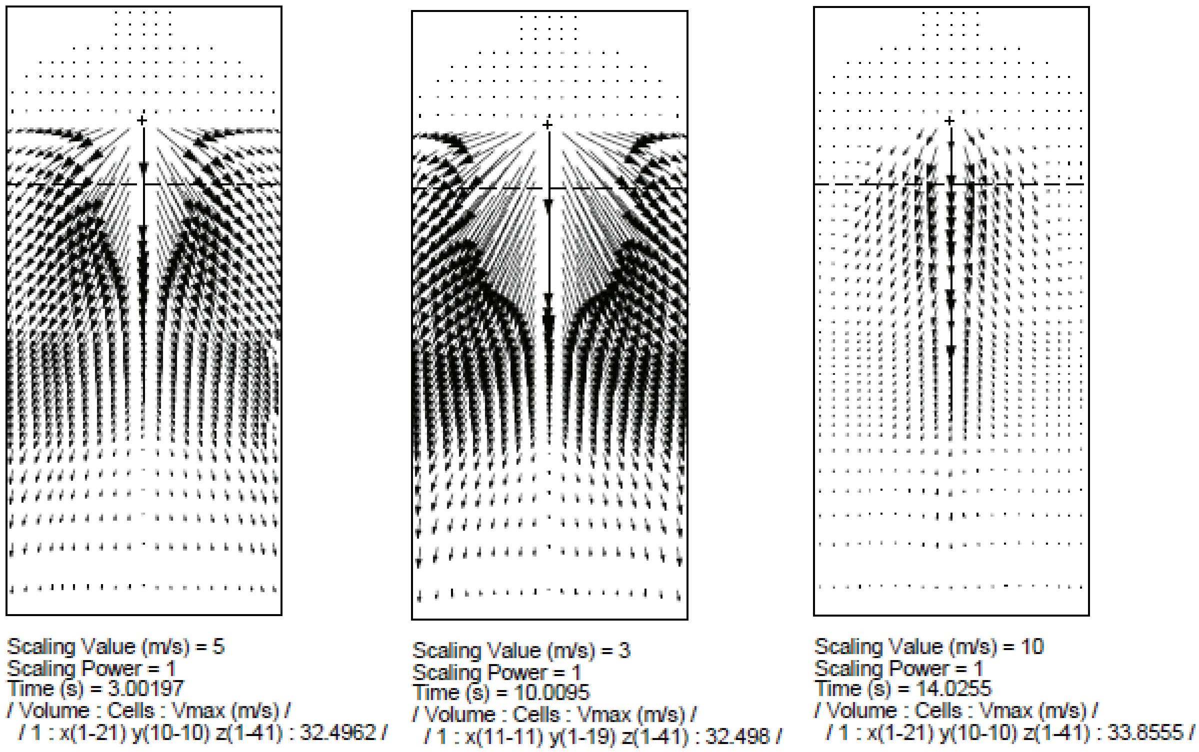

Figure 15. Vector Velocity Profiles predicted for Droplet Injection using FLSOUP.

4. CONCLUSIONS

An investigation of modified approaches and alternative differencing schemes that offers an improved treatment for this unique scenario has provided two new options for consideration (MFOUP and FLSOUP). These will be included in GOTHIC (version 8.1 and later) as a selectable user option. Testing has demonstrated promising results for both a simple test problem as well as the more detailed problem; however, additional testing will be required before either of these schemes could be recommended for a wider range of problems.

ACKNOWLEDGMENTS

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