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# Species Diffusion in ALE3D

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# Species Diffusion in ALE3D (U)

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*ALE3D is a finite element arbitrary Lagrange-Eulerian hydro code with thermal transport and chemical reactions. In order to consider problems of aging a species diffusion capability was added. Species diffusion is the process whereby species move under potential flow from one location in the system to another. The diffusion method needed to work with element-centered concentrations. In order to fit within the ALE3D scheme, the method also needed to work on an arbitrarily connected hexahedral mesh. Since the rate of species diffusion is usually slow compared to other processes, it an explicit method is sufficient. Finally, the method must conserve total species concentration. Three separate finite volume algorithms were developed. These methods share the following characteristics: species fluxes of mass and energy are defined at each face. A second order predictor corrector scheme is used, with the ratio between the corrected mass flux and the predicted mass flux being used to define an accuracy time step constraint. The courant like diffusivity constraint is used for the stability constraint. Examples are shown.*

## 1 Introduction

Understanding the behavior of systems over time is an important part of stockpile stewardship. One aspect of this behavior has to do with the migration of various species within the system. By modeling the process whereby species of interest move from one location to another in a system, we will be better able to define the systems long time environment. The ALE3D code [Sharp et. al.] is an arbitrary Lagrangian Eulerian code used for solving a variety of coupled hydrodynamic, thermal, and chemical problems. Because of ALE3Ds capabilities, it was decided to add species diffusion on top of its existing capabilities.

In this paper we will describe several algorithms for species diffusion implemented in ALE3D. We will first describe the background of ALE3D as it applies to diffusion problems in section 2.1, then consider the underlying diffusion equations as they apply to low temperature species diffusion in section 2.2. We will progressively derive three diffusion algorithms that fit within the ALE3D framework in section 2.3. Results of each of these methods will then be shown in section 3, and we will conclude in section 4.

## 2 Background

### 2.1 Background: ALE3D

Before we can define the method used to solve the species diffusion problem, it is necessary to define the computational environment it will be in. All of the development described here has been done within the framework of the ALE3D code. The thermal transport is based on a finite element scheme derived from TOPAZ3D. With this approach, the temperature field is represented by tri-linear basis functions centered on the nodes. One natural approach to species diffusion, since the underlying equations look similar, would be to use the thermal transport machinery for the species diffusion. There are two problems with this approach. First, while the final solution of a temperature field needs to be continuous, the final species distribution will, in general, have discontinuities, as at boundaries between different solvents. For example, the equilibrium concentration of salt in a system of water and air is a little salt in the air and a lot in the water. Thus, unless one required a mesh discontinuity at solvent boundaries, placing the species concentration at nodes, as is done with the temperature, would not allow one to model the physical system correctly – the solution would have a continuous solution when a discontinuous one was required. One could use the finite element approach if instead of using it on the mesh one used the dual of the mesh, where the nodes of the dual are the elements of the original mesh. However, all of the physics in ALE3D works on an arbitrarily connected hexahedral mesh. The dual of such a mesh is not well posed and would include arbitrary polyhedral elements.

On the other hand, while species concentrations can be discontinuous, their chemical potential will be continuous at equilibrium. Therefore, we can construct a continuous chemical potential field at the nodes or faces. Finally, we must conserve mass. Finite element schemes would conserve the mass of each species globally, but not necessarily locally. Therefore, for these reasons, we have taken a finite volume approach to solving the diffusion equation. We will require that the flux going out of a face of one element will be the flux going into its neighbor through the same face.

### 2.2 Background: Diffusion

Multi-component species diffusion is defined by the equation [Cussler]:

$$\beta \nabla \mu_i = \sum_j \frac{x_j}{D_{ij}} (v_j - v_i) \quad [1]$$

where  $\beta$  is one over the temperature multiplied by the Boltzmann constant,  $\mu_i$ ,  $x_i$  and  $v_i$  are the chemical potential, mole fraction, and drift velocity, respectively, for the  $i^{\text{th}}$  species, and  $D_{ij}$  is the  $ij$ -binary diffusion constant. We can define  $\bar{D}_i$  as the average diffusion constant for  $i$ , and  $\bar{v}_i$  as the average drift velocity felt by  $i$ , with the following definitions:

$$\frac{1}{\bar{D}_i} \equiv \sum_j \frac{x_j}{D_{ij}} \quad [2]$$

$$\frac{\bar{v}_i}{\bar{D}_i} \equiv \sum_j \frac{x_j \underline{v}_j}{D_{ij}} \quad [3]$$

With these definitions we can write the diffusion equation in a more familiar form:

$$\underline{v}_i = \bar{v}_i - \bar{D}_i \beta \underline{\nabla} \mu_i \quad [4]$$

An important consideration is that the chemical potential of a species with no concentration is negative infinity. Because such a condition is not unusual when setting up a problem, and because negative infinite numbers are difficult to deal with within a computational model, it is necessary to restructure these equations in terms of activity coefficients.

$$\beta \mu_i = \beta \mu_i^0 + \beta \Delta \mu_i = \ln(\rho_i) + \beta \Delta \mu_i = \ln(\alpha_i) = \ln(\rho_i z_i) \quad [5]$$

where  $\alpha_i$  is the activity coefficient,  $z_i$  is the excess activity coefficient, and  $\rho_i$  is the density. By substituting Eq [5] into Eq [4], we have

$$\alpha_i \underline{v}_i = \alpha_i \bar{v}_i - \bar{D}_i \underline{\nabla} \alpha_i \quad [6]$$

or

$$\rho_i \underline{v}_i = \rho_i \bar{v}_i - \bar{D}_i (\underline{\nabla} \rho_i + \rho_i \underline{\nabla} \ln z_i) = \rho_i \bar{v}_i - \frac{\bar{D}_i}{z_i} \underline{\nabla} \alpha_i \quad [7]$$

### 2.2.1 General assumptions

Since species diffusion is a slow process when compared to the other processes in most simulations, it was decided to implement an explicit species diffusion algorithm. We construct a mass change operator  $\Delta \underline{M}[M_s]$  that calculates the change in mass for the time step, given the initial concentration  $\underline{M}_s$ . This operator is built by looping over each face to determine the species mass flow between the two elements. The mass flux is then the product of the species density flux and the area through which it travels. The total change of mass for a species is the sum of the mass fluxes into the element. We use a predictor-corrector method to solve for the new concentrations. That is, the first estimate for the new mass concentration is

$$\underline{M}_n^i = \underline{M}_o + \Delta \underline{M}[M_o] \quad [8]$$

The predictor concentration is then used to correct the mass change, so that the final mass concentration is

$$\underline{M}_n^f = \underline{M}_n^i + \frac{1}{2} (\Delta \underline{M}[M_n^i] - \Delta \underline{M}[M_o]) \quad [9]$$

Since we are using an explicit time advance scheme, we need both an accuracy and a stability time step control. We use the initial mass change and its correction to define an accuracy error term:

$$Error = \frac{\|(\Delta M[M_n^i] - \Delta M[M_o])\|}{2\|\Delta M[M_o]\|} \quad [10]$$

This error is compared to a user defined error limit to control the time step. We also use the diffusion equivalent of the courant condition as the stability time constraint:

$$\Delta t \leq \frac{l^2}{D} \quad [11]$$

### 2.3 Tracer Diffusion Approximation

If one can assume that concentration of the diffusing species is small compared to the rest of the system, and that the drift velocity of all non-diffusing species is zero, then  $\bar{v}_i = \underline{0}$  and the original diffusion equation becomes

$$\underline{v}_i = -\bar{D}_i \beta \nabla \mu_i. \quad [12]$$

These assumptions define the tracer diffusion model. The tracer diffusion approximation was made for the initial implementation of all of the models described here.

#### 2.3.1 Method 1

Method 1 is the simplest of the models developed here. The concept is that we need to find a value of the activity at each face center such that when one uses that activity to calculate the activity gradient between the face and the element, the flux calculated from both elements connected to that face are continuous. The species flux is defined as  $\rho_i v_i$ . The flux continuity at each face requires  $\rho_i^1 v_i^1 = \rho_i^2 v_i^2$ . Making the tracer diffusion assumption, defining  $\hat{l}^i$  to be the unit vector between the two elements connecting a face, starting from the  $i^{\text{th}}$  element going toward the face, and defining  $l^i$  as the distance along the unit vector between the element center and the face center (note that this will generally require a projection operation). Then the flux continuity requirement can be written:

$$-\frac{\bar{D}_i^1}{z_i^1} \frac{(\alpha_i^1 - \alpha_i^s)}{l^1} \hat{l}^1 = -\frac{\bar{D}_i^2}{z_i^2} \frac{(\alpha_i^2 - \alpha_i^s)}{l^2} \hat{l}^2 \quad [13]$$

which can be solved for the face activity  $\alpha_i^s$ :

$$\alpha_i^s = \frac{\frac{\alpha_i^1 D_i^1}{z_i^1 l_1} + \frac{\alpha_i^2 D_i^2}{z_i^2 l_2}}{\frac{D_i^1}{z_i^1 l_1} + \frac{D_i^2}{z_i^2 l_2}} \quad [14]$$

The mass flux through that face is then just the product of the flux in the direction of the vector connecting the two elements and the area:

$$\frac{dM_i}{dt} = \rho_i v_i \underline{A} \cdot \hat{l} \quad [15]$$

In the results section, it will be shown that this scheme works well with orthogonal meshes, however does have some issues when the mesh is skewed.

### 2.3.2 Method 2

Method 2 was developed after examining the problems with method 1. The major issue with model 1 is that it creates fluxes that are in the direction between the two element centers connected by a face. And all fluxes flow from the high activity element to the one with low activity. With a sufficiently skewed mesh, it is possible that the correct flow will be from the low activity to the high activity element. Because method 1 only examines the two elements on either side of a face, it is incapable of accommodating the skew of the system. In particular, the flux through the face is independent of the activities of the surrounding elements

In order to correct for this deficiency it is necessary to provide more information about the distribution of the activities around the face. If we examine the formula for the face activity from method 1, we find that it can be considered an average of each

elements activity, weighted by  $\frac{D_i}{z_i l}$ . One way of providing that extra information is to

create an effective nodal activity by averaging the activity of the elements surrounding the node:

$$\alpha_i^n = \frac{\sum_e \frac{\alpha_i^e D_i^e}{z_i^e l_e}}{\sum_e \frac{D_i^e}{z_i^e l_e}} \quad [16]$$

where  $l_e$  is the distance between the element center and the node. With an average activity at each node, and the activity at each element center, one can construct an activity gradient that is centered at the face. We then calculate an face average inverse diffusivity and insert that into Eq. [7]. Solving for the species flux gives

$$\rho_i v_i = - \frac{\nabla \alpha_i}{\frac{1}{2} \left( \frac{z_i^1}{D_i^1} + \frac{z_i^2}{D_i^2} \right)} \quad [17]$$

The total species mass flux across the face is then just the species flux dotted into the area vector of the face:

$$\frac{dM_i}{dt} = \rho_i \underline{v}_i \cdot \underline{A} \quad [18]$$

In the results section it will be shown that method works well in meshes where the mesh lines are parallel to each other, but again has some issues when the mesh lines are kinked.

### 2.3.3 Method 3

As with method 2 building from method 1, the development of method 3 was an attempt to improve on the results of method 2. The central error in method 2 arises from the method to determine the nodal activity. Since it uses an average, the nodal activity will always be bracketed by the activities of the neighboring elements. In severely deformed meshes, it is possible that the node will be outside the volume defined by the element centers. In such a case, it would not be unreasonable for the activity to not be bracketed by the elemental ones. Method 3 addresses this issue by finding the value of the nodal activity and flux that fits the local environment best. We begin by expanding the activity about a node in a Taylor series:

$$\alpha_e^* = \alpha_n + (\underline{r}_e - \underline{r}_n) \cdot \underline{\nabla} \alpha_{ne} \quad [19]$$

where  $\underline{\nabla} \alpha_{ne}$  is the gradient of the activity between node  $n$  and element center  $e$ , and  $\alpha_e^*$  is the predicted activity at the element center. The gradient of the activity is not required to be continuous, however the species flux is. So we solve Eq. [7] for the activity and insert it:

$$\alpha_e^* = \alpha_n - (\underline{r}_e - \underline{r}_n) \cdot \frac{z_e}{D_e} \rho_n \underline{v}_n \quad [20]$$

This equation describes the activity in each element as a function of the nodal activity, nodal flux, and elemental diffusion constant. We can now construct an error measure  $E$  that is the sum of the squares of the difference between the actual elemental activity and the value predicted from the node multiplied by an elemental weight  $w_e$ :

$$E = \sum_e w_e (\alpha_e^* - \alpha_e)^2 = \sum_e w_e \left( \alpha_n - (\underline{r}_e - \underline{r}_n) \cdot \frac{z_e}{D_e} \rho_n \underline{v}_n - \alpha_e \right)^2 \quad [21]$$

We can minimize the error measure by taking its derivative with respect to the nodal activity and species flux, and setting those derivatives to zero:

$$\frac{\partial E}{\partial \alpha_n} = 2 \sum_e w_e \left( \alpha_n - \alpha_e + (\underline{r}_n - \underline{r}_e) \cdot \frac{z_e}{D_e} \rho_n \underline{v}_n \right) = 0 \quad [22]$$

$$\frac{\partial E}{\partial \rho_n \underline{v}_n} = 2 \sum_e w_e (\underline{r}_n - \underline{r}_e) \frac{z_e}{D_e} \left( \alpha_n - \alpha_e + (\underline{r}_n - \underline{r}_e) \cdot \frac{z_e}{D_e} \rho_n \underline{v}_n \right) = \underline{0} \quad [23]$$

This equation can be expressed more simply by defining  $(\underline{r}_n - \underline{r}_e) \frac{z_e}{D_e}$  to be the vector  $\underline{\xi}_{ne}$ , defining the average value of a variable  $\zeta$ , notated as  $\langle \zeta \rangle$ , to be  $\sum_e w_e \zeta / \sum_e w_e$ , and letting the elemental weight be the inverse of the distance between the node and the element center, we can write the minimization as a matrix equation to solve:

$$\begin{pmatrix} 1 & \langle \underline{\xi}_{ne} \rangle \\ \langle \underline{\xi}_{ne} \rangle & \langle \underline{\xi}_{ne} \underline{\xi}_{ne} \rangle \end{pmatrix} \cdot \begin{pmatrix} \alpha_n \\ \rho_n \underline{v}_n \end{pmatrix} = \begin{pmatrix} \langle \alpha_e \rangle \\ \langle \underline{\xi}_{ne} \alpha_e \rangle \end{pmatrix} \quad [24]$$

With this notation, flux boundary conditions are defined as

$$\begin{pmatrix} 1 & \underline{0} \\ \underline{0} & \underline{I} \end{pmatrix} \cdot \begin{pmatrix} \underline{0} \\ \rho_n \underline{v}_n \end{pmatrix} = \begin{pmatrix} \underline{0} \\ \underline{f} \end{pmatrix}, \quad [25]$$

and the activity boundary conditions are defined as

$$\begin{pmatrix} 1 & \underline{0} \\ \underline{0} & \langle \underline{\xi}_{ne} \underline{\xi}_{ne} \rangle \end{pmatrix} \begin{pmatrix} \alpha_n \\ \rho_n \underline{v}_n \end{pmatrix} = \begin{pmatrix} \alpha_n \\ \langle \underline{\xi}_{ne} (\alpha_e - \alpha_n) \rangle \end{pmatrix} \quad [26]$$

In order to define the no external flux boundary condition, it is necessary to define a projection operator for each external surface associated with the element:

$$\underline{\underline{P}} = (\underline{I} - \hat{n}\hat{n}), \quad [27]$$

where  $\hat{n}$  is the outward surface normal of the external face. The outward surface normal is calculated by dividing the external faces about a node into orientation groups, where faces in the same group have similar normals, that is, the absolute value dot product between any two in the group is greater than 0.8. By dividing the external faces into groups, we are able to support multiple surfaces, as one would find at a corner. The average normal for each group is calculated and then the projection operator is created for each group. The projection operator is then applied to the flux field to project out the out of plane driving force. This leads to

$$\begin{pmatrix} \langle 1 \rangle & \langle \underline{\xi}_{ne} \rangle \cdot \underline{\underline{P}} \\ \underline{\underline{P}} \cdot \langle \underline{\xi}_{ne} \rangle & \underline{\underline{P}} \cdot \langle \underline{\xi}_{ne} \underline{\xi}_{ne} \rangle \cdot \underline{\underline{P}} \end{pmatrix} \cdot \begin{pmatrix} \alpha_n \\ \rho_n \underline{v}_n \end{pmatrix} = \begin{pmatrix} \langle \alpha_e \rangle \\ \underline{\underline{P}} \cdot \langle \underline{\xi}_{ne} \alpha_e \rangle \end{pmatrix}. \quad [28]$$

Unless we are defining an activity boundary condition, we actually do not need to know the final nodal activity. Thus, we can reduce the complexity of the equation by conducting the Schur reduction on the matrix equation, reducing the problem to a simple 3x3:

$$\left( \langle \underline{\xi}_{ne} \underline{\xi}_{ne} \rangle \langle 1 \rangle - \langle \underline{\xi}_{ne} \rangle \langle \underline{\xi}_{ne} \rangle \right) \cdot \rho_n \underline{v}_n = \langle \underline{\xi}_{ne} \alpha_e \rangle \langle 1 \rangle - \langle \underline{\xi}_{ne} \rangle \langle \alpha_e \rangle \quad [29]$$

The natural tendency would be to simply solve the resultant matrix equation.

However, it can be shown that at external surfaces the matrix will be singular. This is because the projection operator has the effect of reducing the number of degrees of freedom in the problem. Thus, there exists a zero eigen-value associated with the out of plane motion. Since we know that the final solution will have no component in that direction, and that the matrix can be represented as the product of the outer product of the eigenvectors to the

eigenvectors ( $\underline{M} = \sum_i \lambda_i \underline{v}_i \underline{v}_i$ ), we add the

outer product of the zero eigenvector to the matrix. Once the matrix is no longer singular, we can solve for the species flux  $\rho_i \underline{v}_i$ . The mass flux through each face is then computed by integrating the bi-linear species flux as defined by the nodes over the face.

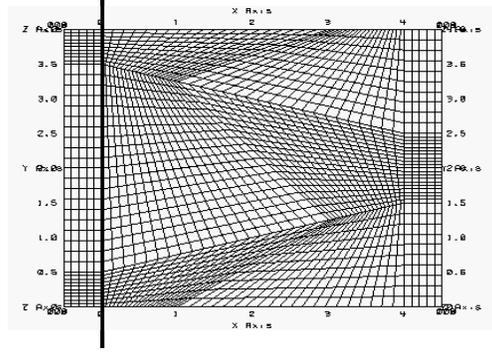


Figure 1. The Kershaw mesh is used to gauge the quality of the diffusion solution for each of the methods defined here. The initial high concentration of the diffusing species is to the left of the solid line at  $x=0$ .

## 2.4 Non Tracer Diffusion

With the development of model 3, we returned to consider the issue of non-tracer diffusion. Rearranging Eq [7] to express the activity gradient in terms of the fluxes and inserting it into equation [19], we get the non-tracer equivalent to [20]:

$$\alpha_{ei}^* = \alpha_{ni} + (r_e - r_n) \cdot \left( z_{ei} \sum_j \frac{x_{ej} \rho_{nj} \underline{v}_{nj}}{D_{ij}^e} - z_{ei} \sum_i \frac{x_{ej} \rho_{ni} \underline{v}_{ni}}{D_{ii}^e} \right)$$

and the error term that must be minimized is:

$$E = \min_{\alpha_{ni}, \rho_{ni} \underline{v}_{ni}} \sum_{ei} w_{ei} (\alpha_{ei}^* - \alpha_{ei})^2$$

such that  $\sum_i \rho_{ni} \underline{v}_{ni} = \underline{0}$

The constraint that the sum of the species fluxes is zero is required to maintain the total mass in each element by requiring that the mass flowing out of a face is balanced by an equivalent inflow. These equations are solved using the LAPACK

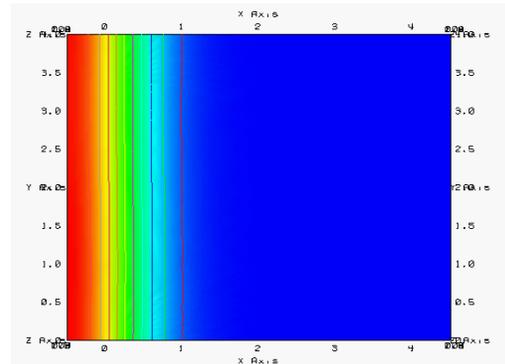


Figure 2. Solution of a finite element thermal problem equivalent to the species diffusion problems. The color is the pseudo-color plot of the concentration, and the lines are the iso-concentration contours.

routine DGGLSE which solves the least squares problem.

### 3 Results

We decided to use a modified Kershaw Z mesh to highlight the issues associated with each of these algorithms, shown in Figure 1. The Kershaw Z mesh consists of many distorted elements that are also oriented in non-orthogonal directions that can lead to rather peculiar interactions between elements. For this study, we the mesh is one element thick. The initial concentration of the diffusion species is set to be a step function at  $x=0$ , shown as a heavy line in Figure 1. The concentration is 0.001 for  $x<0$  and 0.0001 for  $x>0$ . We solved the equivalent thermal problem using the finite element scheme built into ALE3D. The results are shown in Figure 2. Note that the finite element scheme does a good job of maintaining the one dimensional nature of the solution, with the iso-thermal lines showing only a slight deviation from straight vertical lines.

The diffusion on the Kershaw mesh problem was solved for each of the tracer diffusion methods defined here. Figure 3 shows the results from method 1. The solution time for this problem on an SGI 200 MHz R10000 was 119  $\mu$ s per zone-cycle. Note the significant deviation from true one dimensional behavior. In method 1, the species flux tends to follow the mesh lines. As long as the mesh is reasonably orthogonal, the flux behaves properly. But where the mesh stops being orthogonal, the fluxes either pile up or disperse.

Figure 4 shows the results for method 2. The solution time for this problem on an SGI 200 MHz R10000 was 123  $\mu$ s per zone-cycle, approximately 3% more expensive than method 1. There is still some deviation from the one dimensional behavior, but the error is significantly reduced from that found in method 1.

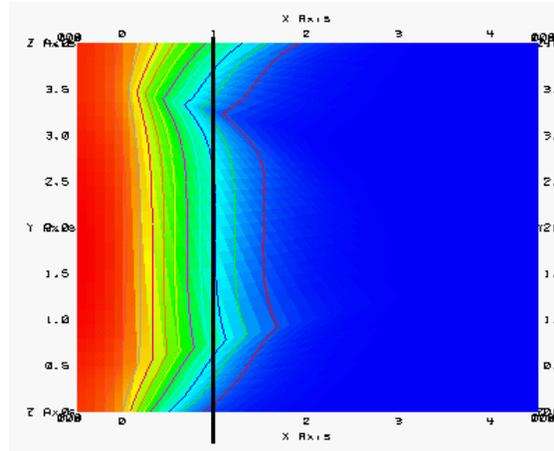


Figure 3. Plot of pseudo-color and contour plots of mass concentration of the trace component solved by on a Kershaw mesh using tracer diffusion method 1. A straight line has been added as a guide the eye.

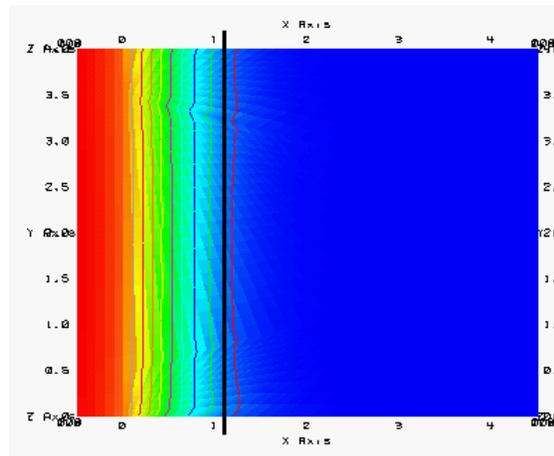


Figure 4. Plot of pseudo-color and contour plots of mass concentration of the trace component solved by on a Kershaw mesh using tracer diffusion method 2. A straight line has been added as a guide the eye.

Figure 5 shows the results for method 3. The solution time for this problem on an SGI 200 MHz R1000 was 192  $\mu$ s per zone-cycle, approximately 60% more expensive than either method 1 or 2. Here the iso-concentration lines are very straight, indicating good one-dimensional behavior, even on this difficult mesh. The deviations in linearity at the creases in the mesh can be ascribed to artifacts in the VisIt contour reconstruction algorithm. With that consideration, method 3 is arguably better at preserving the one dimensional nature of the solution than the finite element approach used for the thermal solver, as shown in Figure 2.

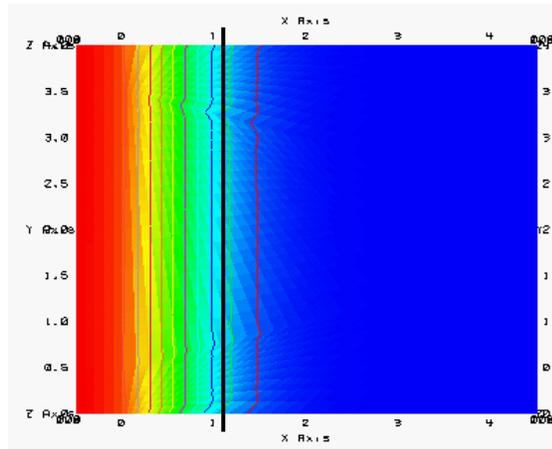


Figure 5. Plot of pseudo-color and contour plots of mass concentration of the trace component solved by on a Kershaw mesh using tracer diffusion method 3. A straight line has been added as a guide the

We show here an example of the solution of a non-tracer diffusion problem in Figure 6. The left face is subject to a species activity boundary condition, and the face on the right has been subject to a species flux boundary condition. Note the flair that is occurring on both sides, as the material is flowing in and swelling the block. The non-tracer scheme is required for this kind of problem because of the large amount of material which is moving about the system

#### 4 Conclusion

In this paper, we have shown the development of three diffusion algorithms that have been implemented in ALE3D, each with their advantages and disadvantages. All three methods use a predictor-corrector method to advance the composition. Method 1 uses information available at each face to define the face flux, and is the fastest. Method 2 averages elemental information to the nodes to construct a face flux using the computed gradient on the face, and is only slightly slower than method 1. Method 3 uses a least squares approach to find the best activity and flux at each node, and then

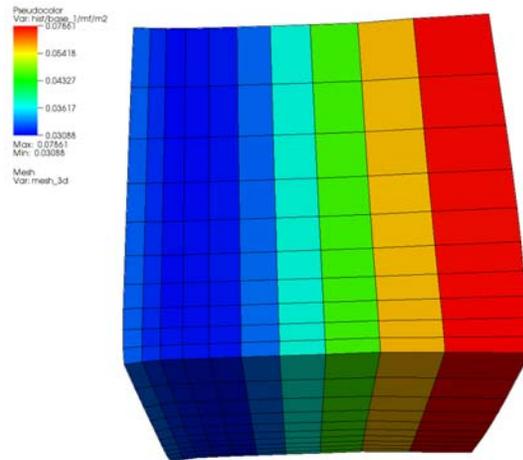


Figure 6. Pseudo-color plot of species mass fraction in a box with a species potential boundary condition on left and in flux boundary condition on the right. Because of the significant inflow of material, a non-tracer diffusion scheme was required.

uses the nodal fluxes to compute a face flux, and is the slowest of the methods. All three methods give accurate results on orthogonal meshes. However, the accuracy of method 1 decreases rapidly as the orthogonal nature of the mesh is reduced. Method 2 and 3 operate well on parallel meshes because they are not wed to the actual mesh connectivity. However, the fact that method 2 depends on averaging of element data to the nodes limits its accuracy as the mesh topology becomes more distorted. Finally, method 3 appears to provide good answers regardless of the topology.

With these considerations, if one were considering diffusion on an orthogonal Eulerian mesh, method 1 would be a suitable choice. If the expected mesh distortion can be expected to be slight, without the creation of significant creases in the mesh, then method 2 appears to be a good compromise in accuracy and speed. Finally, if preserving linear behavior in distorted meshes is a priority, as when one is considering moving parts near a fixed lagrange boundary, then method 3 should be used.

The extension of method 3 to include non-tracer diffusion will allow us to model systems where the diffusing species can be a significant fraction of the system.

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