APPROACHES TO LOCAL GRID REFINEMENT IN TOUGH2 MODELS

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ABSTRACT

In many applications, local refinement of a TOUGH2 model grid is needed where smaller-scale details of the model behaviour must be resolved- for example, around production areas (or even individual wells) in a geothermal field. Because of its flexibility, TOUGH2 makes a range of approaches to local grid refinement possible. TOUGH2's numerical formulation does implicitly require that the connection faces between grid blocks are orthogonal to the lines joining the block centres. However, not all approaches to local grid refinement satisfy this requirement.

This paper surveys the available approaches to horizontal local grid refinement of TOUGH2 models, considering the merits and disadvantages of each with reference to model performance on a test problem. A new approach is also introduced, incorporating a non-linear optimization technique for ensuring maximum compliance with TOUGH2's orthogonality requirement.

1. INTRODUCTION

The TOUGH2 simulator (Pruess, 2004) is widely used for the numerical simulation of many types of subsurface flow and transport problems, including modelling geothermal and other reservoirs. In many cases, a TOUGH2 model contains one or more areas of particular interest, over which either smaller-scale physical processes need to be simulated accurately, or more detailed results are required (or both). The production area of a geothermal reservoir model is an example.

The accuracy of the numerical formulation used by TOUGH2 (and other simulators) varies inversely with the local size of the model grid. Hence, the increased accuracy needed in areas of interest generally requires smaller grid blocks in that area.

The simplest way to achieve this is by refining the grid over the entire model. This increases the model accuracy in the area of interest, but also gives unnecessary increased accuracy outside this area, resulting in a needlessly large model and often excessive computation time (particularly if the area of interest is relatively small).

2. LOCAL GRID REFINEMENT

Hence, local grid refinement is needed, in which block sizes within the area of interest are reduced, while leaving the block sizes in the remainder of the model unchanged. The main difficulty with local grid refinement lies in the treatment of the transition zone- the zone between refined and unrefined blocks at the edge of the area of interest.

In this paper, we will focus mainly on horizontal grid refinement, rather than general 3-D grid refinement. Current 3-D reservoir models typically have a layer/ column structure, with a horizontal 2-D grid projected vertically down through a series of layers. In such models, fully 3-D local grid refinement cannot be carried out without destroying the layer/ column structure. Horizontal and vertical local grid refinement are instead carried out independently.

Hence, vertical refinement in layered reservoir models is carried out over the entire horizontal grid. This results in some wasted vertical refinement outside the horizontal area of interest, but allows the layered structure to be preserved, and keeps the vertical refinement process simple. The vertical transition zone just consists of a transition between thinner and thicker layers, requiring no special treatment beyond ensuring that the change in layer thickness is not too abrupt.

Similarly, horizontal local refinement in such grids extends down through all grid layers, resulting in some wasted horizontal refinement outside (typically below) the area of interest, but preserving the columnar structure of the grid. Handling the horizontal transition zone is more complex and there are various approaches to it.

3. TOUGH2 GRIDS

TOUGH2 uses an 'integrated finite difference' (IFD) numerical formulation (Narasimhan and Witherspoon, 1976), often referred to as a 'finite volume' formulation, in which the model grid is specified only as a set of block volumes and the connections between them. A connection between two blocks (with volumes V_1 and V_2) is defined by its interface area A_{12} and the two perpendicular distances d_1 and d_2 from the block centres to the interface (see Figure 1).

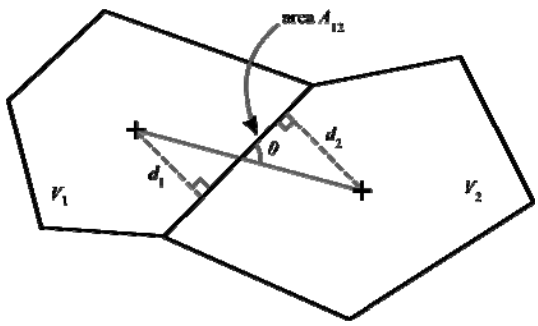

Figure 1: TOUGH2 blocks and connections

This formulation is very flexible, allowing grid blocks of almost arbitrary shape and a wide variety of grid configurations. However, as for other formulations, such as finite elements or finite differences (which IFD reduces to for regular rectangular blocks), solution accuracy can be degraded by the use of block shapes that are very irregular- e.g. blocks that have large aspect ratios (or more generally, large variations in block interface area), or are very skewed.

In addition, the IFD formulation's accuracy is reduced whenever the connection interface between two blocks is not orthogonal to the line joining the block centres- i.e.

whenever the angle θ in Figure 1 is less than 90°. This is because the pressure difference between the block centres, divided by the distance $d_1 + d_2$, is used to approximate the normal component of pressure gradient driving flow through the interface (Pruess and Garcia, 2000). As θ decreases, this becomes increasingly inaccurate. Hence, designing TOUGH2 grids with orthogonal connections ($\theta = 90°$) "may be difficult to achieve in practice but should be approximated as closely as possible" (Narashimhan and Witherspoon, 1976). The most common way to achieve this is simply to use rectangular grids. However, even then the problem may reappear when local refinement is carried out, depending on the approach taken.

4. LOCAL GRID REFINEMENT APPROACHES

Figure 2 shows three commonly-used approaches to local refinement of a rectangular grid. A small section of example grid is shown, originally consisting of three coarse blocks, the rightmost of which has been refined by a factor of two in both the *x*- and *y*-directions (the transition zone is shown in grey). Refinement of a real reservoir model grid consists mostly of repetitions of patterns similar to this (for irregular grids, the shapes may vary but the grid topology is the same).

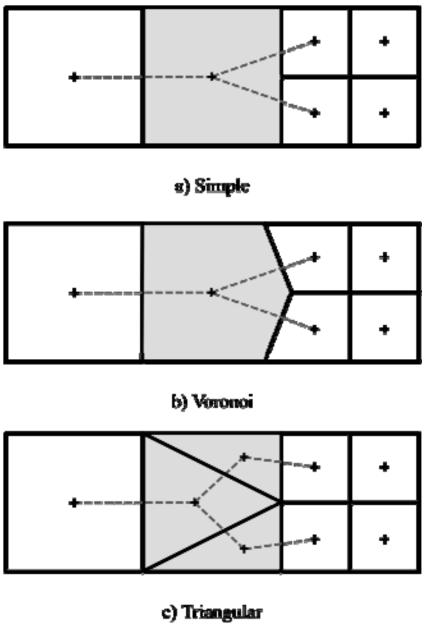

Figure 2: Three approaches to local grid refinement

4.1 Simple local refinement

The simplest approach to local refinement is just to add extra faces to the transition zone blocks, connecting them to the newly refined blocks, and leave the grid otherwise unchanged. In the Figure 2a example, the transition zone block has five horizontal faces. This approach has the virtue of simplicity, but has the drawback that the connections from the transition blocks to the refined blocks are almost never orthogonal.

Noting this, Pruess and Garcia (2000) proposed a modification of the simple scheme, in which additional "interpolation nodes" are introduced into the transition blocks, to enable correct pressure gradients to be calculated across the connections to the refined blocks. This approach performs well but is limited to regular rectangular grids.

Simple refinement results in transition blocks with more than four horizontal faces. This poses no problem for TOUGH2 itself but can cause difficulties for auxiliary software (e.g. visualization, data fitting or solid mechanics) that uses a finite-element formulation, which may only permit 2-D elements with a maximum of four sides.

4.2 Voronoi local refinement

Voronoi grids are constructed from a specified set of block centres (and a boundary), with the faces formed by the perpendicular bisectors of the lines joining pairs of blocks. Hence, the connections in a Voronoi grid are always orthogonal. The Voronoi grid in Figure 2b is constructed from the block centres of the simple refinement in Figure 2a. Specifying different block centres would result in other refinement configurations.

Like simple refinement, Voronoi refinement usually results in transition blocks with more than four horizontal faces. Voronoi grid generators can also produce blocks with some very small faces (see Figure 3). Sieger et al. (2010) noted that these can cause numerical instability, even if only one block in the grid has a small face, and presented a method for eliminating them from Voronoi grids; however, no implementations of this method appear to be widely available as yet.

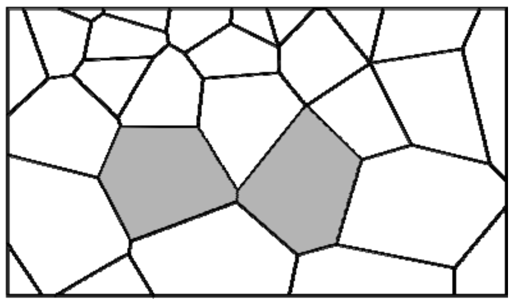

Figure 3: Blocks in a Voronoi grid with a small connection interface

4.3 Triangular local refinement

Another approach to local grid refinement is to triangulate the transition zone- essentially performing a Delaunay triangulation on it. This is a common local refinement approach for finite element grids. As can be seen in Figure 2c, more transition blocks are created than in the previous two approaches, but they are of intermediate size, making a less abrupt change in block volumes across the transition zone. No blocks with more than four horizontal faces are created. However, the transition zone connections are usually not orthogonal.

5. GRID OPTIMIZATION

The problem of non-orthogonal connections in TOUGH2 grids can be addressed by adjusting the positions of the grid nodes to make the connections as orthogonal as possible. This process can be formulated as a non-linear least squares optimization problem. The nodal coordinates are the optimization parameters, and the functions to be minimized are the cosines of the connection angles (calculated for each connection from the dot product of the vector along the connection face with the vector difference between the block centres).

When this optimization process is used in conjunction with local grid refinement, usually only grid nodes within the transition zone need be optimized. Nodes in neighbouring blocks can be added in as well if needed.

Optimization of a grid with simple local refinement gives something very similar to the Voronoi grid generated from the original block centres. An optimization of the triangulated grid from Figure 2c is shown in Figure 4.

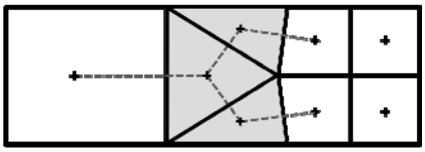

Figure 4: Optimized triangular local refinement

This optimization scheme has been implemented as part of the PyTOUGH Python scripting library (Croucher, 2011; Wellmann et al., 2012) for TOUGH2. It makes use of the ‘leastsq’ routine from the SciPy library (www.scipy.org), or optionally the parameter estimation software PEST (Doherty, 2010), to do the optimization, and can carry out horizontal optimization of layer/ column grids. The user can also include, with appropriate weighting, other grid quality measures in the optimization (aspect ratio and skewness).

The optimization scheme could also be extended, with little effort, to arbitrary unstructured 3-D grids. The formulation would be essentially the same, but the calculation of the connection angle θ would be slightly different.

6. TEST PROBLEM

A test problem was formulated to illustrate the importance of maintaining orthogonal connections in TOUGH2 grids, the performance of different local refinement approaches and the effect of the grid optimization scheme described above. The problem consists of a very simple isothermal, one-dimensional uniform flow caused by a constant pressure gradient in the x-direction. In this flow a square grid is located, which can be rotated about its centre to various orientations with respect to the flow direction. As the grid orientation angle φ varies, the boundary conditions on the grid are adjusted so that the underlying solution stays the same (see Figure 5).

The parameters of the problem are given in Table 1. Neglecting any variation of fluid density or viscosity with pressure, a simple application of Darcy’s Law yields the analytical solution for the pressure P at any position x,y :

$$P(x, y) = P_0 - \mu\, q\, x \,/\, (\rho\, k)$$

Pressure boundary conditions, given by the analytical solution, are applied on the upstream boundaries via inactive blocks connected to the boundary. Fluid is extracted via sink terms from the blocks on the downstream boundaries, so that the total mass extracted from the top and right-hand side boundaries is $q\ h\ l \sin(\varphi)$ and $q\ h\ l \cos(\varphi)$ respectively. (Top and bottom boundary conditions are not applied for φ = 0 or 90°.)

Starting from the 36-block φ = 0 grid, all 18 blocks to the right of the grid centre were refined by a factor of two in each direction, using four different local grid refinement approaches (simple, Voronoi, triangular and optimized triangular). The steady-state problem was then solved numerically using TOUGH2 for all angles φ between 0 and 90°, in 5° increments. The pressure and flow results in each case were compared with the analytical solution. The PyTOUGH scripting library was used to set up, run, and post-process all 76 TOUGH2 models from a Python script.

TOUGH2 strictly does not give the modelled pressures at particular points, but rather the average pressure over each block. Hence, in comparing modelled pressures with an analytical solution, the average of the analytical solution over each block should be computed, via e.g. Gaussian quadrature, and used for comparison. For the present problem the pressure varies only linearly in space, so the averages can be computed exactly using only a low-order Gaussian quadrature scheme.

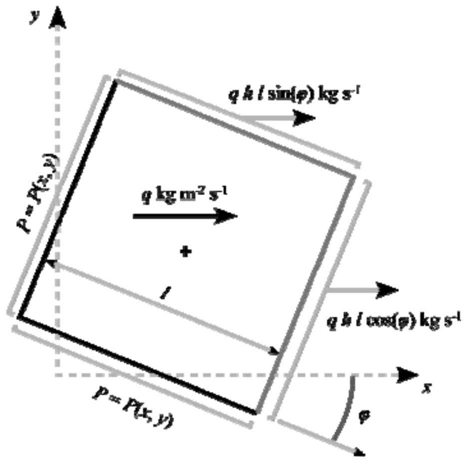

Figure 5: Test problem configuration

Parameter	Value
Grid side length l	6000 m
Grid depth h	100 m
Unrefined grid block size	1000 m
Permeability (k)	10^{-13} m^2
Porosity	0.1
Fluid flux in x-direction (q)	0.5×10^{-5} kg m^{-2} s^{-1}
Pressure at x = 0 (P_0)	5 bar
Temperature (constant)	20 °C
Fluid viscosity μ	1.0017×10^{-3} kg m^{-1} s^{-1}
Fluid density ρ	998.44 kg m^{-3}

Table 1: Test problem parameters

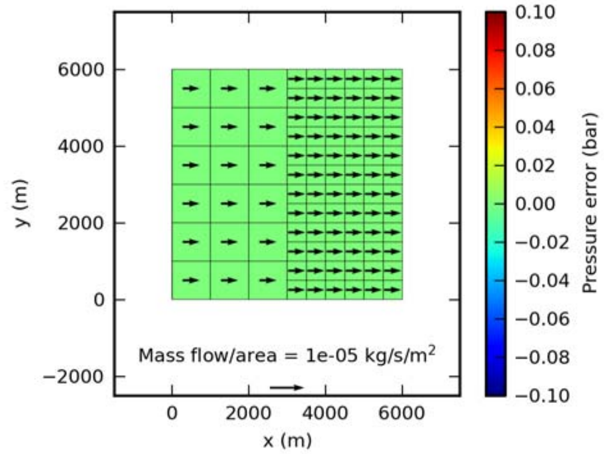

Figure 6: Test results for simple refinement, $\varphi = 0°$

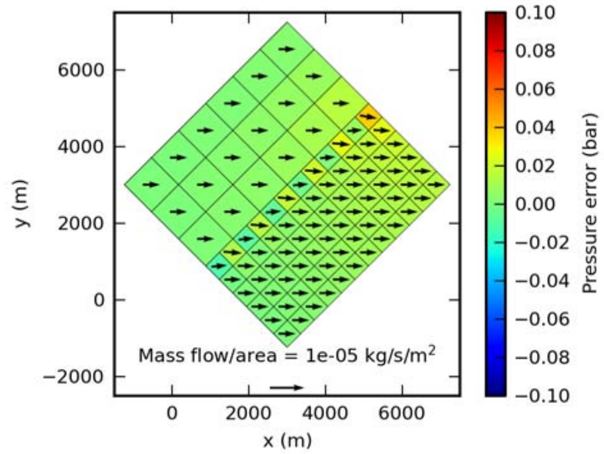

Figure 7: Test results for simple refinement, $\varphi = 45°$

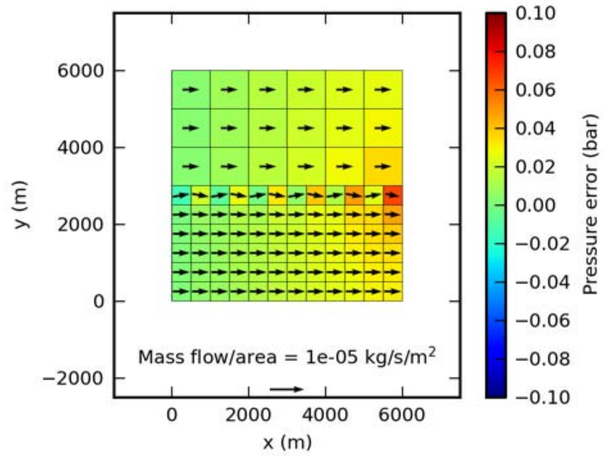

Figure 8: Test results for simple refinement, $\varphi = 90°$

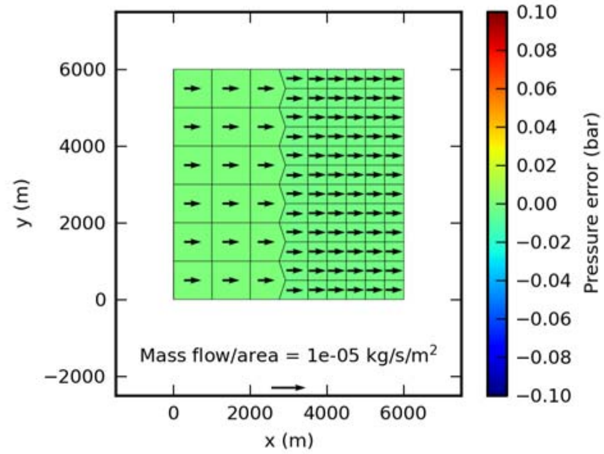

Figure 9: Test results for Voronoi refinement, $\varphi = 0°$

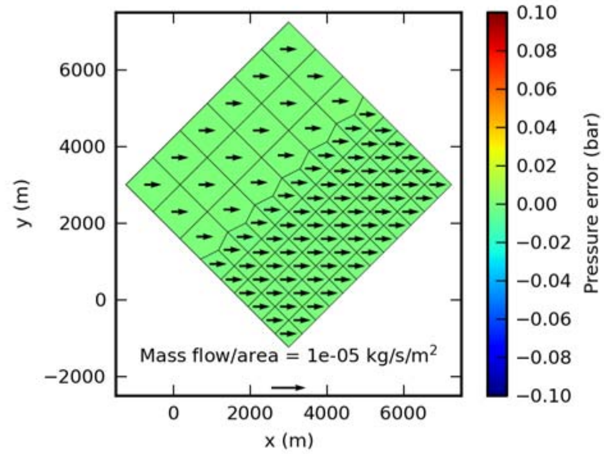

Figure 10: Test results for Voronoi refinement, $\varphi = 45°$

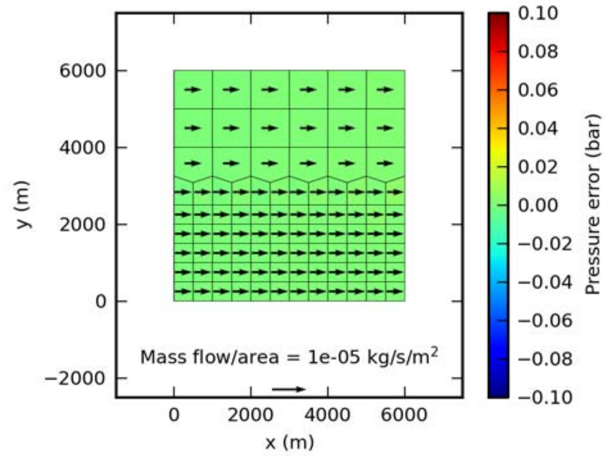

Figure 11: Test results for Voronoi refinement, $\varphi = 90°$

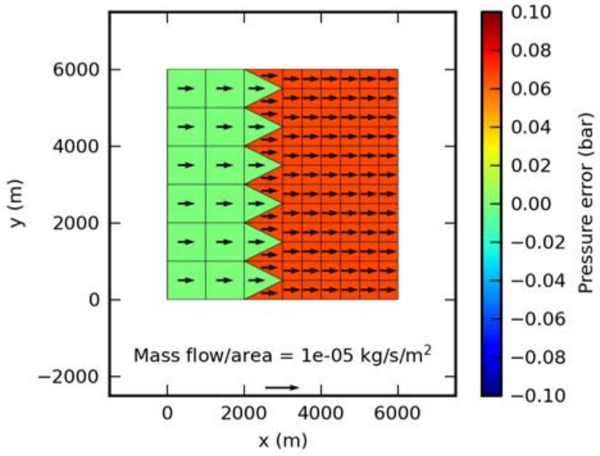

Figure 12: Test results for triangular refinement, φ = 0°

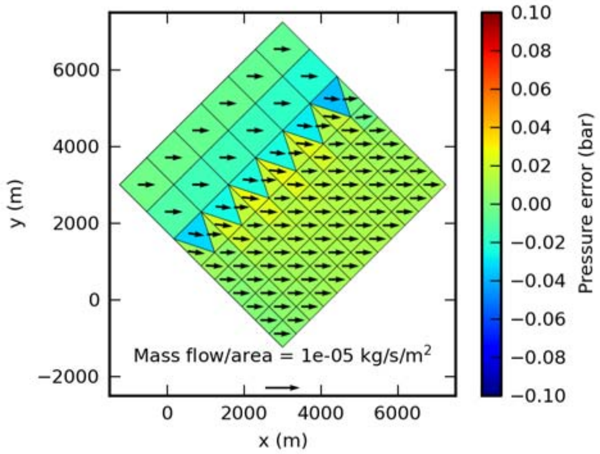

Figure 13: Test results for triangular refinement, *φ* = 45°

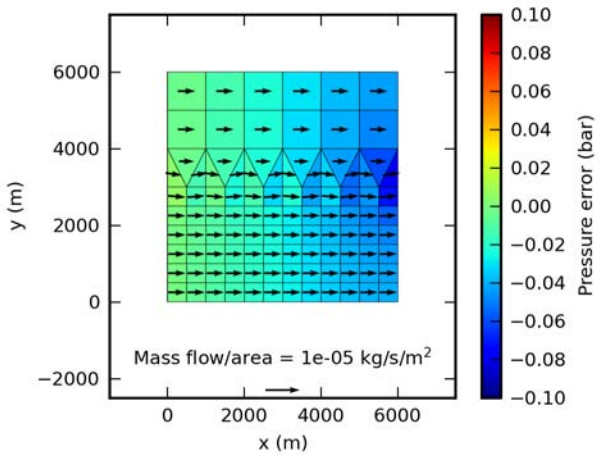

Figure 14: Test results for triangular refinement, *φ* = 90°

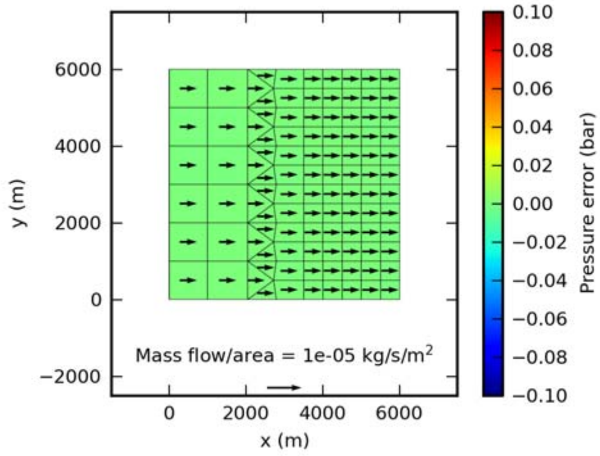

Figure 15: Test results for optimized triangular refinement, *φ* = 0°

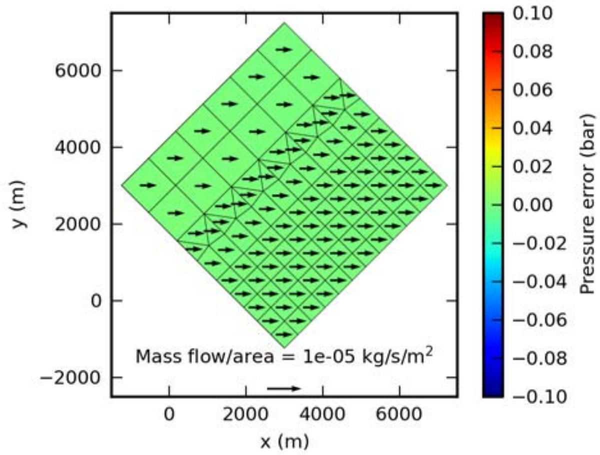

Figure 16: Test results for optimized triangular refinement, *φ* = 45°

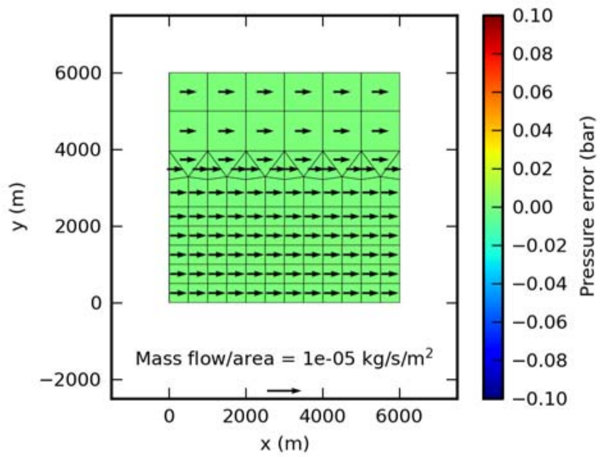

Figure 17: Test results for optimized triangular refinement, *φ* = 90°

7. RESULTS

Figures 6 – 17 show the results for φ = 0, 45° and 90°, for each of the four types of local grid refinement. In each case the pressure error in each block is shown, together with the block-averaged mass flux vector (calculated from the connection mass flows). The exact solution for the flux is a constant vector of length q in the x-direction.

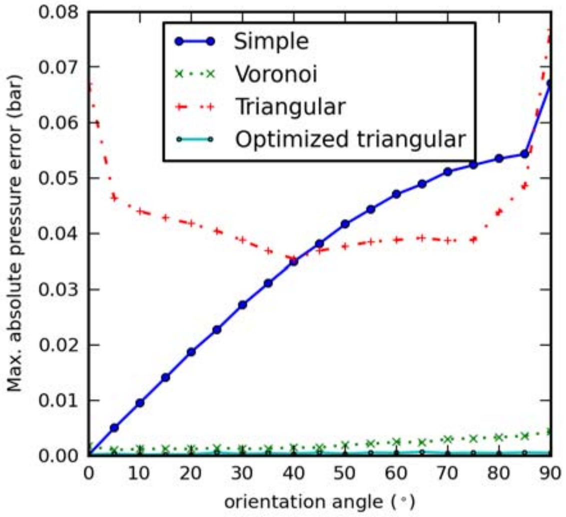

Figure 18: Maximum absolute pressure errors as a function of orientation angle φ, for four refinement types

Figure 18 shows the maximum absolute pressure error over the grid as a function of orientation angle φ, again for each of the four types of local grid refinement.

8. DISCUSSION

The results for simple refinement (Figures 6 - 8) show pressure errors in the transition zone increasing in magnitude to nearly 0.1 bar (5%) for the φ = 90° case. These errors are solely an artefact of the non-orthogonal connections in the transition zone, and have an alternating pattern between adjacent blocks along the edge of the zone. Figure 19 shows the effect of this pressure distribution on the mass flows through the block connections. The oscillating pressures give rise to mass flows of alternating sign, forming small flow loops in and out of the transition zone. This effect shows up in Figure 8 as an oscillation in the block-averaged mass fluxes. It has also been observed in real reservoir models using simple refinement.

The simple refinement scheme does not, however, introduce any pressure errors for φ = 0. Again, this can be understood by considering the connections between the refined part of the grid and the transition zone. As pointed out by Pruess and Garcia (2000), a line from the centre of a refined block perpendicular to its connection interface with a transition block does not pass through a transition block centre, but rather through a point some distance above or below it. Hence, in calculating the pressure gradient at the interface from the pressures at the block centres, the position of the transition block centre is effectively incorrect only in its y-coordinate. However, when φ = 0 this does not matter, because the pressure for this problem does not depend on the y coordinate.

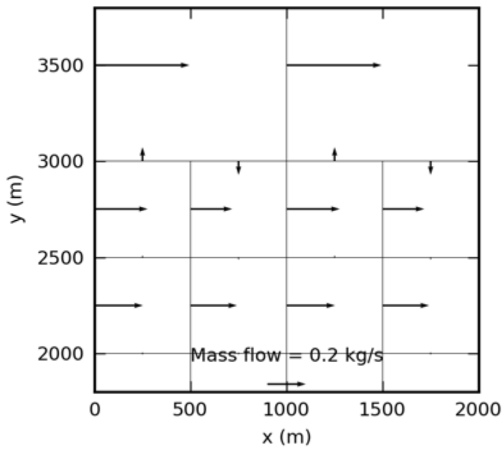

Figure 19: Connection mass flows around the transition zone for simple refinement, φ = 90°

Figures 9 - 11 show that using a Voronoi grid to regain orthogonal connections practically eliminates the errors seen in the case of simple refinement. All the block-averaged mass fluxes are aligned with the x-axis and have the correct magnitude of 0.5×10^{-5} kg m^{-2} s^{-1}, and the pressure errors are close to zero.

There are again obvious pressure errors when triangular refinement is used (Figures 12 - 14). When φ = 0, all blocks downstream from the transition zone have pressures nearly 0.1 bar too high. For intermediate angles, the magnitude of the pressure error reduces somewhat and takes on an alternating pattern, like that of the simple refinement case, which again causes oscillations in the mass flows. Interestingly, the downstream errors are near zero for the φ = 45° case, indicating that some of the errors introduced in the transition zone have fortuitously cancelled each other out. However, as φ increases further to 90° the errors increase again in magnitude (though reversed in sign) to nearly 0.1 bar, and are larger at the downstream end of the grid.

Figures 15 - 17 show that optimizing the triangular refinement grid is sufficient to regain correct performance, with near-zero pressure errors and correctly aligned mass fluxes.

Finally, Figure 18 shows that the error behaviour is similar for intermediate orientation angles. The errors for the simple refinement scheme increase steadily with the angle φ, while those for the triangular scheme are lowest at around φ = 40°. Pressure errors for the optimized triangular scheme are practically zero at all angles, while those for the Voronoi scheme are small but still detectable, particularly at larger angles. A closer analysis of the grids reveals that the connection angles (θ) in the Voronoi grid are not all exactly 90° (as would be expected in theory), but depart from this by up to 1°, possibly from loss of precision when the grid data were written to file. By comparison, the connections in the optimized triangular grid are all within 0.4° of being orthogonal, while the worst connections in both the simple refinement and triangular grids are 18.4° from orthogonal.

9. CONCLUSIONS

As previous authors have stated (but is sometimes overlooked), it is important to use TOUGH2 grids with connections that are as close to orthogonal as possible. Rectangular grids (regular or irregular) automatically satisfy this requirement, but local grid refinement even on a regular rectangular grid can result in non-orthogonal connections, depending on the refinement approach used.

TOUGH2 solutions on grids with non-orthogonal connections will usually contain pressure errors. The test problem used here to demonstrate this is very simple, but representative of the general situation of pressure gradients causing flow at various angles to any computational grid. The nature of the pressure errors will depend on the refinement approach and the orientation of the flow with respect to the grid. Even relatively small pressure errors can lead to unphysical flow patterns, e.g. flow loops at the edge of the refinement area.

To avoid these problems, it is recommended to use either Voronoi grids for local refinement, or the optimized triangular scheme presented in this paper. (Optimized simple refinement is essentially the same as Voronoi refinement.) Both approaches give grids with very nearly orthogonal connections. Grids with Voronoi local refinement have somewhat fewer blocks than those created using the optimized triangular scheme: 90 blocks instead of 102 for the test problem shown here. More generally, when refining a rectangular grid by a factor of two in each direction, over a rectangular area of interest, the number of extra blocks created by the optimized triangular scheme is twice the number of transition zone blocks in the corresponding Voronoi grid. However, the optimized triangular approach gives block sizes that vary less abruptly across the transition zone.

The optimization scheme also avoids the problem of the very small connection faces often created by Voronoi grid generators. Also, with optimized triangular refinement, blocks with more than four horizontal faces are not needed, which can be advantageous for interfacing with finite-element based auxiliary software. The optimization scheme could be extended to local refinement of unstructured 3-D TOUGH2 grids.

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