

SCIENTIFIC NOTEBOOK

by

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INITIAL ENTRIES

Scientific notebook: #282E Vol. 16
Issued to: S. L. Painter
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By agreement with CNWRA QA this electronic notebook contains material transferred from the hardcopy notebook issued on 17-July-1998. This notebook will be printed at approximate quarterly intervals. This computerized electronic notebook is intended to address the criteria of CNWRA QAP-001.

Development of the Multiflo code

Account number: 20.14002.01.071 and 20.14002.01.074

Description: Near-field environment code development - Multiflo.

Collaborators:

Objective:

Development, testing, and documentation of the Multiflo code, including the GEM and METRA modules and the MULTIFLO GUI. Assorted tasks associated with quantity and chemistry of water ISI.

Evolution of the Near Field Environment/ Quantity and Chemistry of Water

Account number: 20.14002.01.071
Description: Evolution of the near-field environment.
Collaborators: J. Myers, L. Sabido, A. Sun

Objective:

Application of MULTIFLO to understand the evolution of the near-field coupled thermal-hydro-chemical environment.

1.18.2007 Thermal conductivity as function of temperature

Used a work-in-progress MULTIFLO THC simulation to answer a question posed by staff from ENG 2 ISI: can we use MULTIFLO TH simulation results to define a temperature-dependent thermal conductivity for use in a conduction-only model. The question arises because thermal conductivity is saturation dependent. However, if a strong relationship exists between temperature and saturation in the simulations, then an effective thermal conductivity can be defined that captures some aspects of the TH model in a conduction-only model.

The model is a standard chimney-type (see 2.04.2004 entry Vol 14 of this notebook) updated with thermal properties from the DOE report Drift-scale THC Seepage Model MDL-NBS-HS-000001 Rev 04. Multiflo Version 2.0.1 was used. Note that they wet and dry thermal conductivity for TSw35 hydrogeological unit are 1.89 W/m-K and 1.28 W/m-K, respectively. Input/output files are stored in the directory KTH.

A cross-plot of temperature and saturation (or saturation-dependent thermal conductivity) suggest that after 100 years of heating, a temperature-dependent thermal conductivity can be defined. The following equation was used to fit the results:

$$K_{eff} = 1.86 - \frac{0.26}{1 + \text{Exp}[-(T - 95)/1.4]} \quad \text{for } T < 110$$

$$K_{eff} = 1.6 - 0.08 \times (110 - T) \quad \text{for } 110 < T < 114$$

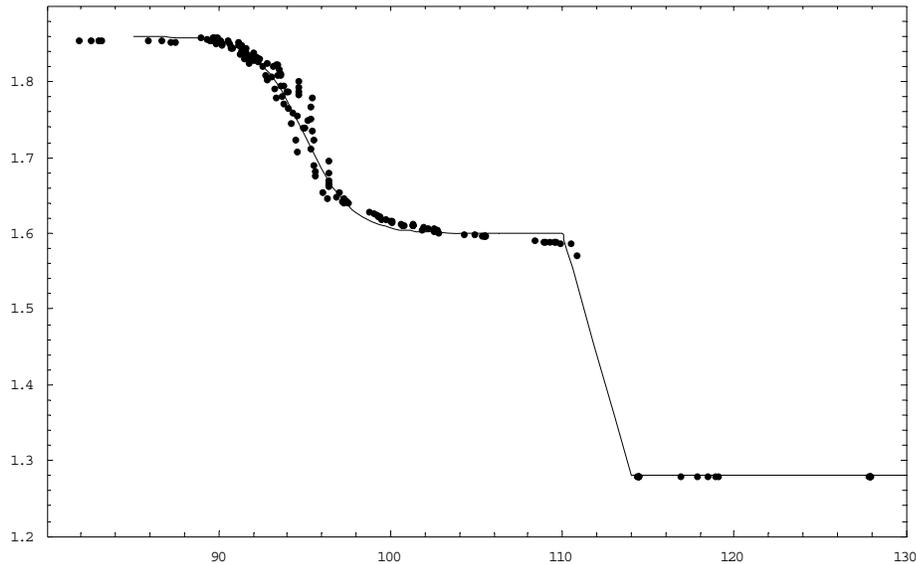
$$K_{eff} = 1.28 \quad \text{for } T > 114$$

where K_{eff} is in units of W/m-K and temperature is in degrees Celsius.

The fit is shown in the following figure. This figure was generated by extracting temperatures and saturations from the simulation at times 250, 500, 1000, 1750, and 3600 years. The
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saturation was then converted to thermal conductivity using the relationship $K = K_{dry} + (K_{wet} - K_{dry}) \sqrt{\text{saturation}}$ where K_{dry} and K_{wet} are dry and wet thermal conductivity, respectively.

Thermal conductivity versus temperature as extracted from MULTIFLO simulation (data points) and fitted (solid curves).



1.22.2007 Effect of rubble on drift-wall temperature

Simulations were performed to assess the effects of rubble on drift wall temperature. The hypothesis is that rubble resulting from drift collapse will have only a minimal effect on in-rock thermal conditions (although the effect on waste package temperature may be large). This hypothesis is based on a simple scoping calculation, which is described first.

A typical thermal conductivity value for rubble is approximately 0.5 W/m-K. Specific heat should be similar to that of intact rock (~1000 J/kg-K). Bulk density is that of intact rock with adjustments for the larger porosity of rubble: (~2000 kg/m³). Thus, the thermal diffusivity is $0.5 / (1000 \times 2000) \text{ m}^2/\text{s} = 2.5 \times 10^{-7} \text{ m}^2/\text{s} = 7.9 \text{ m}^2/\text{yr}$. The characteristic thermal time constant is the cross-sectional area divided by the thermal diffusivity. For a 5 meter diameter rubble pile, the characteristic thermal time constant is $\pi 2.5^2 / 7.9 \approx 2.5 \text{ yr}$. This is the characteristic time required for the rubble pile to equilibrate with the waste package. Given the long time scales of interest and the relatively slow variations in the waste package heat output, the 2.5 year lag is relatively unimportant, and it is thus adequate to consider the rubble in instantaneous equilibrium with the waste package. Once the rubble pile is equilibrated, the total heat flux entering the intact rock mass is the same as the waste package heat output. Thus, the rubble pile has little effect on in-rock thermal conditions.

Two MULTIFLO/METRA simulations were performed to test this hypothesis. The simulations are based on standard 2-d “chimney” models of one drift (for 3-d version, see *Painter, S.L. Modeling Ventilation Effects in Three-Dimensional Thermal Hydrological Simulations of a Potential Waste Repository at Yucca Mountain, Nevada. 2005 Transactions of the Society for Mining, Metallurgy and Exploration, Vol. 318, pp. 36-40, 2006.*). In the intact-drift simulation, heat from the waste package is applied instantaneously to the drift wall (the primary heat transfer mechanisms are thermal radiation and thermal convection; thermal capacity of air is very small and ignored). In the second simulation, the drift is assumed to be filled with rubble (thermal conductivity = 0.5 W/m-K; specific heat =1000 J/kg-K; bulk density=2000 kg/m³). The two simulations are identical in all other respects. Note that these are full two-phase thermal-hydrological simulations.

Temperature fields in the intact rock for the two models at 60 years are shown in Figure 1. The temperatures in the intact-drift case are slightly higher, but the difference is relatively small and confined to a very narrow region near the drift wall. A similar plot at 100 years is shown in Figure 2.

Figure 3 shows temperature at the drift crown versus time for the two cases. The case without rubble is shown in blue. The case with rubble is shown in black. The maximum temperature without rubble is 143 C; with rubble, the maximum temperature occurs a few years later and is about 141 C.

Thus it would appear that rubble has little effect on thermal conditions in the intact rock. However, the waste package temperature may be strongly affected by the presence of the thermally insulating rubble.

The result showing little-to-no effect of rubble is consistent with previous MULTIFLO simulations (Manepally et al. DRIFT-SCALE THERMOHYDROLOGICAL PROCESS MODELING—IN-DRIFT HEAT TRANSFER AND DRIFT DEGRADATION, 2004) which showed only negligible effect of rubble on the drift-wall temperature at the horizontal spring line.

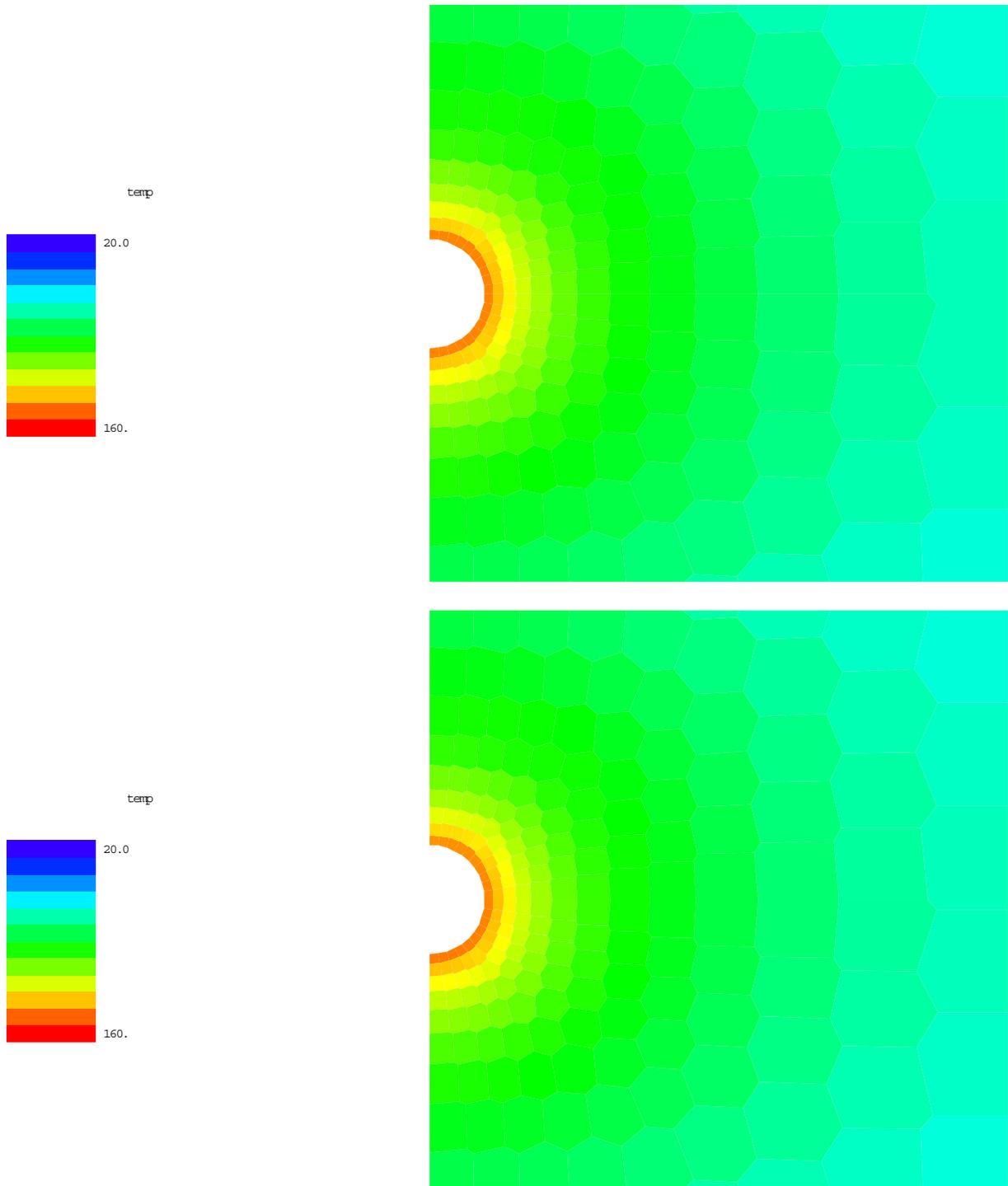


Figure 2. Temperature field in a 30 x 30 meter region near the drift at 100 years (50 years post-closure) with (bottom) and without (top) rubble in the drift. The in-drift temperatures are not shown. Note that only half the drift is modeled because of symmetry.

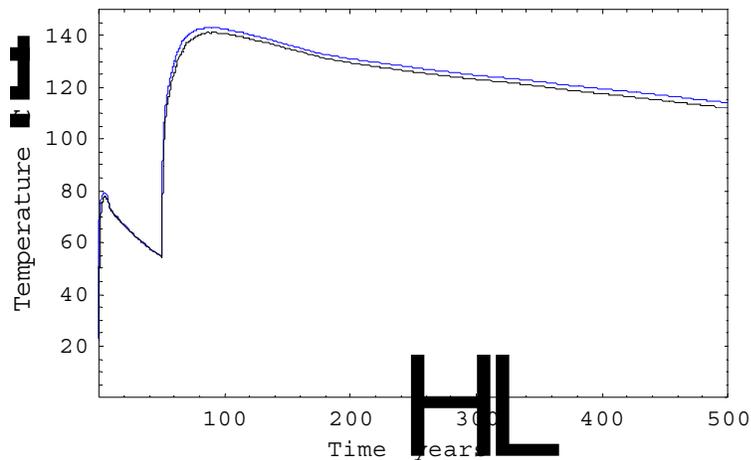


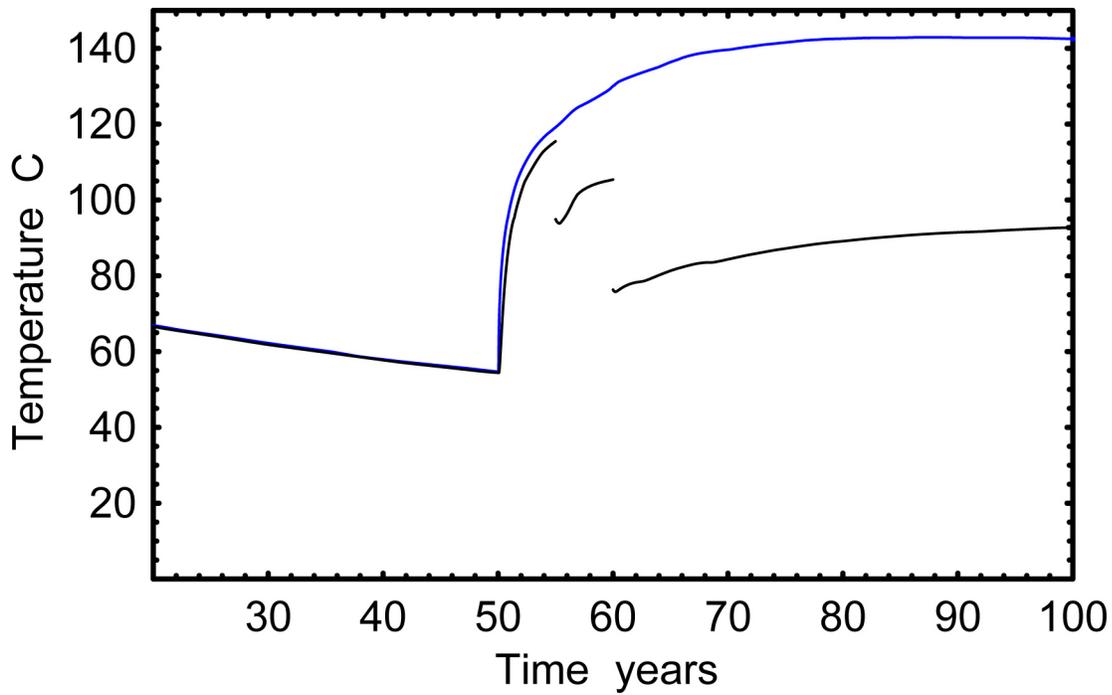
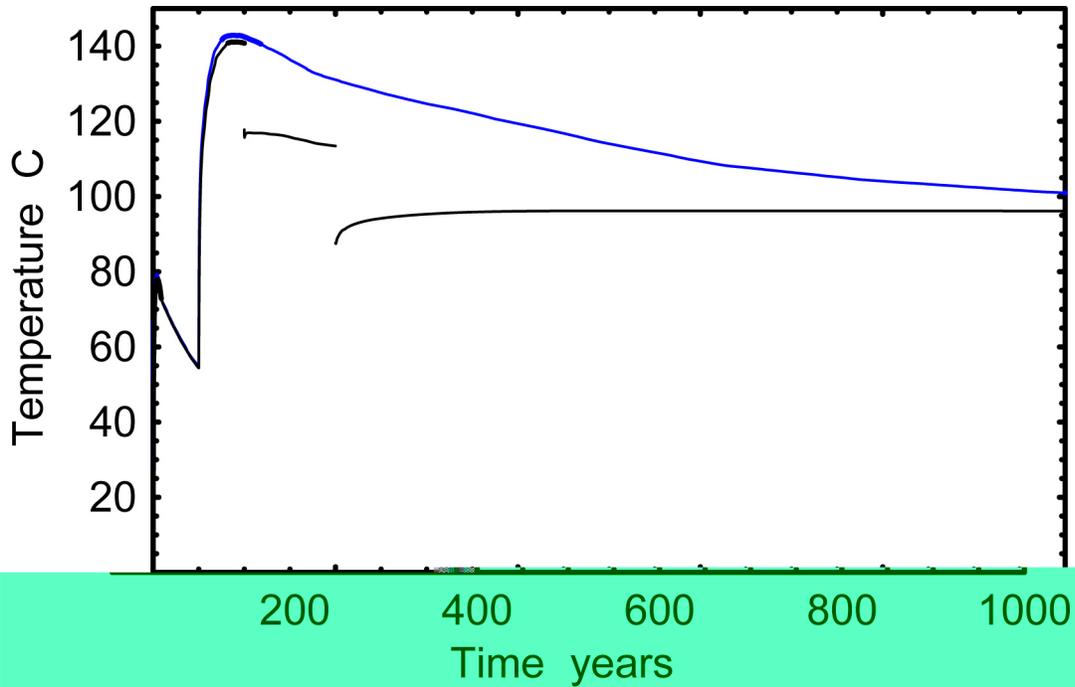
Figure 3. Temperature at the drift crown for the case of an open drift (blue) and a rubble-filled drift (black). The scenario modeled has forced ventilation up to 50 years, which is the reason for the sudden jump in temperature at that time.

1.26.2007 Temperature at drift wall following drift degradation

MULTIFLO/METRA simulations were performed to estimate temperatures at drift crown taking into account drift degradation. The issue is whether thermal spalling from drift crown will be a self-limiting process taking into account the fact that the intact rock wall will be receding from the heat source as thermal spalling occurs. The thermal insulating effects of a rubble pile may also have an effect if the rubble zone is large enough and asymmetrical.

The simulations used the same grid, thermal-hydrological properties, and heat load as the previous entry. The simulations started with an intact drift. At $t = t_1$, a zone extending 5 meters vertically from the drift center with the same footprint of the drift was converted to rubble. At that time the temperature monitoring point was moved from the original drift crown to a point 5 meters above the drift center. At $t = t_2$, the rubble zone was extended to 10 meters with corresponding relocation of the temperature monitoring point.

Two scenarios were considered. In the first scenario $t_1=100$ years and $t_2=200$ years. In the second scenario $t_1=55$ years and $t_2=60$ years. Results are shown in the following two figures. Note that the heat removal effect of forced ventilation is removed at $t=50$ years (i.e., repository closure occurs at 50 years). The blue curves are temperature without drift degradation and the black curves are temperature at the drift crown with drift collapse. The discontinuities in the black curves are due to the discrete failure events.



Temperature at drift crown versus time for two drift failure scenarios. In the top figure, drift failure occurs in a 5 meters zone at 100 years and in a 10 meter zone at 200 years. In the bottom figure the two failure events occur at 55 and 60 years. The blue curve in each is the temperature with no drift degradation.

3/12/07 Thermal-hydrological chemical simulations for M&C SNA07 conference

Thermal-hydrological-chemical simulations were created for the American Nuclear Society Mathematics, Computing and Supercomputing in Nuclear Applications in Monterey CA. April 2007.

Simulations were done with MULTIFLO V2.0.1 using a standard single-drift chimney-type configuration with 21 aqueous species, 7 mineral, and CO₂ gas. See input files for details.

Several runs are documented here. The simulations have identical physical and chemical. Runs differ only in the numerical parameters affecting the coupling between reactions and transport. Results of these simulations are documented in the attached Mathematica notebooks titled. *THC Simulations for M&C SNA'07 Conference* and *THC Simulations for M&C SNA'07 Conference-2*.

Specific runs are

Meth1 -- global implicit time stepping
Meth2-2 -- Strang splitting with wtkin=1
Meth2-2_wtkin -- Strang splitting with wtkin=0.5
Meth2-2_wtkin0 -- Strang splitting with wtkin=0
Meth2-1 -- ordinary operator splitting with wtkin=1
Meth2-1_wtkin0 -- operator splitting with wtkin=0

Meth2-2_wtkin0_delcmax2 -- Strang, wtkin=0, delcmax = 2 mol/kg
Meth2-1_wtkin0_delcmax2 -- Ordinary operator splitting with wtkin=0, delcmax= 2 mol/kg

Input and output files are archived with the notebook SN858E, which is issued to Lynn Sabido.

7/21/2007 Evaluation of conduction only models for temperature near emplacement drifts

MULTIFLO V2.0.1 simulations were used to evaluate the accuracy of models based on heat conduction only for evaluating temperatures in the host rock near emplacement drifts. Four simulations were conducted. The reference case simulation used the full two-phase thermal hydrology capabilities of MULTIFLO. A standard single-drift (chimney-type) domain was used with typical time-dependent heat load and rock properties. Three conduction-only simulations were performed using the same configuration. These three simulations had a thermal conductivity independent of temperature with value K_{dry} , $0.9 K_{wet}$, $1.0 K_{wet}$ and $1.1 K_{wet}$, where K_{dry} and K_{wet} are dry and wet thermal conductivities, respectively.

Input and output files are in the directory THforTPA. Results for drift-wall temperature can be found in the Mathematica Notebook *TH compared with Conduction Only.nb*. The results suggest that setting thermal conductivity K equal to K_{dry} significantly overestimates drift wall temperature. Setting $K = K_{wet}$ underpredicts the peak of the drift-wall temperature slightly – a better fit to the peak temperature is obtained by setting $K = 0.9 K_{wet}$. During the cool-down

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period, thermal hydrological processes cause the drift wall to cool faster than the conduction-only models predict. Taking $K=1.1K_{wet}$ provides the best fit during the cool-down period. These simulations were used to refine sampled values of thermal conductivity for the TPA Version 5.1 code.

Note added 7/25/07: Infiltration rate for the TH run was 4.8 mm/yr for the first 600 years, 14.4 mm/yr for the period 600-2000 years, and 24.4 mm/yr for times greater than 2000 years.

Entries into Scientific Notebook No. 282E Vol. 16, pages for the period of 1.18.07 to 7.25.07 were made by Scott Painter. No original text entered into this scientific notebook has been removed.

Scott Painter

ESP 1/21/2010

THC simulations for M&C SNA'07

Conference -2

This notebook is similar to the notebook. THC for Monterey.nb, except that the allowed concentration change is reduced to 2 mol/kg.

3/12/2007

Scott Painter

Preliminaries

```
<< "D:\\multiflo\\mflo2.0\\mfloPlot\\mfloPlot.m"
```

? GetMesh

GetMesh[filename] reads a segmt file (amesh output) containing the mesh to be plotted

? GetData

GetData[filename] reads the unstructured xyp files written by Metra or Gem

? PlotUnstructured

PlotUnstructured[mesh, data] constructs a two-dimensional plot from unstructured grid.

The 'mesh' and 'data' objects are the result of GetMesh[] and GetData[] commands

```
mesh1 = GetMesh["h:\\minc\\amesh\\segmt"];
```

Porosity: 500 years

■ fully implicit: Del C Max 10

```
data = GetData["H:\\Lynn\\THC_meth1\\fi_volf18.xyp"];
```

```
!time= 500.0 y Mon Jan 15 21:34:24 2007
```

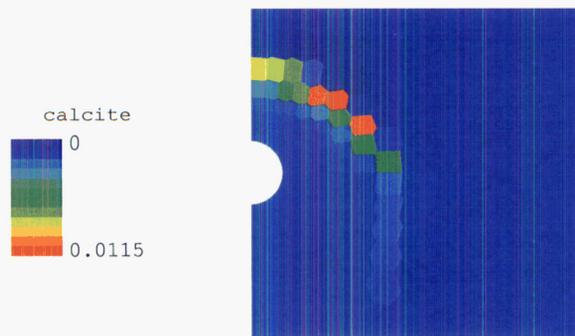
```
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,  
5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,  
PlotRange -> {{0, 30}, {-15, 15}}, DataRange -> {0.85, 1}, WarmColor -> False]
```



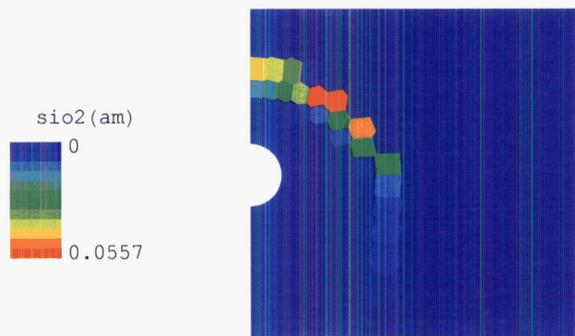
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",  
NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



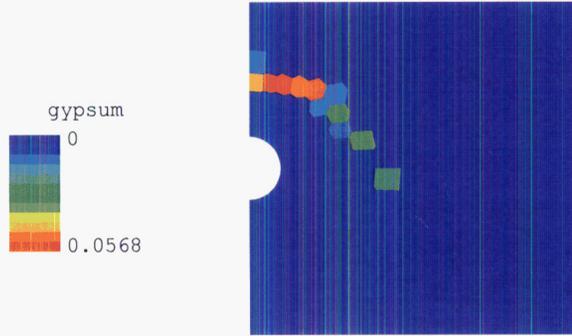
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",  
NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



- Graphics -

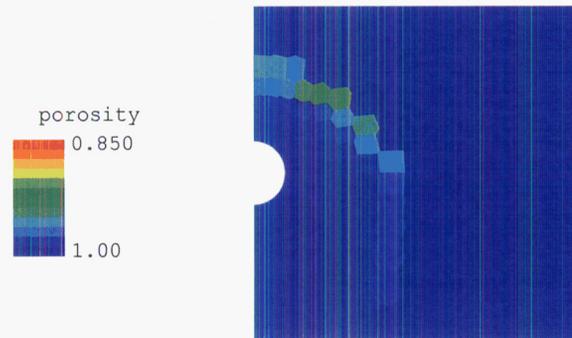
```
PlotUnstructured[mesh1, data, "gypsum",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

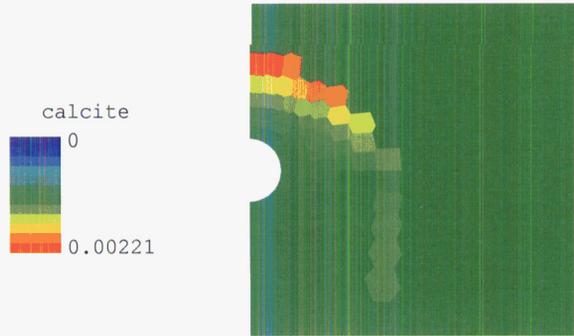
■ **strang splitting. wtkin=0**

```
data = GetData[ "H:\\Lynn\\THC_meth2-2_wtkin0\\fi_vol18.xyp" ];
!time= 500.0 y Mon Mar 05 20:07:28 2007
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
PlotUnstructured[mesh1, data, "porosity", NumberCells → 446,
  PlotRange → {{0, 30}, {-15, 15}}, DataRange → {0.85, 1}, WarmColor → False]
```



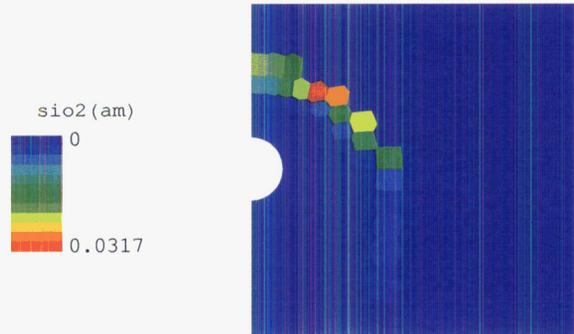
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



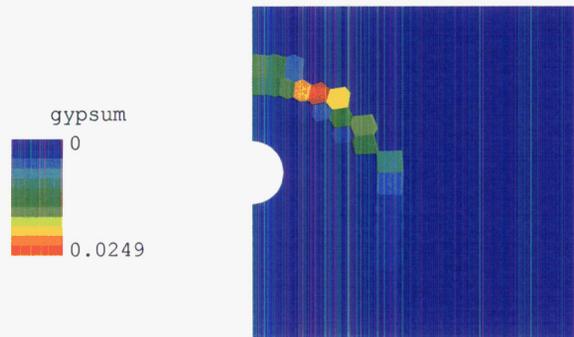
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

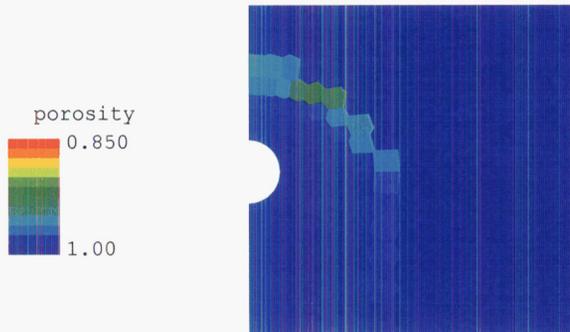
```
PlotUnstructured[mesh1, data, "gypsum",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

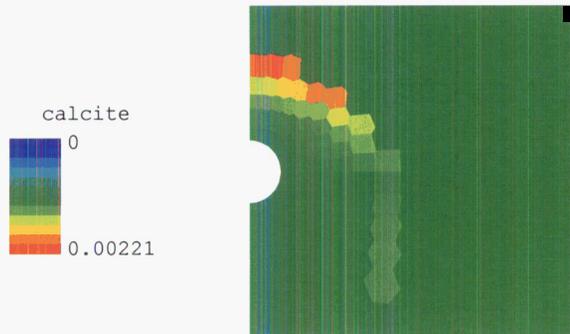
■ strang splitting. wtkin=0. delcmax = 2

```
data = GetData[ "H:\\Lynn\\THC_meth2-2_W0_dcx2\\fi_volf18.xyp" ];
!time= 500.0 y Tue Mar 06 18:36:20 2007
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,
PlotRange -> {{0, 30}, {-15, 15}}, DataRange -> {0.85, 1}, WarmColor -> False]
```



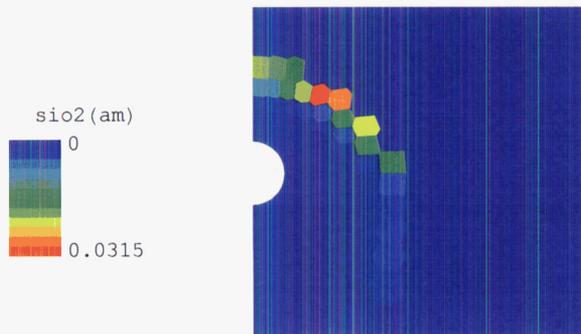
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",
NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



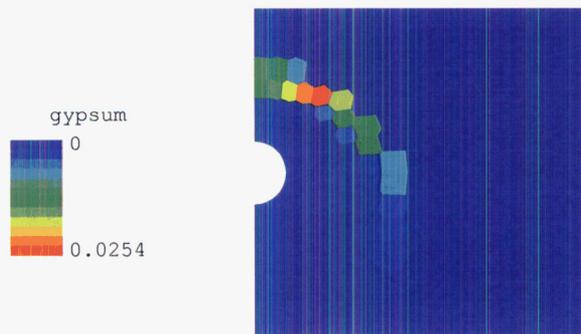
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

```
PlotUnstructured[mesh1, data, "gypsum",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



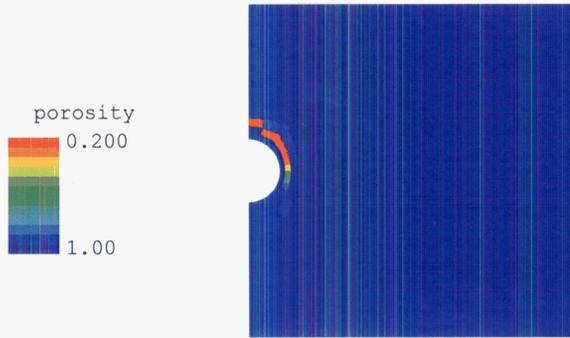
- Graphics -

Porosity: 2000 years

■ fully implicit: Del C Max 10

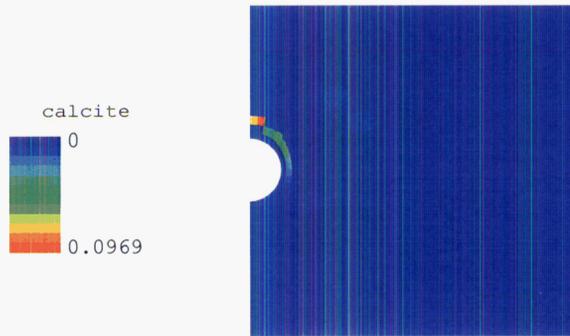
```
data = GetData[ "H:\\Lynn\\THC_meth1\\fi_volf21.xyp" ];
!time= 2000.    y    Tue Jan 16 06:08:49 2007
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,  
PlotRange -> {{0, 30}, {-15, 15}}, DataRange -> {0.2, 1}, WarmColor -> False]
```



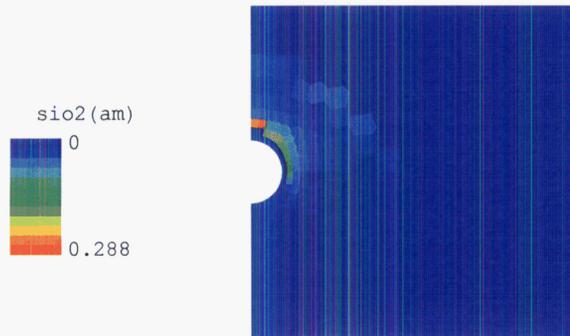
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",  
NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



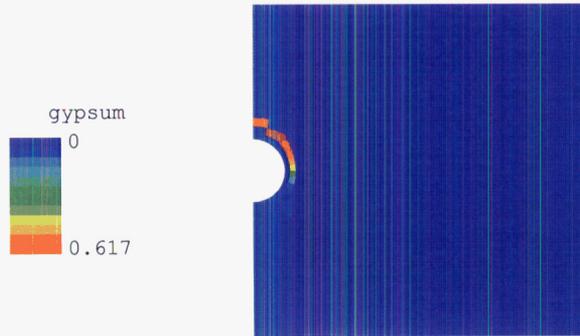
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",  
NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



- Graphics -

```
PlotUnstructured[mesh1, data, "gypsum",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

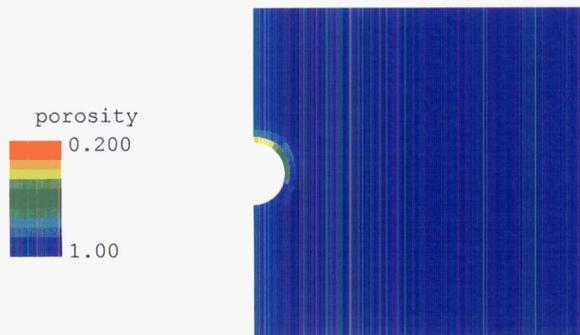
■ **strang splitting. wtkin=0, delcmax=10**

```
data = GetData[ "H:\\Lynn\\THC_meth2-2_wtkin0\\fi_volf21.xyp" ];
```

```
!time= 2000. y Mon Mar 05 21:49:26 2007
```

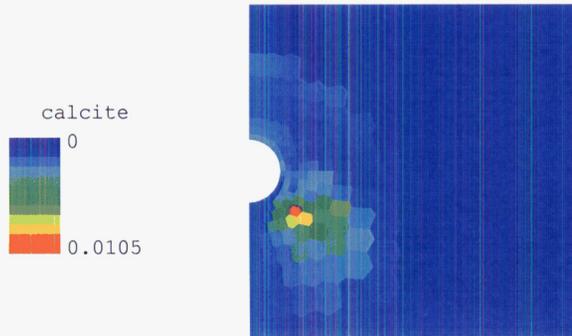
```
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells → 446,
  PlotRange → {{0, 30}, {-15, 15}}, DataRange → {0.2, 1}, WarmColor → False]
```



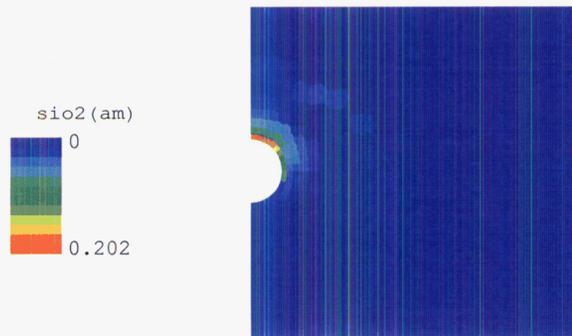
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",  
NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



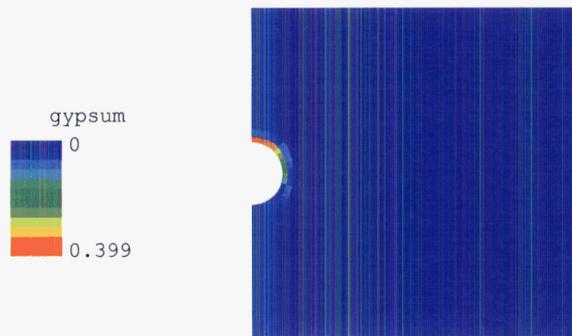
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",  
NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

```
PlotUnstructured[mesh1, data, "gypsum",  
NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

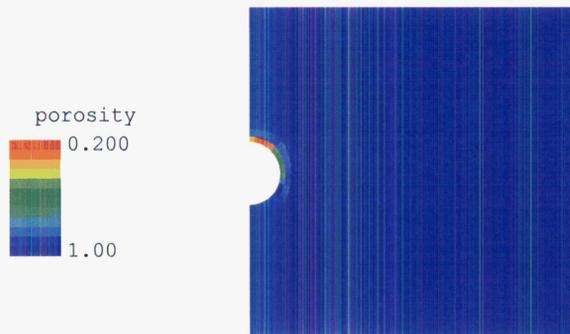
■ **strang splitting. wtkin=0, delcmax = 2**

```
data = GetData[ "H:\\Lynn\\THC_meth2-2_W0_dcx2\\fi_volf21.xyp" ];
```

```
!time= 2000. y Tue Mar 06 22:27:08 2007
```

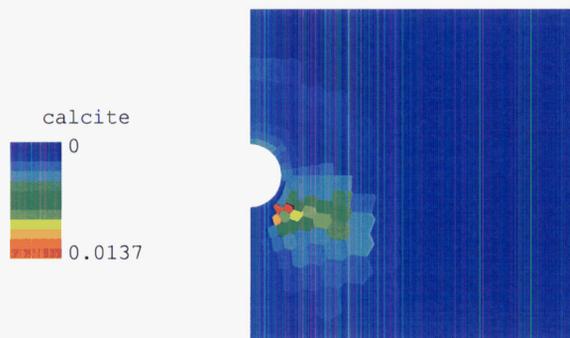
```
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,  
5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,  
PlotRange -> {{0, 30}, {-15, 15}}, DataRange -> {0.2, 1}, WarmColor -> False]
```



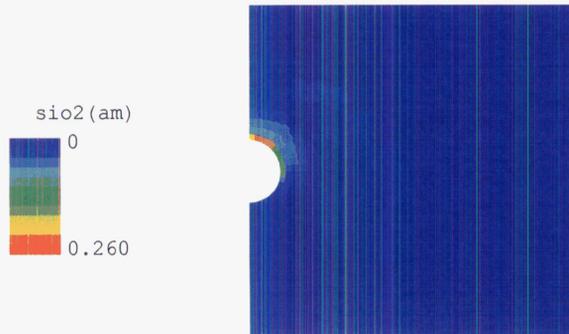
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",  
NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



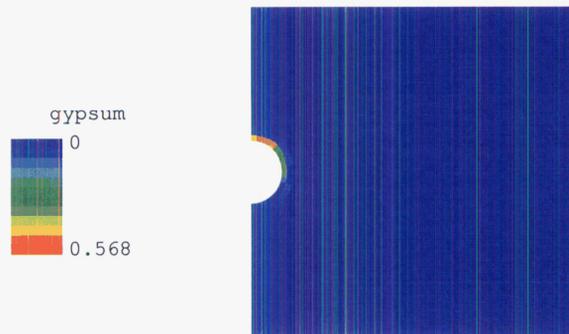
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

```
PlotUnstructured[mesh1, data, "gypsum",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

■ meth 2-1 . wtkin=0, delcmax=10

```
data = GetData[ "H:\\Lynn\\THC_meth2-1_wtkin0\\fi_volf21.xyp" ];
```

```
!time= 2000. y Mon Mar 05 21:57:51 2007
```

```
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,
  PlotRange -> {{0, 30}, {-15, 15}}, DataRange -> {0.2, 1}, WarmColor -> False]
```



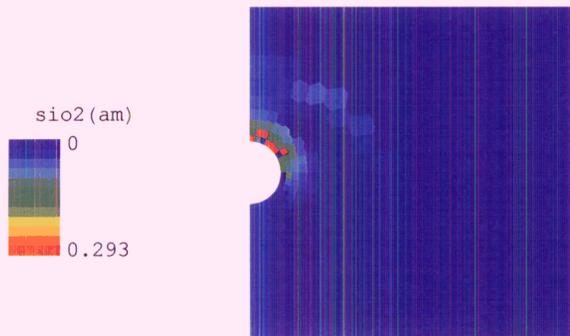
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",
  NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



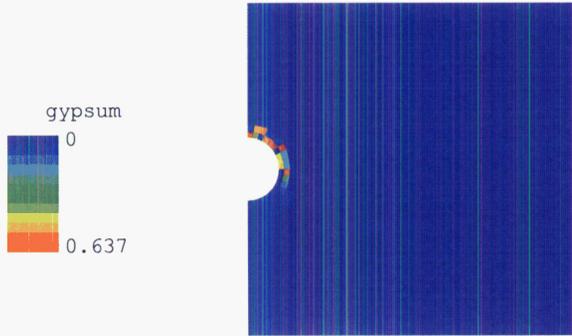
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",
  NumberCells -> 446, PlotRange -> {{0, 30}, {-15, 15}}]
```



- Graphics -

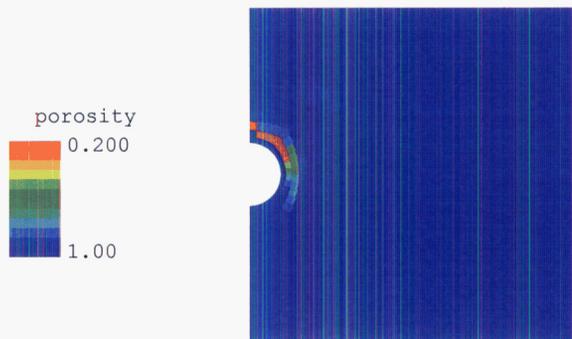
```
PlotUnstructured[mesh1, data, "gypsum",
  NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

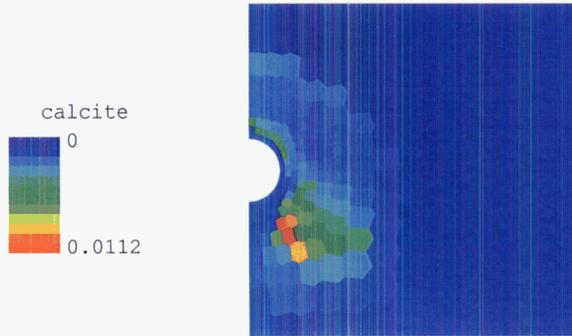
■ meth 2-1, wtkin=0, delcmax = 2

```
data = GetData[ "H:\\Lynn\\THC_meth2-1_W0_dcx2\\fi_volf21.xyp" ];
!time= 2000. y Wed Mar 07 00:19:48 2007
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
PlotUnstructured[mesh1, data, "porosity", NumberCells → 446,
  PlotRange → {{0, 30}, {-15, 15}}, DataRange → {0.2, 1}, WarmColor → False]
```



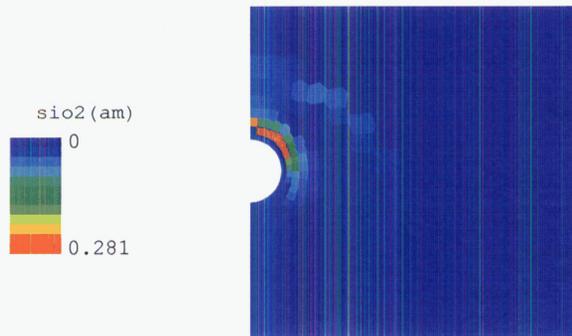
- Graphics -

```
PlotUnstructured[mesh1, data, "calcite",  
NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



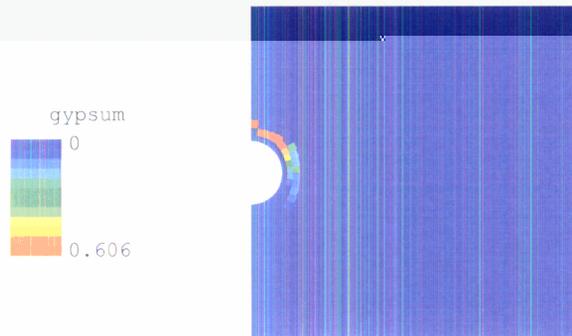
- Graphics -

```
PlotUnstructured[mesh1, data, "sio2(am)",  
NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -

```
PlotUnstructured[mesh1, data, "gypsum",  
NumberCells → 446, PlotRange → {{0, 30}, {-15, 15}}]
```



- Graphics -