

# THC simulations for M&C SNA'07

## Conference

This notebook documents material to be presented at 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. Physical and chemical input is identical in each. Runs differ only in the numerical parameters affecting the coupling between reactions and transport. 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 -- Operator splitting with wtkin=1  
Meth2-1\_wtkin0 --Operator splitting with wtkin=0

3/12/2007

Scott Painter

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## Preliminaries

```
<< Graphics `Graphics`
```

```
<< "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**

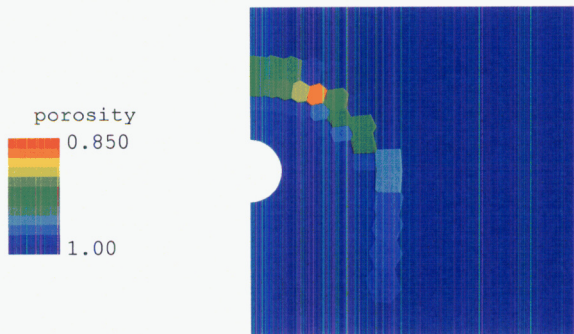
PlotUnstructured[mesh, data] constructs a two-dimensional plot from unstructured grid.  
The 'mesh' and 'data' objects are the result of GetMesh[] and GetData[] commands

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

## Porosity: 500 years

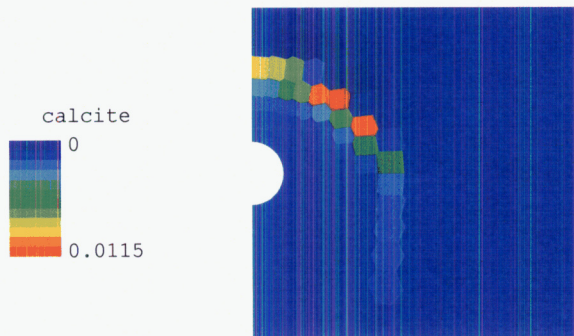
### ■ fully implicit

```
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]
```



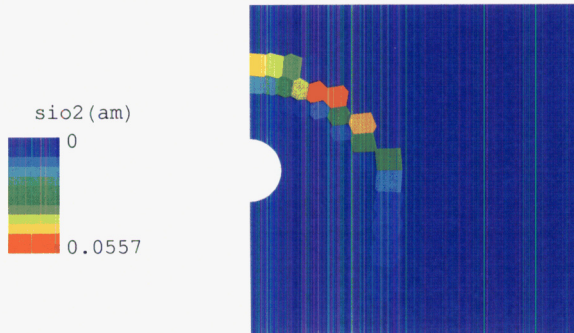
- Graphics -

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



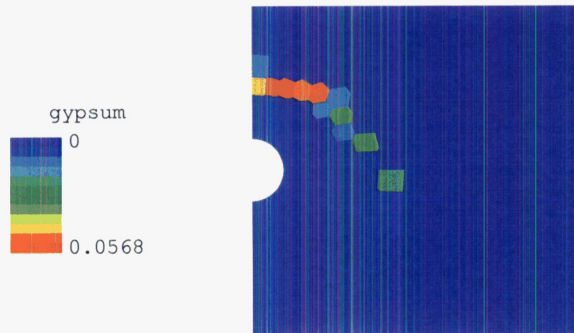
- Graphics -

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



- Graphics -

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

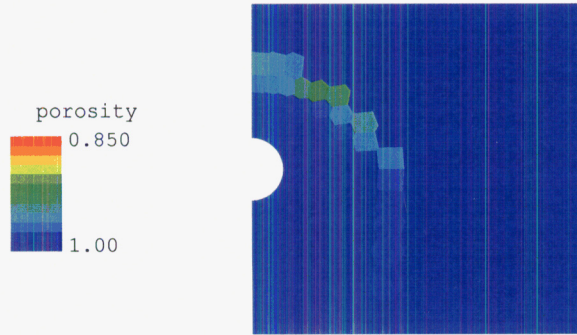


- Graphics -

■ **strang splitting. wtkin=0**

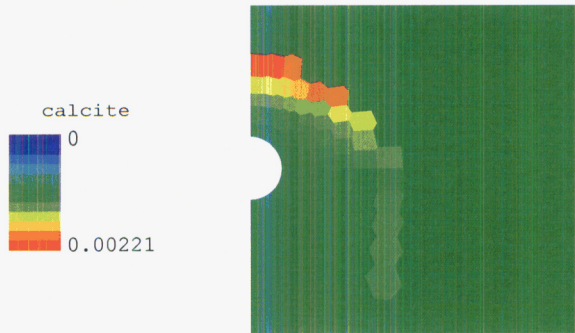
```
data = GetData[ "H:\\Lynn\\THC_meth2-2_wtkin0\\fi_volf18.xyp" ];
!time= 500.0 y Mon Mar 05 20:07:28 2007
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

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



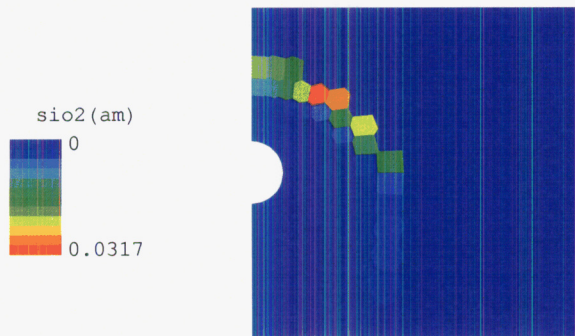
- Graphics -

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



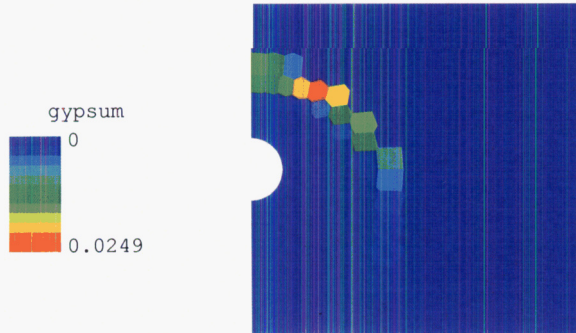
- Graphics -

```
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 -

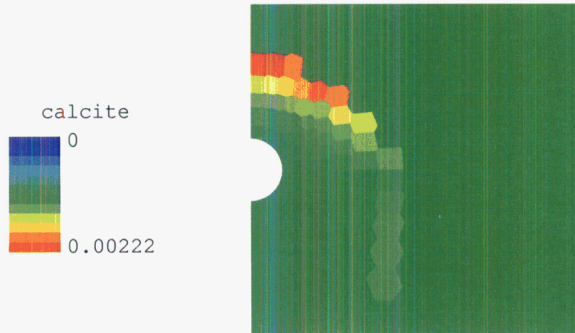
■ **strang splitting. wtkin=0.5**

```
data = GetData[ "H:\\Lynn\\THC_meth2-2_wtkin\\fi_volf18.xyp" ];
!time= 500.0 y Mon Feb 26 19:39:58 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]
```



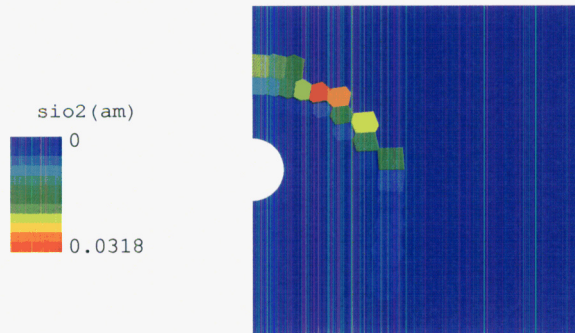
- Graphics -

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



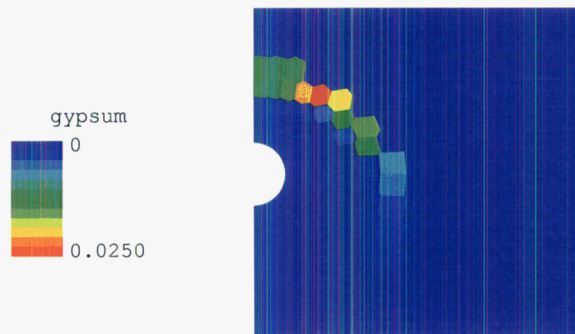
- Graphics -

```
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 -

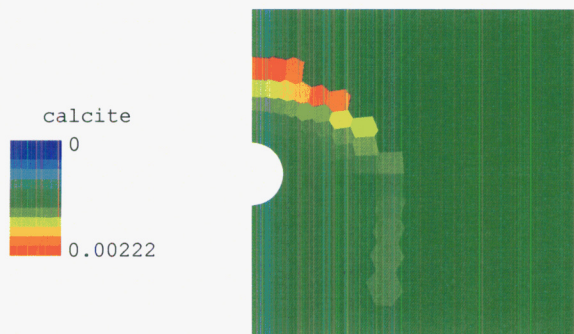
## ■ strang splitting. wtkin=1

```
data = GetData[ "H:\\Lynn\\THC_meth2-2\\fi_volf18.xyp" ];  
  
!time= 500.0 y Wed Jan 10 17:01:20 2007  
  
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,  
 5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}  
  
foo = Transpose[data[[2]]];  
data1 = {data[[1]], Transpose[Take[foo, 471]]};  
  
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,  
  PlotRange -> {{0, 30}, {-15, 15}}, DataRange -> {0.85, 1}, WarmColor -> False]
```



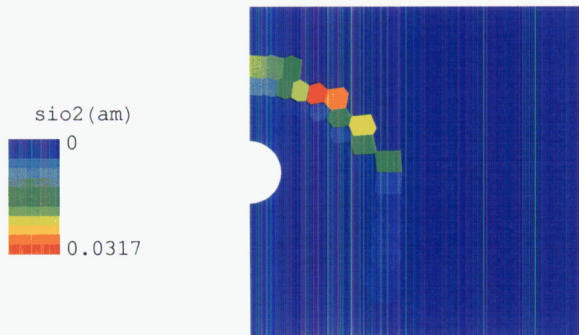
- Graphics -

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



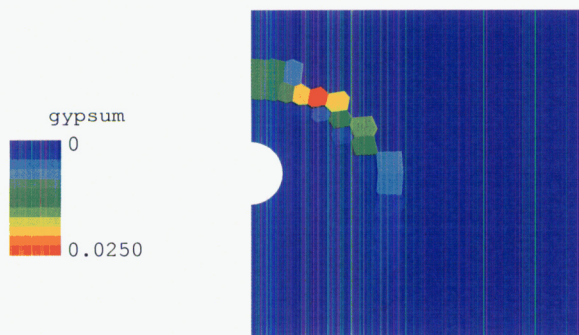
- Graphics -

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



- Graphics -

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



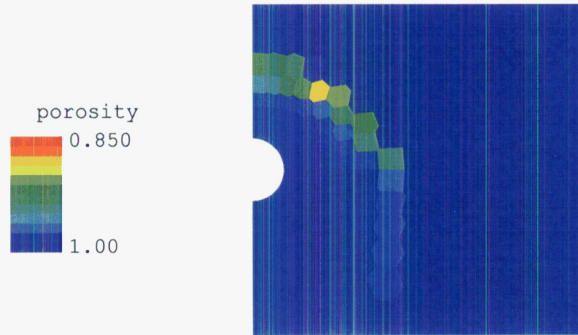
- Graphics -

■ method 2-1 wtkin = 0.0

```
data = GetData[ "H:\\Lynn\\THC_meth2-1_wtkin0\\fi_volf18.xyp" ];
!time= 500.0 y Mon Mar 05 19:44:09 2007
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

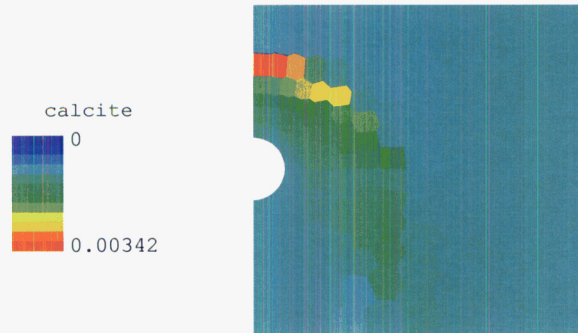


```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,
  PlotRange -> {{0, 30}, {-15, 15}}, DataRange -> {0.85, 1}, WarmColor -> False]
```



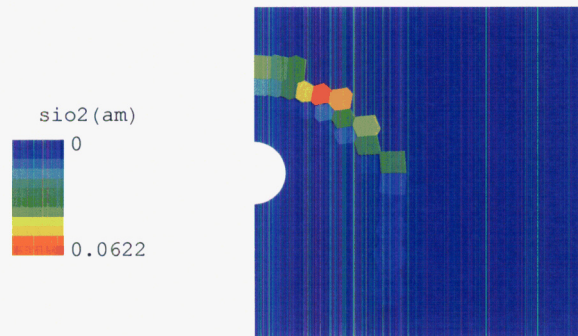
- Graphics -

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



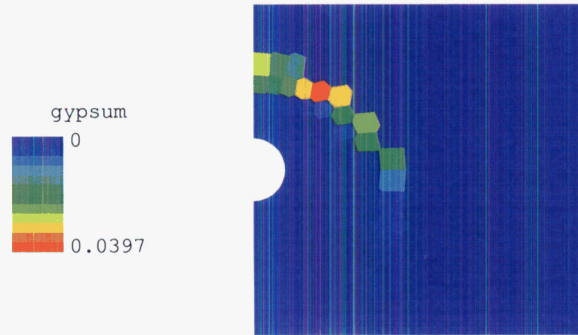
- Graphics -

```
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 -

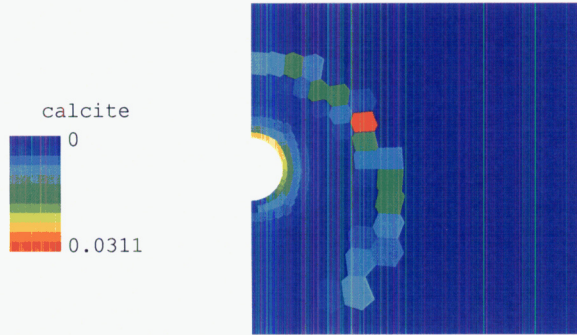
■ method 2-1 wtkin = 1

```
data = GetData[ "H:\\Lynn\\THC_meth2-1\\fi_volf18.xyp" ];
!time= 500.0 y Mon Jan 15 20:19:28 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]
```



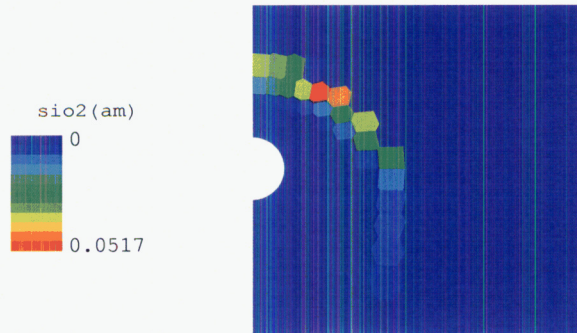
- Graphics -

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



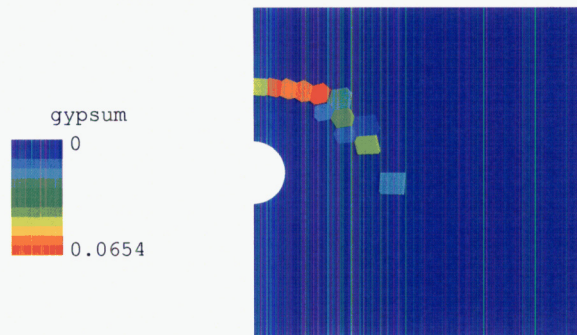
- Graphics -

```
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 -

## Porosity: 2000 years

### ■ fully implicit

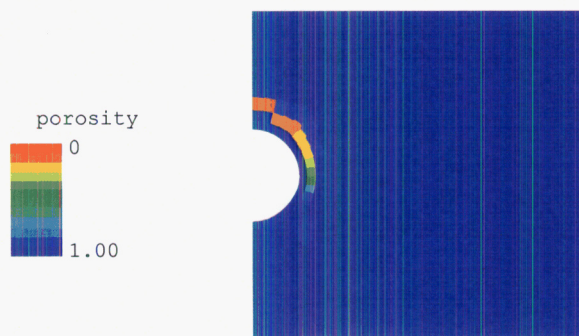
```

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}

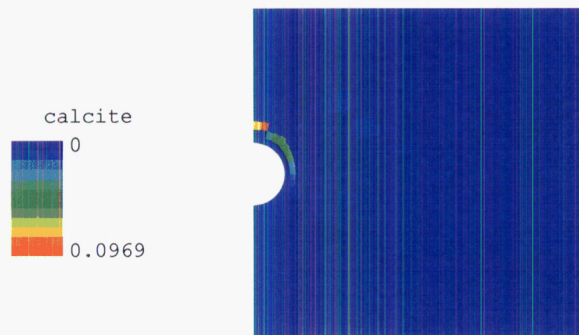
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,
  PlotRange -> {{0, 20}, {-10, 10}}, DataRange -> {0.0, 1}, WarmColor -> False]
    
```



- Graphics -

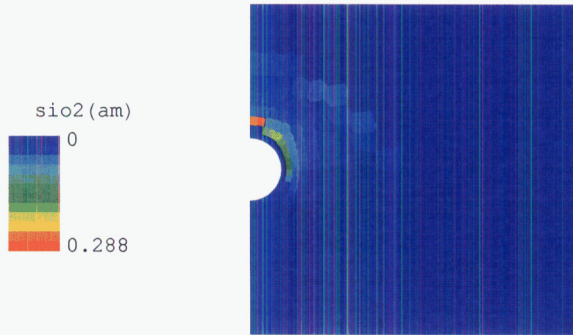
```

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



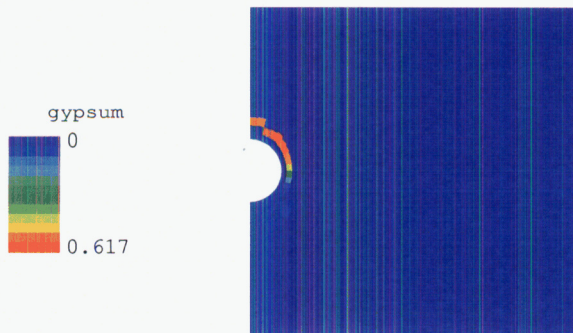
- Graphics -

```
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 -

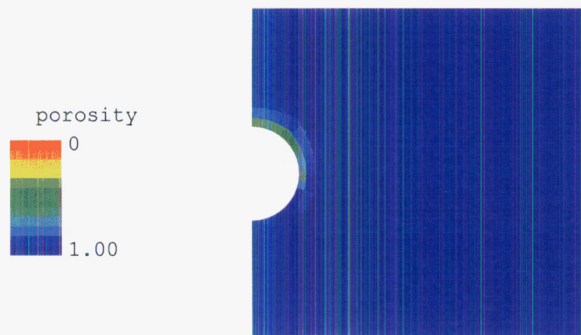
## ■ strang splitting. wtkin=0

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

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

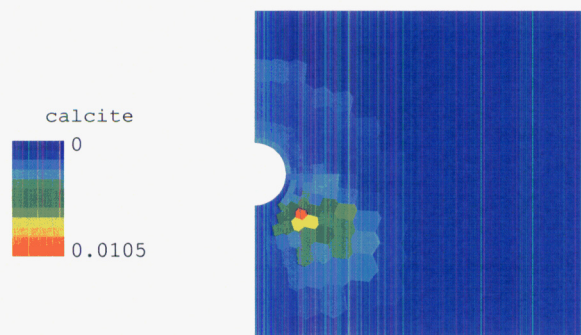
```
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells → 446,
  PlotRange → {{0, 20}, {-10, 10}}, DataRange → {0.0, 1}, WarmColor → False]
```



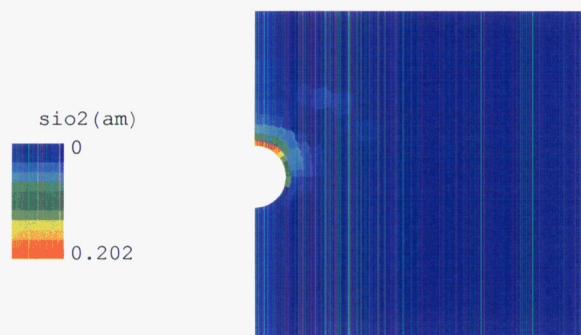
- Graphics -

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



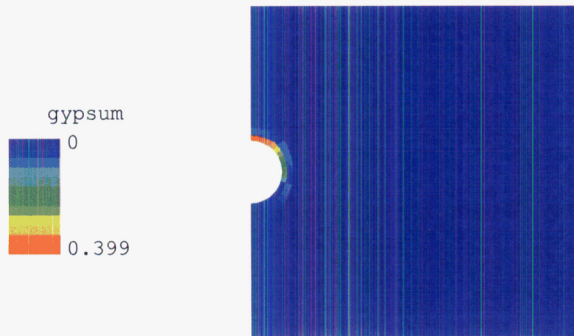
- Graphics -

```
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=0.5

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

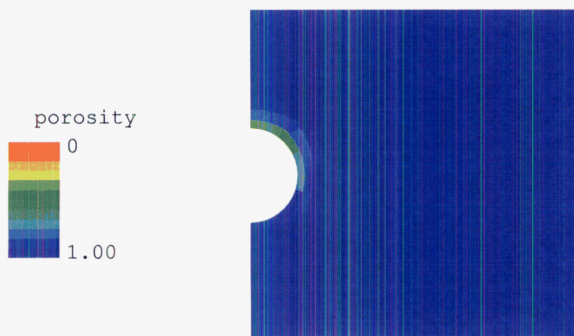
```
!time= 2000. y Mon Feb 26 22:02:17 2007
```

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

```
foo = Transpose[data[[2]]];
```

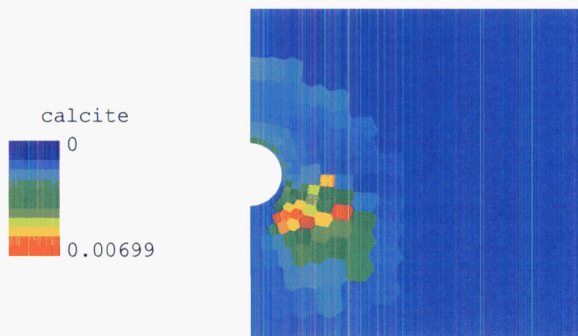
```
data1 = {data[[1]], Transpose[Take[foo, 471]]};
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells → 446,
  PlotRange → {{0, 20}, {-10, 10}}, DataRange → {0.0, 1}, WarmColor → False]
```



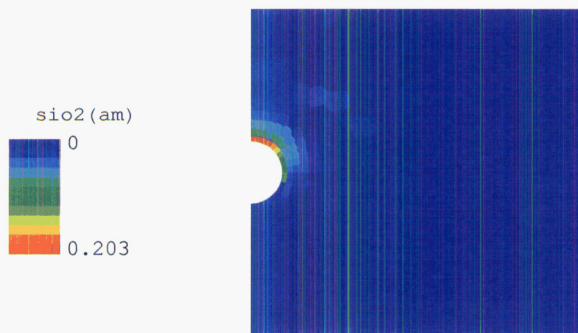
- Graphics -

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



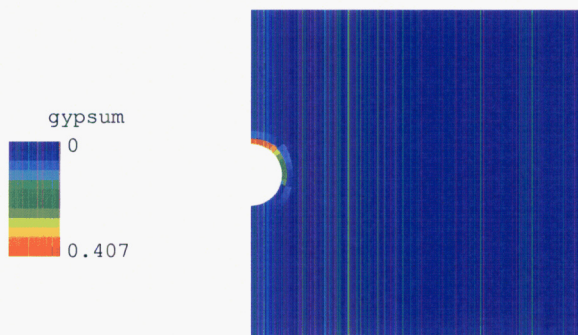
- Graphics -

```
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=1

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

```
!time= 2000. y Wed Jan 10 18:34:54 2007
```

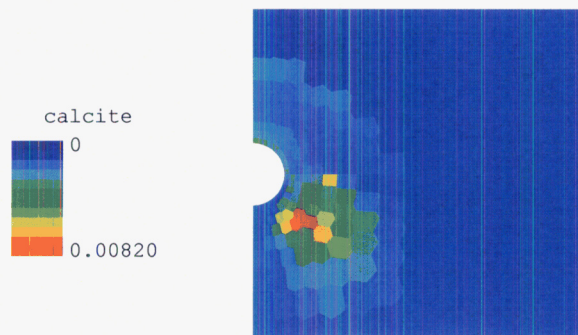
```
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,
PlotRange -> {{0, 20}, {-10, 10}}, DataRange -> {0.0, 1}, WarmColor -> False]
```



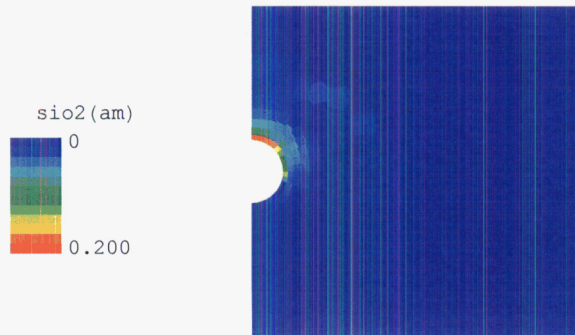
- Graphics -

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



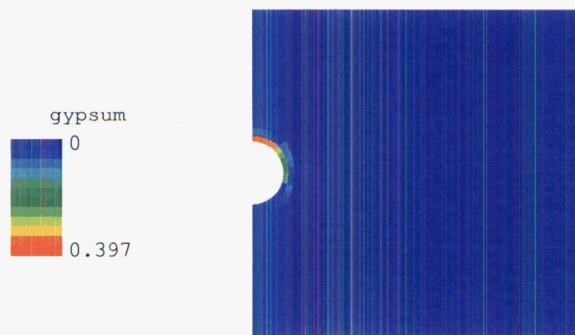
- Graphics -

```
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 -

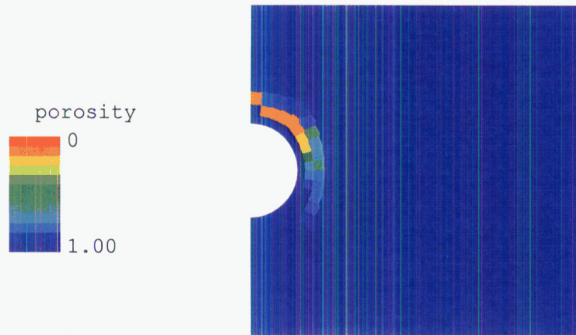
## ■ method 2-1 wtkin = 0.0 reduced time step

```
data = GetData[ "H:\\Lynn\\THC_meth2-1_w0_dcx2\\fi_volf21.xyp" ];
```

```
!time= 2000. y Wed Mar 07 00:19:48 2007
```

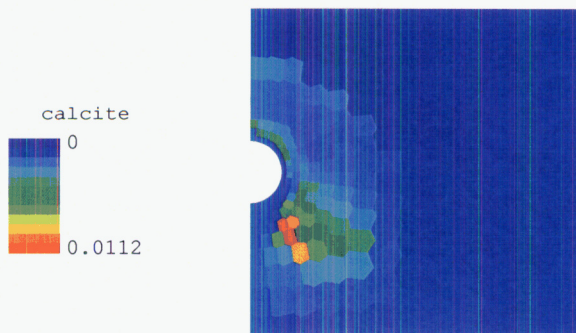
```
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
  5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}
```

```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,
  PlotRange -> {{0, 20}, {-10, 10}}, DataRange -> {0.0, 1}, WarmColor -> False]
```



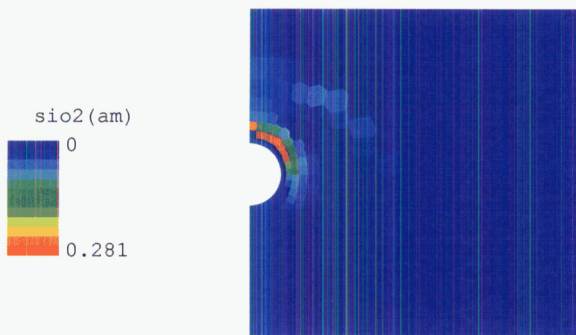
- Graphics -

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



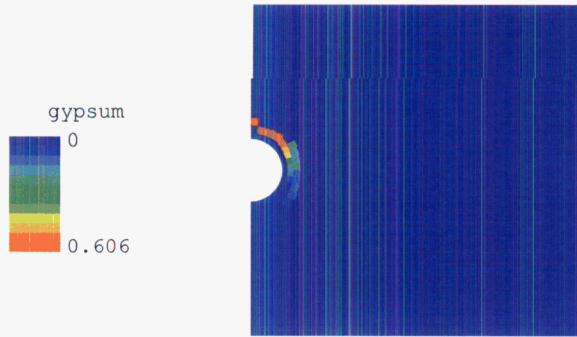
- Graphics -

```
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 -

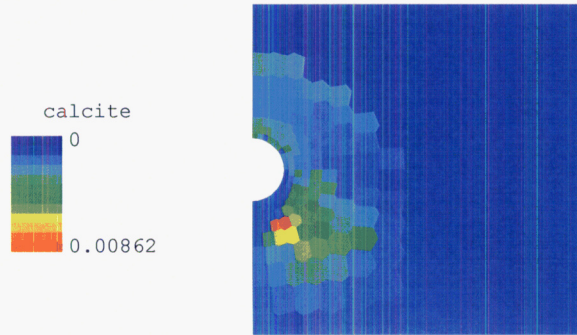
■ method 2-1 wtkin = 0.0

```
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, 20}, {-10, 10}}, DataRange → {0.0, 1}, WarmColor → False]
```



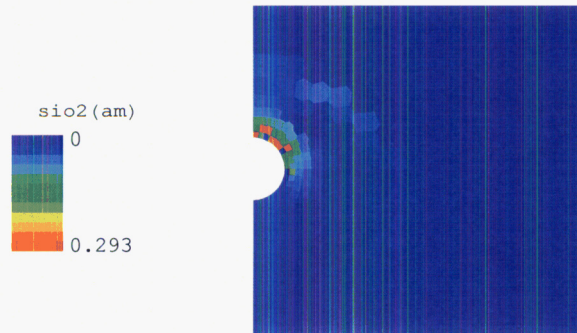
- Graphics -

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



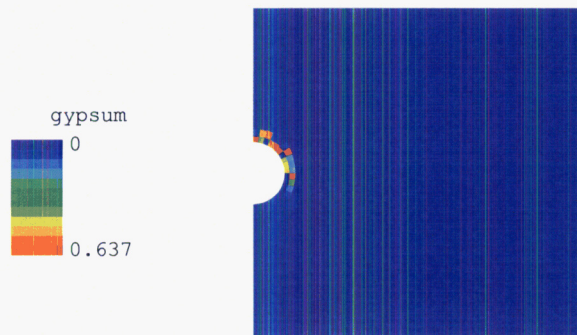
- Graphics -

```
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 -

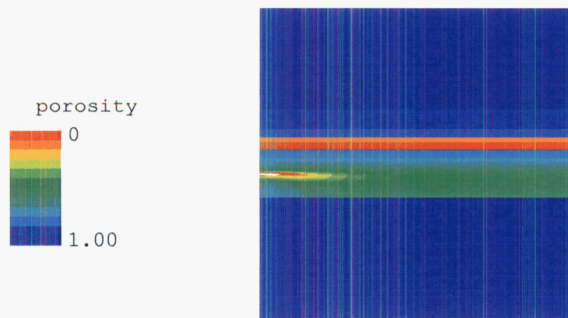
## Numerical Artifact

Method 2-1 with `wtkin .ne. 0` produced a numerical artifact. specifically, fractures plugged in unit above repository

### ■ method 2-1 wtkin = 1

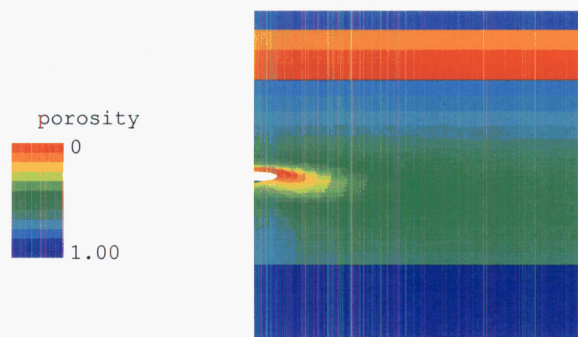
```
data = GetData[ "H:\\Lynn\\THC_meth2-1\\fi_volf25.xyp" ];
!time= 4500.    y    Thu Jan 18 13:27:22 2007
{!distance, 1-gypsum, 2-calcite, 3-fluorite, 4-cristobalite,
 5-tridymite, 6-sio2(am), 7-glass, 8-quartz, 9-burkeite, porosity, por}

PlotUnstructured[mesh1, data, "porosity",
  NumberCells -> 446, DataRange -> {0.0, 1}, WarmColor -> False]
```



- Graphics -

```
PlotUnstructured[mesh1, data, "porosity", NumberCells -> 446,
  DataRange -> {0.0, 1}, PlotRange -> {{0, 40}, {-100, 100}}, WarmColor -> False]
```



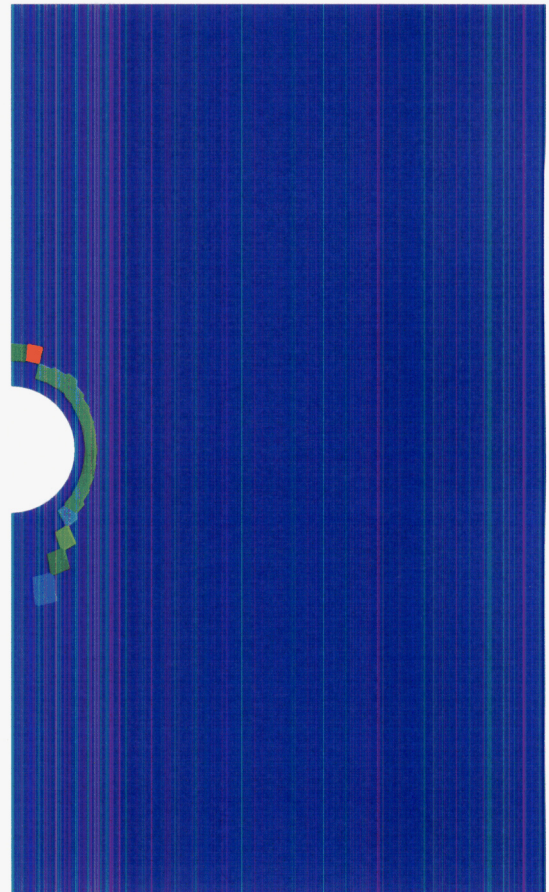
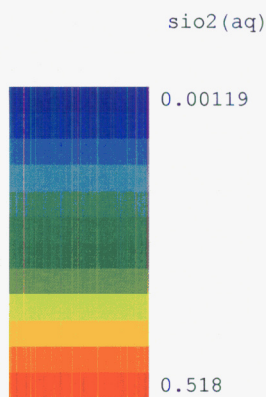
- Graphics -

---

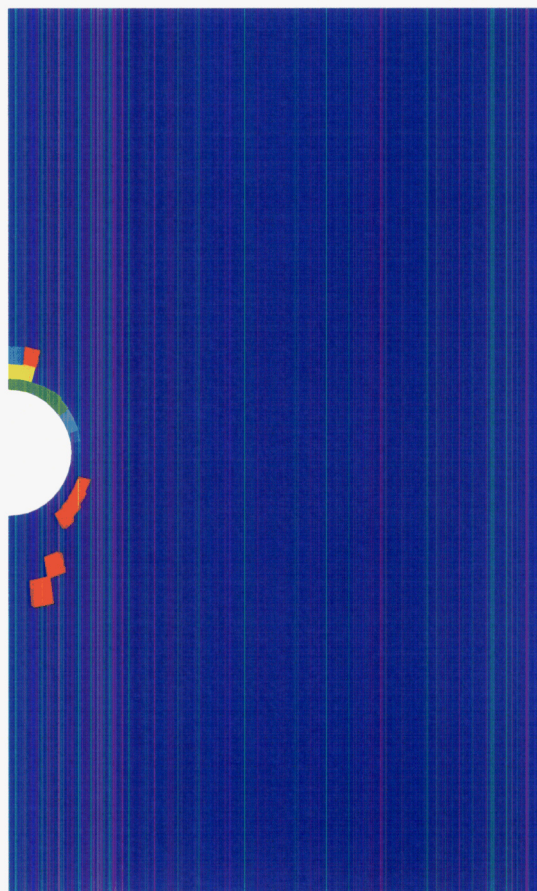
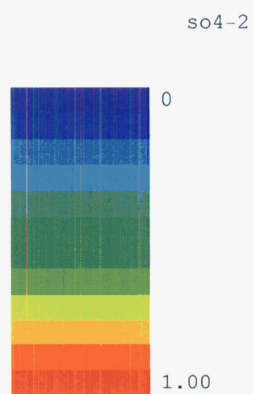
## Aqueous Concentrations

### ■ Fully implicit

```
data = GetData[ "H:\\Lynn\\THC_meth1\\fi_aqf21.xyp" ];  
!time= 2000. y Tue Jan 16 06:08:48 2007  
{!distance, pH, 2-cl-, 3-ca+2, 4-h+, 5-hco3-, 6-sio2(aq), 7-na+, 8-so4-2, 9-f-, dliq}  
  
foo = Transpose[data[[2]]];  
data1 = {data[[1]], Transpose[Take[foo, 471]]};  
  
PlotUnstructured[mesh1, data1, "sio2(aq)",  
NumberCells -> 446, PlotRange -> {{0, 40}, {20, -20}}]
```



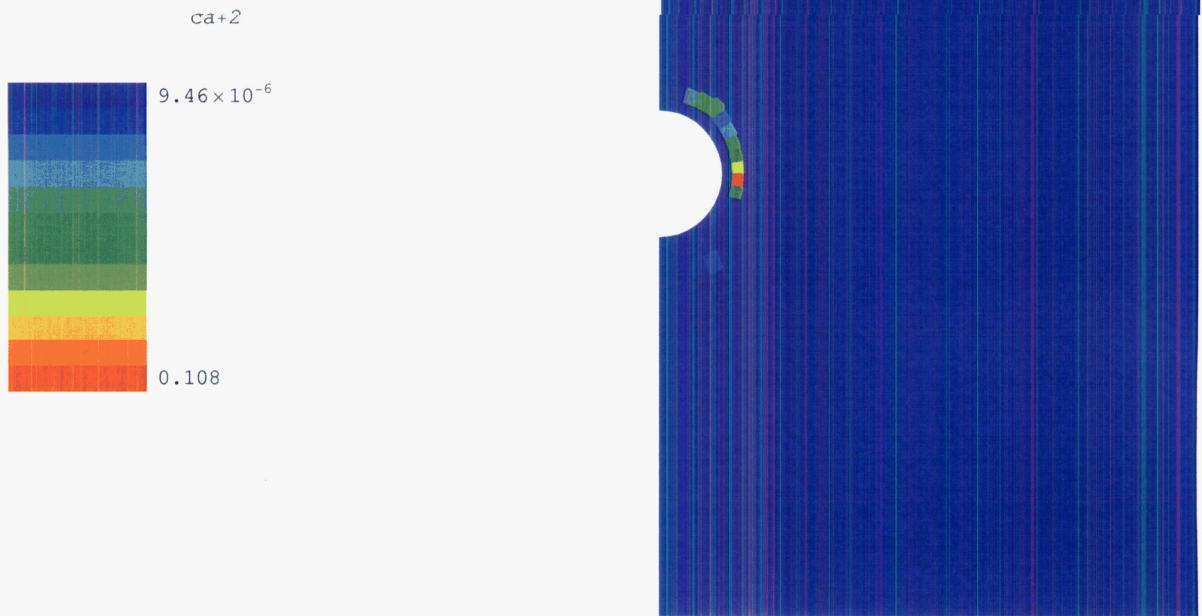
```
PlotUnstructured[mesh1, data1, "so4-2", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 1}]
```



- Graphics -



```
PlotUnstructured[mesh1, data1, "ca+2",
  NumberCells -> 446, PlotRange -> {{0, 40}, {20, -20}}]
```



- Graphics -

---

## TH

Show the temperature field evolution . Note there are differences for the different runs because of effect of mineral precipitation on the flow field. Result shown is for meth1.

## ■ Plot the heat load

```
tmp = OpenRead["H:\\Lynn\\THC_meth1\\multi.src"]
Read[tmp, {String}];
data = ReadList[tmp, Number];
data = Partition[data, 2];
data = Transpose[data];
Close[tmp];
```

```
InputStream[H:\\Lynn\\THC_meth1\\multi.src, 15]
```

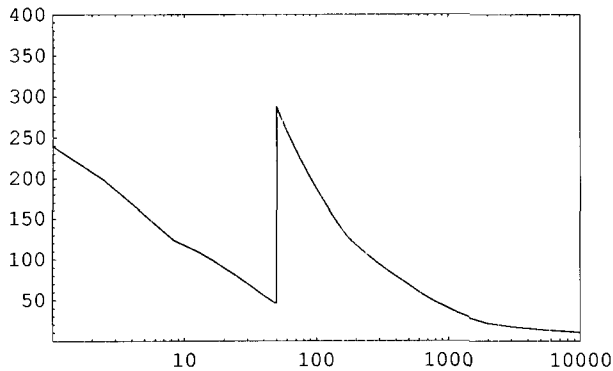
```
Read::readn : Syntax error reading a real number from H:\\Lynn\\THC_meth1\\multi.src. More...
```

Convert from seconds to years

```
data[[1]] = data[[1]] / (365 * 24 * 3600);
data = Transpose[data];

LogLinearListPlot[data, PlotJoined -> True,
  Frame -> True, PlotRange -> {{1, 10000}, {0, 400}}]
```

```
Graphics::gptn : Coordinate Indeterminate in {Indeterminate, 572.28} is not a floating-point number. More...
```

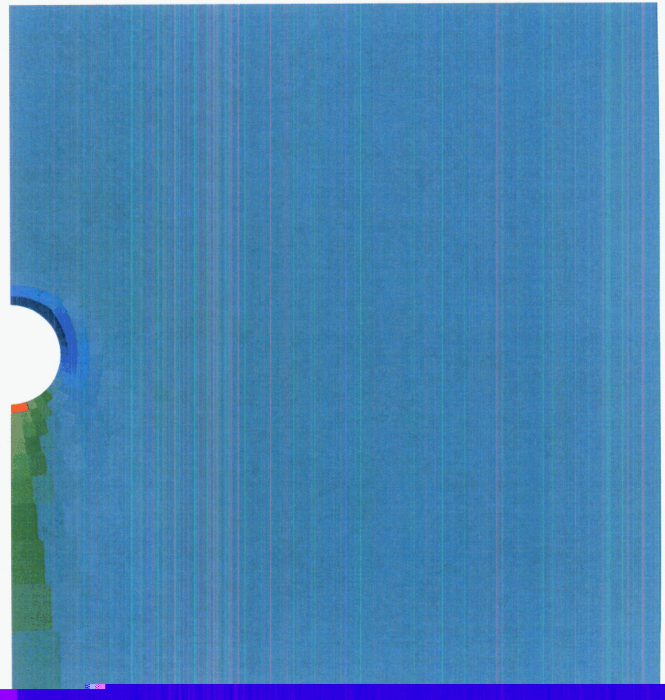
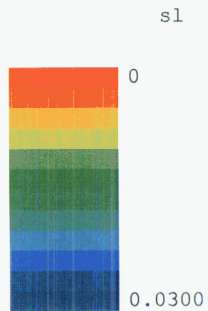


- Graphics -

## ■ 50 years

```
data = GetData["H:\\Lynn\\THC_meth1\\multifldf9.xyp"];
TITLE=" 50.00 y n1= 942 Mon Jan 15 17:25:02 2007"
{x, press, temp, sl, sg, xa1rl, xa1rg, pcap, zh, psat, rho1, rho2, por}
```

```
PlotUnstructured[mesh1, data, "s1", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```

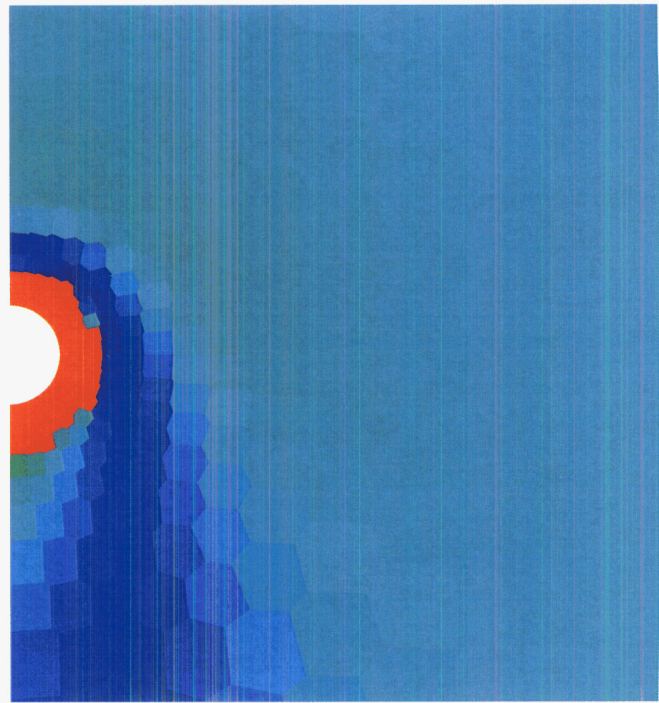
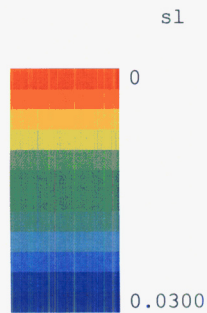


- Graphics -

## ■ 55 years

```
data = GetData["H:\\Lynn\\THC_meth1\\multifldf10.xyp"];  
TITLE=" 55.00 y nl= 942 Mon Jan 15 17:50:23 2007"  
{x, press, temp, s1, sg, xair1, xairg, pcap, rh, psat, rho1, rhog, por}
```

```
PlotUnstructured[mesh1, data, "s1", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```

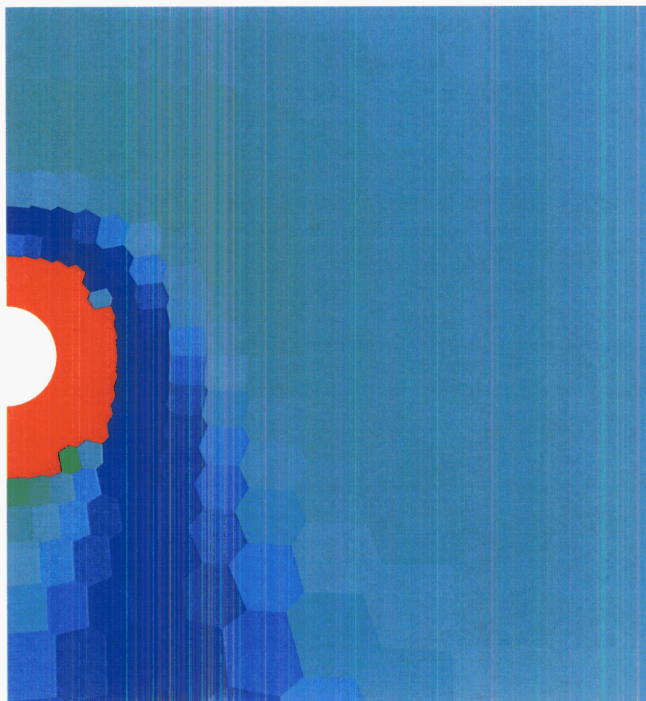
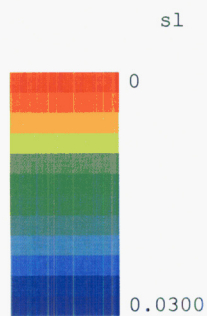


- Graphics -

## ■ 60 years

```
data = GetData[ "H:\\Lynn\\THC_meth1\\multifldf11.xyp" ];  
TITLE=" 60.00 y n1= 942 Mon Jan 15 18:10:39 2007"  
{x, press, temp, s1, sg, xairl, xairg, pcap, rh, psat, rho1, rhog, por}
```

```
PlotUnstructured[mesh1, data, "sl", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```

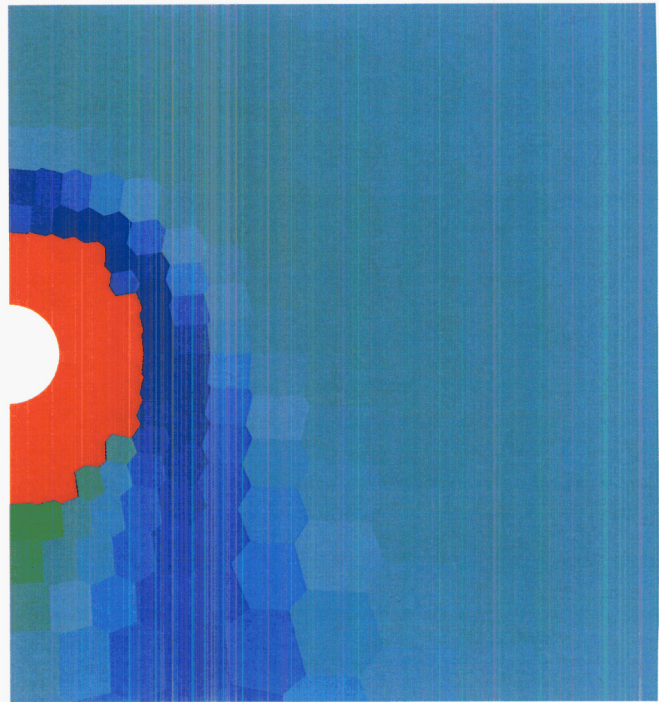
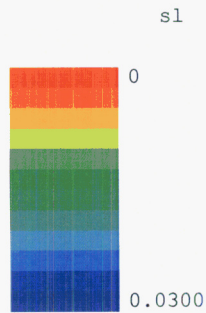


- Graphics -

## ■ 70 years

```
data = GetData[ "H:\\Lynn\\THC_meth1\\multifldf12.xyp" ];  
TITLE=" 70.00 y n1= 942 Mon Jan 15 18:41:48 2007"  
{x, press, temp, sl, sg, xair1, xairg, pcap, rh, psat, rho1, rhog, por}
```

```
PlotUnstructured[mesh1, data, "s1", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```

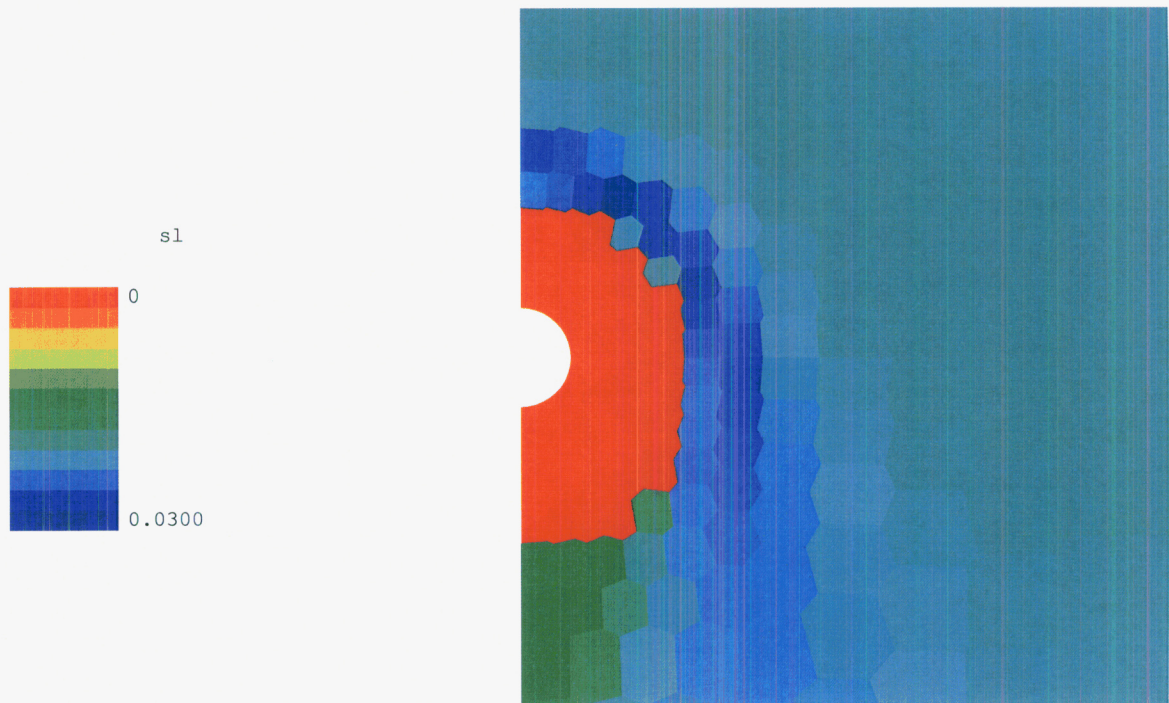


- Graphics -

## ■ 100 years

```
data = GetData["H:\\Lynn\\THC_meth1\\multifldf14.xyp"];  
TITLE=" 100.0 y n1= 942 Mon Jan 15 19:52:31 2007"  
{x, press, temp, s1, sg, xair1, xairg, pcap, rh, psat, rho1, rhog, por}
```

```
PlotUnstructured[mesh1, data, "sl", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```

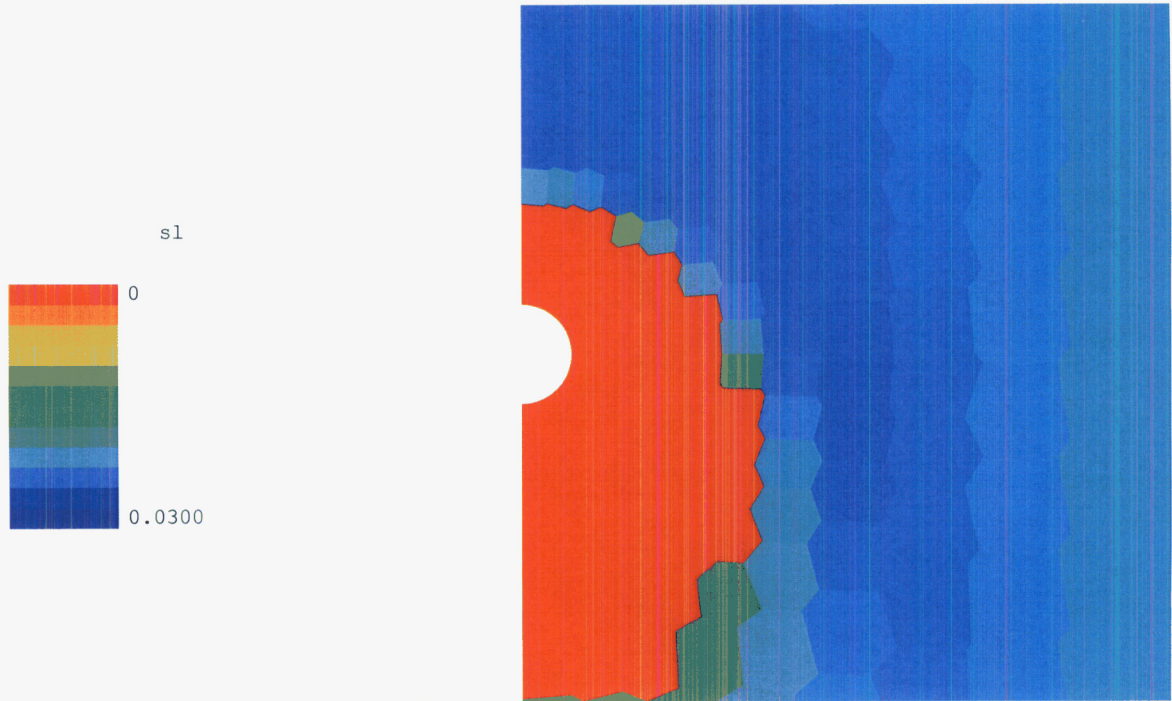


- Graphics -

## ■ 500 years

```
data = GetData[ "H:\\Lynn\\THC_meth1\\multifldf18.xyp" ];  
TITLE=" 500.0 y n1= 942 Mon Jan 15 21:34:21 2007"  
{x, press, temp, sl, sg, xair1, xairg, pcap, rh, psat, rho1, rhog, por}
```

```
PlotUnstructured[mesh1, data, "sl", NumberCells -> 446,
  PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```



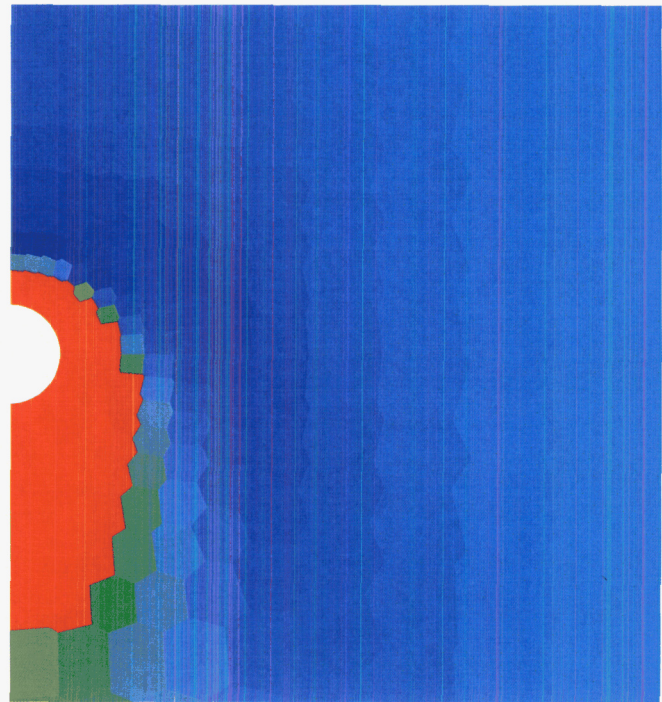
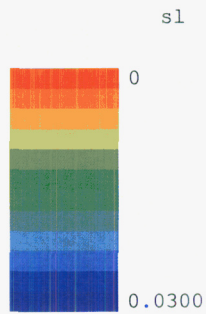
- Graphics -

■ 1000 years

```
data = GetData[ "H:\\Lynn\\THC_meth1\\multifldf20.xyp" ];
TITLE=" 1000. y n1= 942 Tue Jan 16 00:29:39 2007"
{x, press, temp, sl, sg, xairl, xairg, pcap, rh, psat, rho1, rhog, por}
```



```
PlotUnstructured[mesh1, data, "s1", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```



- Graphics -

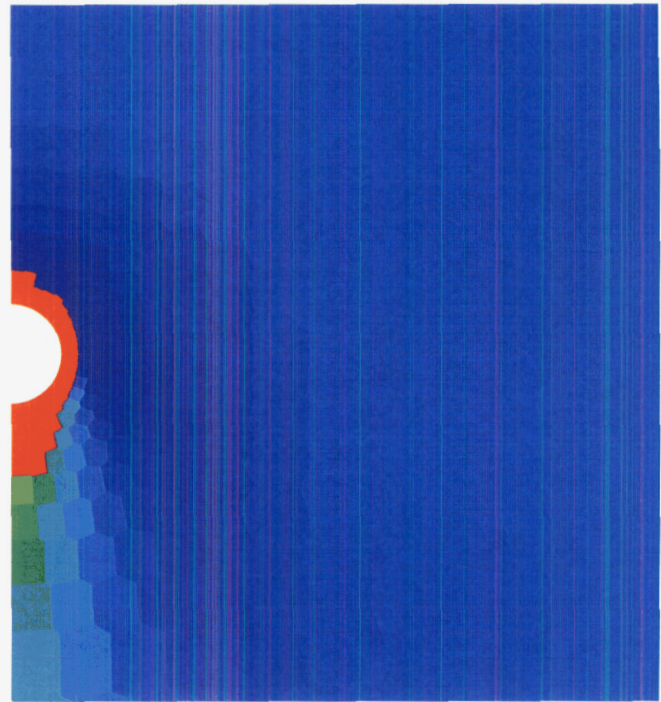
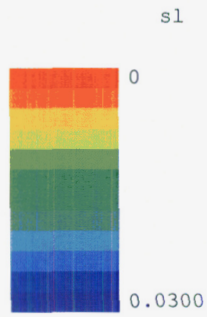
## ■ 2000 years

```
data = GetData["H:\\Lynn\\THC_meth1\\multifldf21.xyp"];
```

```
TITLE=" 2000. y n1= 942 Tue Jan 16 06:08:33 2007"
```

```
{x, press, temp, s1, sg, xairl, xairg, pcap, rh, psat, rho1, rhog, por}
```

```
PlotUnstructured[mesh1, data, "s1", NumberCells -> 446,  
PlotRange -> {{0, 40}, {20, -20}}, DataRange -> {0, 0.03}, WarmColor -> False]
```



- Graphics -

# Defining an effective thermal-conductivity versus T

Scott Painter

1/18/2006

Read the data for 5 times

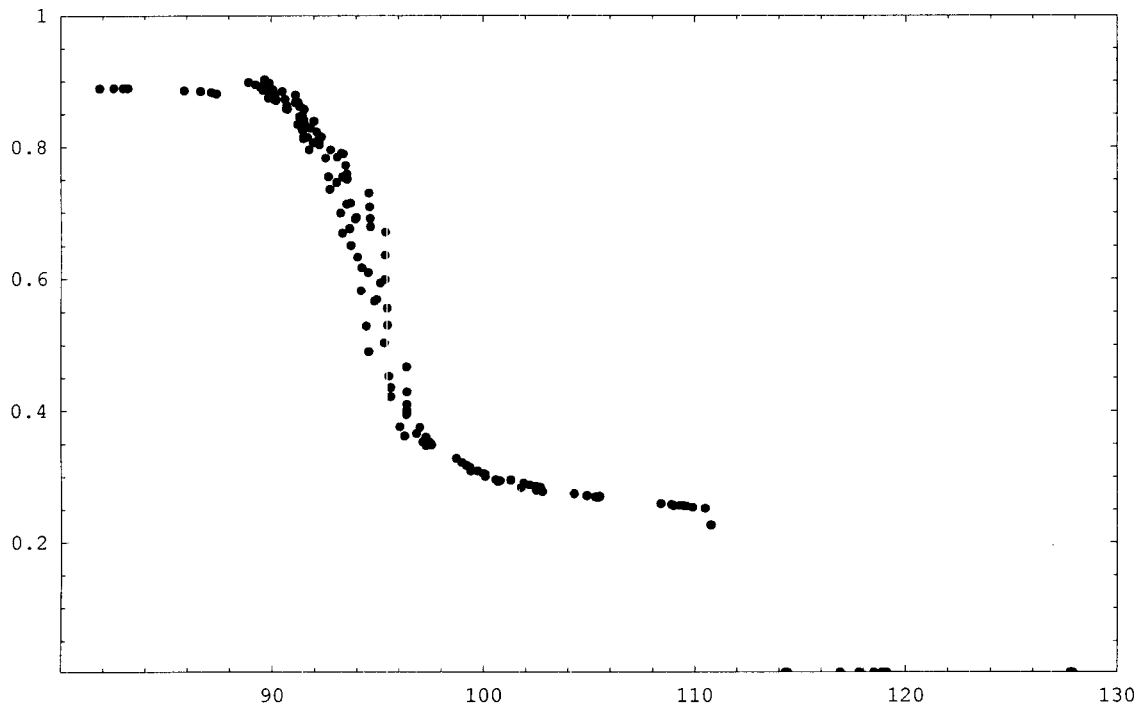
```

slbig = {};
tempbig = {};
Do[
  fn = StringJoin["H:\\THforGoodluck\\multifldm", ToString[i], ".xyp"];
  tmp = OpenRead[fn];
  Read[tmp, {String, String, String}];
  data = ReadList[tmp, Number, 444];
  data = Partition[data, 13];
  data = Transpose[data];
  sl = data[[4]];
  temp = data[[3]];
  Close[tmp];
  slbig = Join[slbig, sl];
  tempbig = Join[tempbig, temp], {i, 11, 15}]

```

16 (SP)

```
ListPlot[ Transpose[{tempbig, slbig}], PlotRange -> {{80, 130}, {0, 1}}, Frame -> True]
```



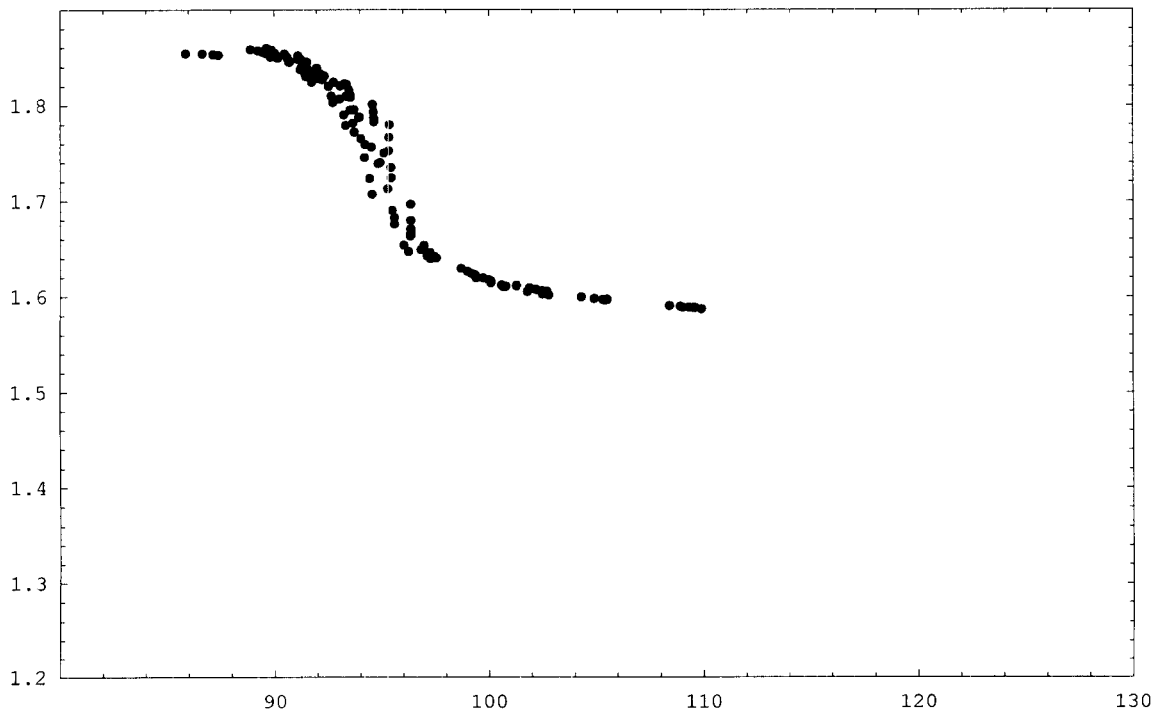
- Graphics -

Limit the range for the fit

```
indx = Position[tempbig, _? (85 < # < 110 &)];  
temp2 = Extract[tempbig, indx];  
sl2 = Extract[slbig, indx];  
kdry = 1.28; kwet = 1.89;  
kth = kdry + (kwet - kdry) * Sqrt[sl2];
```

1c (SP)

```
ListPlot[ Transpose[{temp2, kth}], PlotRange -> {{80, 130}, {1.2, 1.9}}, Frame -> True]
```



- Graphics -

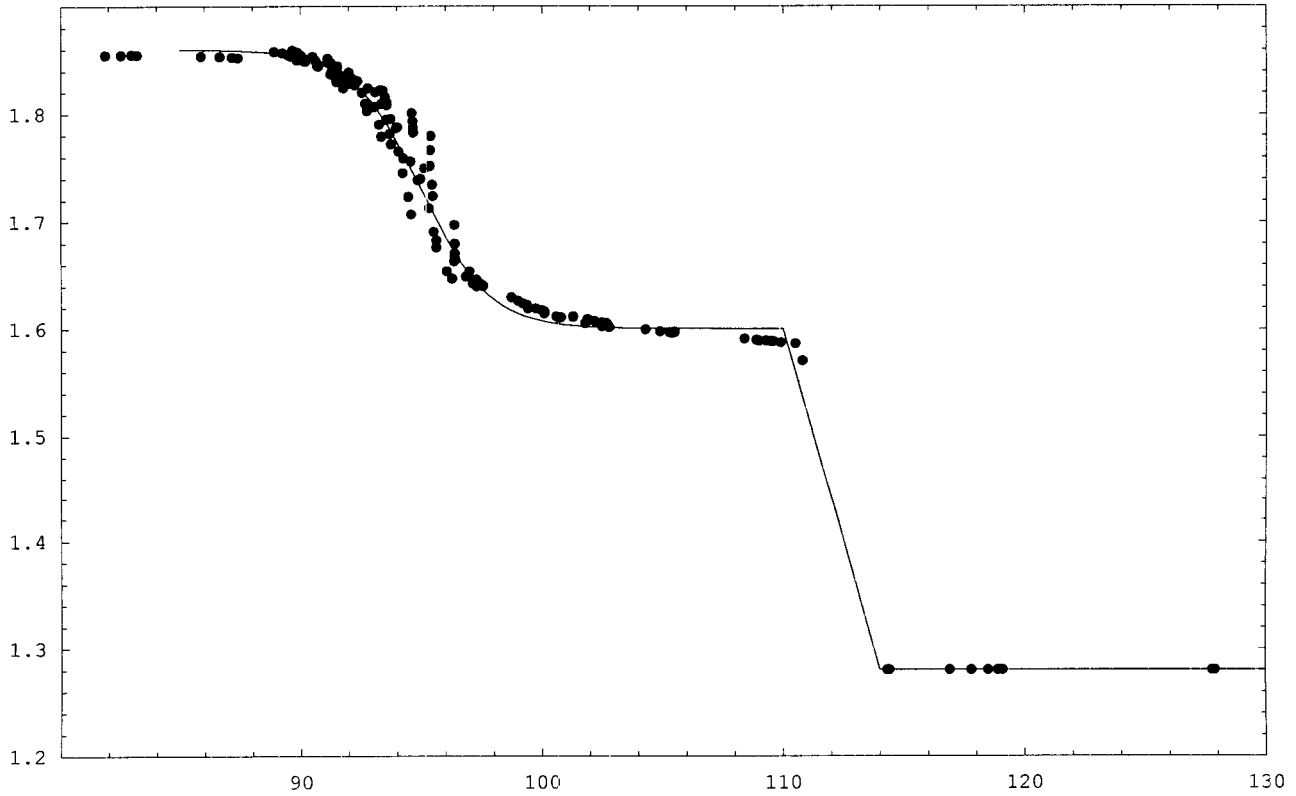
The fit

```
f[x_] := 1.86 - 0.26 / (1. + Exp[-(x - 95) / 1.4])
```

```
ff[x_] := If[ x < 110, f[x], 1.60 + (110 - x) * 0.32 / 4. ]
```

16 (SP)

```
DisplayTogether[  
  ListPlot[ Transpose[{tempbig, kdry + (kwet - kdry) * Sqrt[slbig]}],  
    PlotRange -> {{80, 130}, {1.2, 1.9}}, Frame -> True],  
  Plot[ ff[x], {x, 85, 114}],  
  Plot[ 1.28, {x, 114, 130}]  
]
```



- Graphics -

# Corrosion product Surface Areas

This notebook compares corrosion product specific surface area distribution used by DOE with an alternative model that assumes HFO transformation to goethite. (Goethite-only model).

Units here are m<sup>2</sup>/g.

Scott Painter

3/2/09

```
<< Statistics`ContinuousDistributions`
```

```
<< Graphics`Graphics`
```

HFO surface area Distribution used by DOE (ANL-WIS-PA-000001 REV 03).

```
hfodist = LogNormalDistribution[ 5.541, 0.396]
```

```
LogNormalDistribution[5.541, 0.396]
```

goethite surface area Distribution used by DOE (ANL-WIS-PA-000001 REV 03).

```
gdist = LogNormalDistribution[ 3.793, 0.543]
```

```
LogNormalDistribution[3.793, 0.543]
```

Uncertain mixture used by DOE (ANL-WIS-PA-000001 REV 03).

```
fraction = Table[ Random[ Real, {0.45, 0.80}], {1000}];
```

Sample from DOE's mixture.

```
mixture = Table[ Random[hfodist], {1000}] * (1 - fraction) +  
  Table[ Random[gdist], {1000}] * fraction;
```

```
Mean[mixture]
```

```
135.387
```

Sample assuming goethite only

```
goethiteonly = Table[ Random[gdist], {1000}];
```

```
Mean[goethiteonly]
```

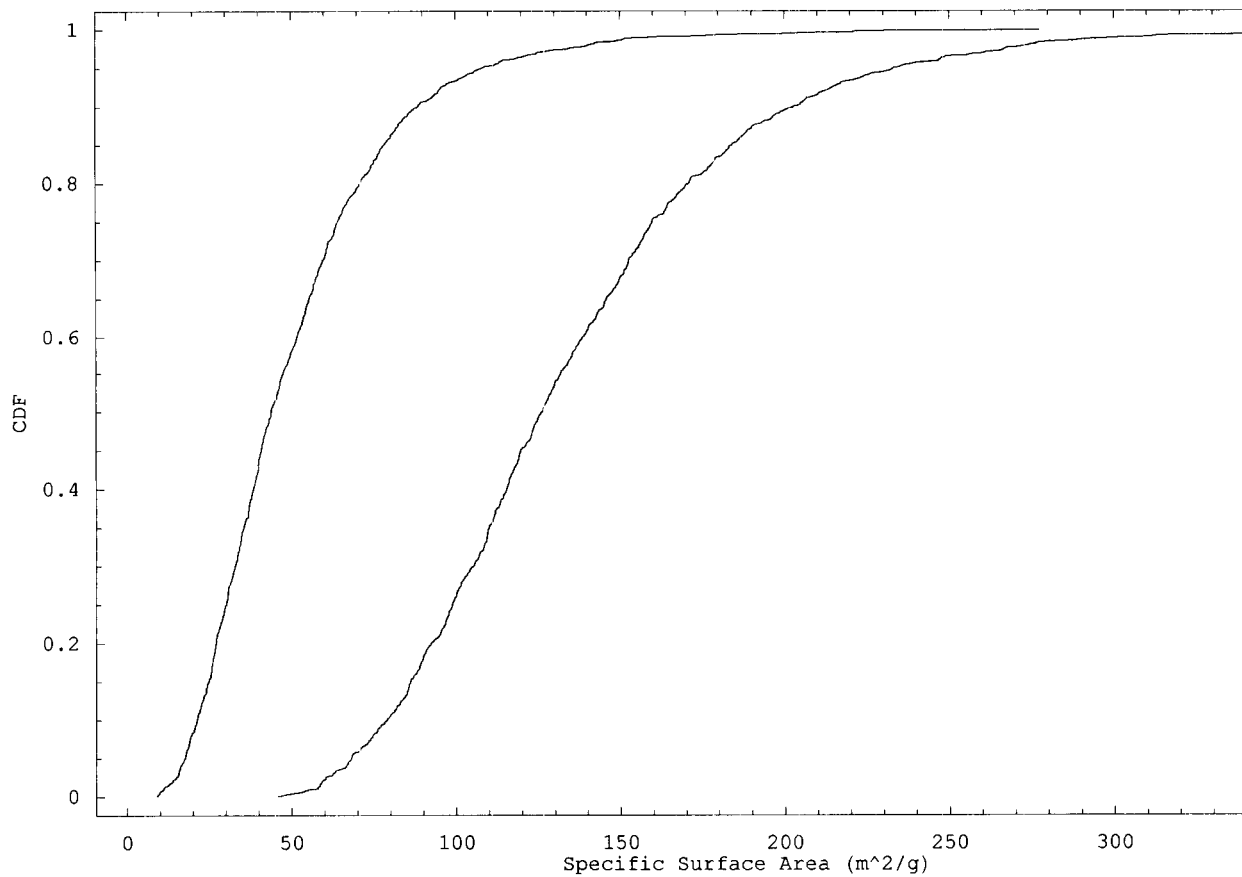
```
51.5056
```

CDFs

```
mixture = Sort[mixture];
olddist = Transpose[{mixture, (Range[Length[mixture]] - 0.5) / Length[mixture]}];

goethiteonly = Sort[goethiteonly];
newdist =
  Transpose[{goethiteonly, (Range[Length[goethiteonly]] - 0.5) / Length[goethiteonly]}];

DisplayTogether[
  ListPlot[olddist, PlotJoined → True],
  ListPlot[newdist, PlotJoined → True], Frame → True,
  FrameLabel → {"Specific Surface Area (m2/g)", "CDF"} ]
```



- Graphics -

```
InterpolatedQuantile[mixture, 0.05]
```

68.0452

```
InterpolatedQuantile[goethiteonly, 0.05]
```

17.5452

```
%%/%
```

3.87828



InterpolatedQuantile[mixture, 0.01]

56.5847

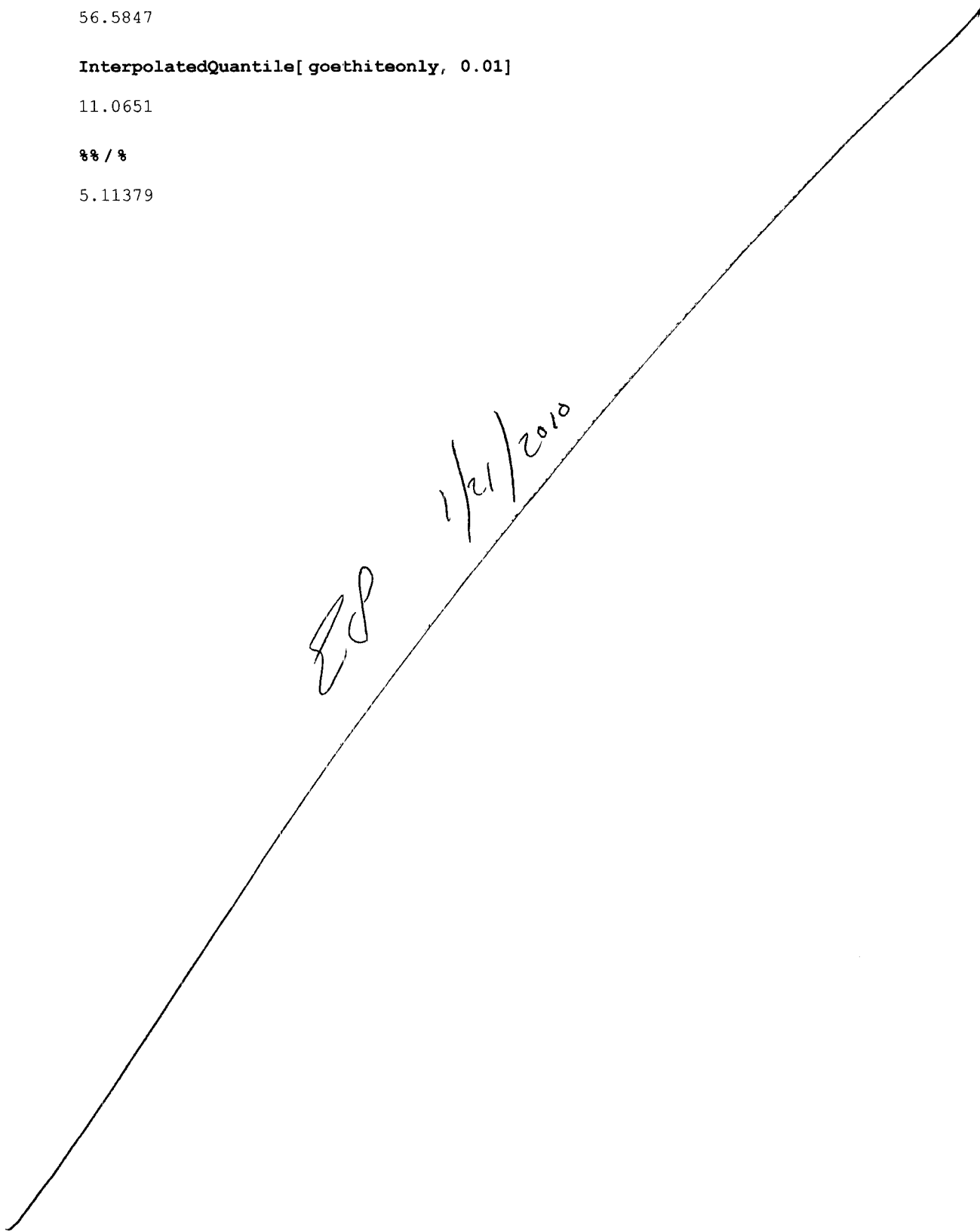
InterpolatedQuantile[goethiteonly, 0.01]

11.0651

%% / %

5.11379

ES 1/21/2010



## ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 282E

<b>Document Date:</b>	7/14/1998
<b>Availability:</b>	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
<b>Contact:</b>	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
<b>Data Sensitivity:</b>	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
<b>Date Generated:</b>	01/21/2010
<b>Operating System:</b> (including version number)	Windows
<b>Application Used:</b> (including version number)	
<b>Media Type:</b> (CDs, 3 1/2, 5 1/4 disks, etc.)	1 DVD
<b>File Types:</b> (.exe, .bat, .zip, etc.)	xls, jps, inp, arp
<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material

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<b>Date Generated:</b>	03/27/2003
<b>Operating System:</b> (including version number)	UNIX, sunOS 5.9
<b>Application Used:</b> (including version number)	gzip 1.3, tar
<b>Media Type:</b> (CDs, 3 1/2, 5 1/4 disks, etc.)	1 CD
<b>File Types:</b> (.exe, .bat, .zip, etc.)	.gz, tar
<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material

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<b>Data Sensitivity:</b>	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
<b>Date Generated:</b>	10/2003
<b>Operating System:</b> (including version number)	Windows NT
<b>Application Used:</b> (including version number)	
<b>Media Type:</b> (CDs, 3 1/2, 5 1/4 disks, etc.)	1 CD
<b>File Types:</b> (.exe, .bat, .zip, etc.)	.phk, .s, .con, .int, .dat, .xyp, .inp
<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material

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<b>Data Sensitivity:</b>	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
<b>Date Generated:</b>	09/2004
<b>Operating System:</b> (including version number)	Windows XP
<b>Application Used:</b> (including version number)	
<b>Media Type:</b> (CDs, 3 1/2, 5 1/4 disks, etc.)	1 CD
<b>File Types:</b> (.exe, .bat, .zip, etc.)	ASCII Files
<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material

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<b>Data Sensitivity:</b>	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
<b>Date Generated:</b>	09/2004
<b>Operating System:</b> (including version number)	Windows XP
<b>Application Used:</b> (including version number)	
<b>Media Type:</b> (CDs, 3 1/2, 5 1/4 disks, etc.)	1 CD
<b>File Types:</b> (.exe, .bat, .zip, etc.)	.nb, .xyp
<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material

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<b>Data Sensitivity:</b>	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
<b>Date Generated:</b>	4/9/2001
<b>Operating System:</b> (including version number)	Windows NT
<b>Application Used:</b> (including version number)	
<b>Media Type:</b> (CDs, 3 1/2, 5 1/4 disks, etc.)	1 zip
<b>File Types:</b> (.exe, .bat, .zip, etc.)	ASCII Files
<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material

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<b>Operating System:</b> (including version number)	Windows NT
<b>Application Used:</b> (including version number)	
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<b>File Types:</b> (.exe, .bat, .zip, etc.)	ASCI I Files
<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material



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