Modeling of Couplex1 case
with IPARS TRCHEM module.

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1   Introduction

Modeling of reactive transport phenomena in porous media is important and interesting in enviromental engineering and challenges numerical analysts and computational scientist [4, 5, 6, 7, 12, 13]. The ANDRA Couplex1 case [10, 11] is essentially an experiment to test the transport chemistry capabilities of IPARS [1] and to find out what improvements can be made to the IPARS transport chemistry (TRCHEM) module [8] in order to make it more applicable to general chemical problems. Notation: in the text below we use subscripts or superscripts $_A,^A$ to denote original Andra notation/units and sub-(or super-)scripts $_I,^I$ to denote IPARS notation/units.

2   Setup of single phase flow problem.

The problem Couplex1 is essentially 2D ($0 \leq x_A \leq 25000, 0 \leq z_A \leq 695$) where the lengths are given in units of $[m]$ and z_A is the gravity direction with gravity pointing in negative z direction. The origin is at the bottom left of the computational domain. A detailed description of Couplex1 is in Appendix 1 attached to this layout.

IPARS grid used here is ($0 \leq x_I \leq 695, 0 \leq y_I \leq 25000, 0 \leq z_I \leq 10$). See the discussion on units below. For simplicity we use origin at the same place as Couplex1 so we set $DOWN_I = (-1, 0, 0)$. Note that z_I is a "dummy" direction and that $(x_A, z_A) \mapsto (y_I, x_I)$.

We choose the x_I discretization to reflect the material boundaries so that dogger, clay, limestone and marl layers are covered by independent gridlines. When grid is refined, the gridlines do not cross material boundaries. In the following example discretization, we approximate the sloping clay/limestone boundary as a horizontal line.

```
DOWN(1 TO 3,1) = -1 0 0
NX(1) = 109
DX(,1) = 20.[ft]*10.[m] 19.[ft]*5.[m] 60.[ft]*5.[m] 10.[ft]*10.[m]
```

Note that default units are $[ft]$. IPARS is capable of performing unit conversions, however care must be taken to establish when the default units are being used in order to ensure that proper units are being used. Also note that the use of unit conversion capability with the following wrinkle. When using mutipliers like in DX below

```
20*10.[m] 19[ft]*5.[m]
```

you need to put a (default) unit $[ft]$ around the multiplier (19) that arises after unit conversion ($[m]$) has been used. Otherwise, the statement

```
20*10.[m] 19*5.[m]
```

may lead the code to translate the multiplier to a default unit ($[ft]$) thereby effectively changing the statement to

```
20*10.[m] 62*5.[m]
```

The use of [ft] around first multiplier (20) is not necessary.

For discretization in $y_I = x_A$ direction, we choose gridlines that will not cross the boundaries of the repository as below:

```
NY(1) = 101
DY(,1) = 73*250.[m] 1[ft]*190.[m]
6[ft]*250.[m]   1[ft]*240.[m] 6[ft]*250.[m]
2[ft]*160.[m]   12[ft]*250.[m]
```

DZ is the size of the (pseduo-) third dimension with only 1 grid. DZ can be choosen as any number as long as we are consistent.

The discretization described above can be used to generate the pressure solution. To this end, we need to set up flow parameters and the boundary conditions prescribed in Couplex1 for use with IPARS flow model. The flow problem as set up in Couplex1 is of incompressible single phase type and boundary conditions are fixed in time therefore the problem is time independent. Still we are going to use the IPARS single phase implicit model SINGLEI model which is set up to accurately solve compressible single phase fluid problems with Peaceman wells, general boundary conditions, etc.

The relevant parameters to be determined are compressibility (0.), viscosity and density for water. We use the following values

```
FLCOMP  = 0.
STFLDEN = 62.428[lb/cu-ft]
FLVIS   = 1.0[cp]
```

Also, permeabilities (intrinsic permeabilities in units consistent with $[md]$ or $[m^2]$) need to be set up. Note that Couplex1 definition uses hydraulic conductivities $K[m/year]$ so that the filtration velocity is given by

$$U_A = -K\nabla h; \quad h = \frac{P}{\rho G} + z_A \tag{1}$$

$$U_I = -\frac{k}{\mu}\nabla(P - \rho G Depth_I) \tag{2}$$

From this equation, we compute that $K = \frac{k\rho G}{\mu}$. If at $20^o C$, water has viscosity $\mu = 1.002.E - 3[Pa*s]$ and gravity is $G = 9.81 m/s^2$ and water density is $\rho = 1.E + 3[kg/cu - m]$, then $1md = 0.987 10^{-15}[sq-m] = 0.966 10^{-8}[m/s] = 0.966*10^{-8}*365.25*24*60*60[m/y] = 0.966 10^{-8}*8766* 3600[m/y]$. In other words, $k[md] \approx 0.305 K[m/year]$.

Using the conversion factors, permeabilities used are

```
XPERM1(1 TO 20,,) = 7.62       $ dogger:    25.[m/year]
XPERM1(21 TO 40,,) = .9E-6      $ clay:      3.E-6[m/year]
XPERM1(41 TO 99,,) = 1.92       $ limestone: 6.3[m/year]
XPERM1(100 TO 109,,) = .9E-5    $ marl:      3.E-5[m/year]
```

We also need to distinguish between rock types so that diffusivity can be input for each separate layer.

```
NROCKTYPE = 4
ROCK1(1 TO 20,,) = 1
ROCK1(21 TO 40,,) = 2
ROCK1(41 TO 99,,) = 3
ROCK1(100 TO 109,,) = 4
```

This defines the permeabilities for the simplified couplex case in which the slanted boundary between the limestone and the clay layers is approximated as a straight line at $z^A = 300m$. See Figure 1.

In order to simulate the more complicated case with the slanted boundary a stairstep is established to change the permeabilities and rock types of the grid squares. The permeabilities and rock types are all assigned as above, then the following grid lines are reassigned to be part of the clay layer:

```
XPERM1(40,14 TO 101,) = .9E-6                    $ clay: top
XPERM1(41 TO 42,28 TO 101,) = .9E-6             $ clay: top
XPERM1(43 TO 44,42 TO 101,) = .9E-6             $ clay: top
XPERM1(45 TO 46,56 TO 101,) = .9E-6             $ clay: top
XPERM1(47 TO 48,70 TO 101,) = .9E-6             $ clay: top
XPERM1(49 TO 50,84 TO 101,) = .9E-6             $ clay: top


ROCK1(41 TO 42,28 TO 101,) = 2
ROCK1(43 TO 44,42 TO 101,) = 2
ROCK1(45 TO 46,56 TO 101,) = 2
ROCK1(47 TO 48,70 TO 101,) = 2
ROCK1(49 TO 50,84 TO 101,) = 2
```

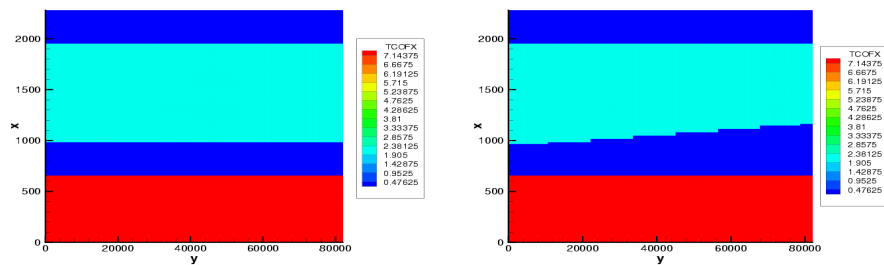The results can be seen in Figure 1.

Figure 1: PERMEABILITIES for simplified Couplex1 (left) and Couplex1 with stairs (right) in millidarcies

Boundary conditions. Boundary conditions for the flow model need to specified for five regions: two at the left side $x_A = y_I = 0$, two at the right side $x_A = y_I = 25000$ and one on top $z_A = x_I = 695$. These are defined in IPARS as boundary volumes as follows:

```
$              nreg nblk  x1 y1 z1      x2 y2 z2
BND_VOL(1 TO 2,1) = 1[ft]      1
```

```
BND_VOL(3 TO 8,1) =       0. 0. 0.      200.[m] 0.  10.
BND_VOL(1 TO 2,2) = 2[ft]      1
BND_VOL(3 TO 8,2) =       300.[m] 0. 0.   595. 0.  10.
BND_VOL(1 TO 2,3) = 3[ft]      1
BND_VOL(3 TO 8,3) =       0.[m] 25000. 0.   200. 25000.  10.
BND_VOL(1 TO 2,4) = 4[ft]      1
BND_VOL(3 TO 8,4) =       300.[m] 25000. 0.  595. 25000.  10.
BND_VOL(1 TO 2,5) = 5[ft]      1
BND_VOL(3 TO 8,5) =       695.[m] 0. 0.  695. 25000. 10.
```

for the simplified case and

```
$              nreg nblk  x1 y1 z1     x2 y2 z2
BND_VOL(1 TO 2,1) = 1[ft]      1
BND_VOL(3 TO 8,1) =       0. 0. 0.      200.[m] 0.  10.
BND_VOL(1 TO 2,2) = 2[ft]      1
BND_VOL(3 TO 8,2) =       295.[m] 0. 0.   595. 0.  10.
BND_VOL(1 TO 2,3) = 3[ft]      1
BND_VOL(3 TO 8,3) =       0.[m] 25000. 0.   200. 25000.  10.
BND_VOL(1 TO 2,4) = 4[ft]      1
BND_VOL(3 TO 8,4) =       350.[m] 25000. 0.  595. 25000.  10.
BND_VOL(1 TO 2,5) = 5[ft]      1
BND_VOL(3 TO 8,5) =       695.[m] 0. 0.  695. 25000. 10.
```

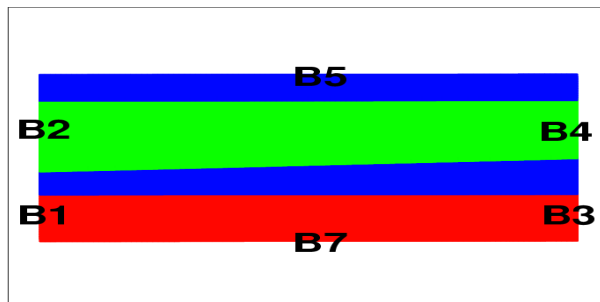for the stairstep case. See schematic cartoon of boundary regions on Figure 2. The boundary

Figure 2: Boundary regions for Couplex1. Region B6 is in the complement of B1..B5,B7.

conditions for pressure in Couplex1 are defined in terms of hydraulic head. Currently this is not yet an option directly available in SINGLEI model. The hydraulic head values need to be "converted" to values of pressure or potential. One way to do it is through the use of TBDMOD functionality in IPARS. The example for region 1 is as follows.

```
BOUND_TYPE(1) = 3
TBDMOD(1) Block
   EXTERNAL XB,YB,ZB,VALB
   VALB = 62.428*.006944445* ( 286./.3048 - XB)
EndBlock
```

Note that the numbers delivered by TBDMOD are treated as if they came in default units or in other words from hydraulic head measured in [ft]. If other units than [ft] are used, TBDMOD
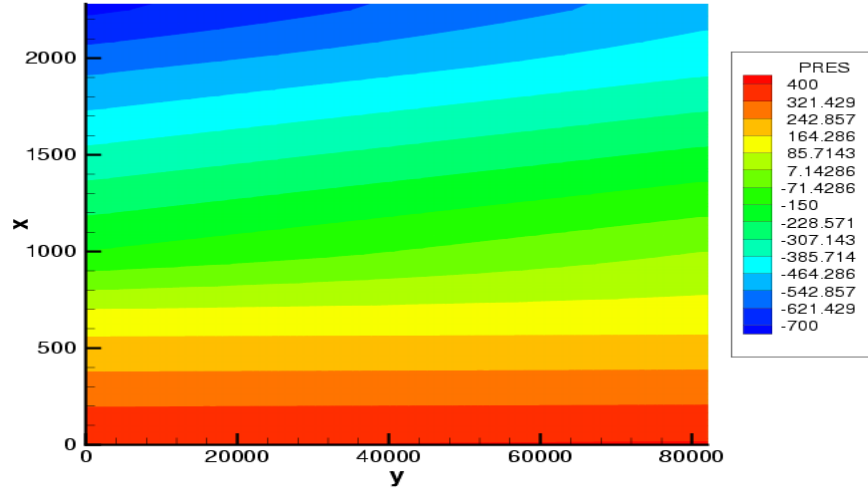
Figure 3: PRESSURE for simplified Couplex1 in psi.

needs to include conversion factor $[ft] \mapsto [m]$ and that's where the number .3048 comes from. The above specification results in the pressure field shown in figure 3. The hydraulic head can be post processed and visualized in IPARS by using the flag

```
VIS_SCL_NAMES(1) = "PRESHEAD"
```
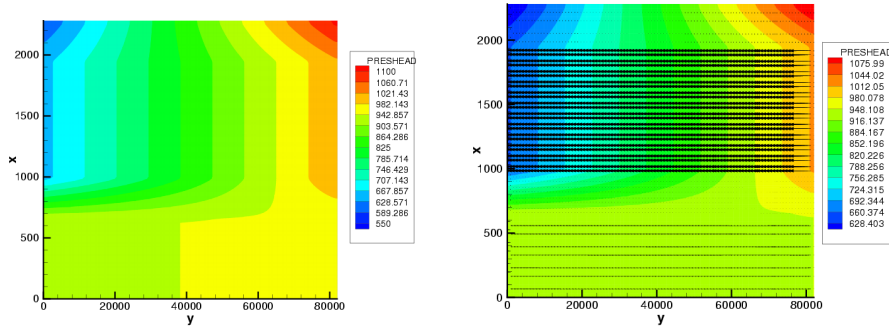

Figure 4: HYDRAULIC HEAD in feet for simplified Couplex1 and velocity profile of flow field.

in the visual output section of the data file. The resulting hydraulic head field is shown in Figure 4.

The head and pressure fields are virtually identical for both the simplified and the stairstep case so only the simplified fields are shown.

The pressure and boundary conditions create the flow field of x and y velocities shown in Figure 5 for the simplified case.
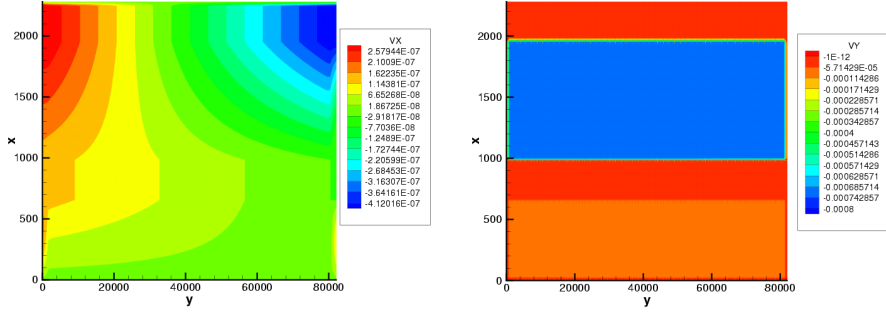
5

Figure 5: X and Y mass velocities[lb/day] for the simplified single phase flow problem.

3 Reactive Transport

The transport equation for ANDRA case written in IPARS notation is as follows.

$$(\Phi + \sigma_i)\left(\frac{\partial C_i}{\partial t} + \frac{\ln 2}{T_i}C_i\right) - \nabla \cdot (\mathbf{D}_i \nabla C_i) + \mathbf{u} \cdot \nabla C_i = f_i$$

where, Φ is the porosity of porous media, σ is the effective adsorption capacity, T is the half life time, $\mathbf{D}$ is the effective diffusion/dispersion tensor, $\mathbf{u}$ is the Darcy's velocity, f is the source term due to wells.

This equation is solved by operator splitting in which we solve separately advection step as described below and diffusion step as described in Section 4, see [9] for details.

Boundary conditions are split between these two steps and described below. Source terms are handled in the advection step and described below. Chemistry in Couplex1 which encompasses adsorption and first order decay, are not handled by a separate call to chemistry step, as it is done in more complicated cases. Adsorption terms related to σ_i are present in both advection and diffusion steps. First order decay related to the $\ln 2$ terms are handled in the diffusion step.

Boundary conditions. Boundary conditions relevant to reactive transport need to be specified for all the regions where flow boundary conditions are specified and for completeness in all the other regions for both advection and diffusion steps.

So in addition to the boundary regions defined for the flow problem, we need to set up two extra boundary volumes: one for the bottom (region 7) and another one which will hold all the remaining parts of the boundary (region 6).

```
BND_VOL(,6) = 6[ft]      1,    200.[m] 0. 0.      300. 0.   10.
BND_VOL(,7) = 6[ft]      1,    595.[m] 0. 0.      695. 0.   10.
BND_VOL(,8) = 6[ft]      1,    200.[m] 25000. 0.    300. 25000.  10.
BND_VOL(,9) = 6[ft]      1,    595.[m] 25000. 0.    695. 25000.  10.
BND_VOL(,10) = 7[ft]     1,     0.[m] 0. 0.  0. 25000. 10.
```

From pressure solution it appears that regions 1, 2 and 5 are outflow regions for advection code and that regions 3 and 4 are inflow where

$$C = 0 \tag{3}$$

is prescribed.

Diffusion code imposes condition

$$\nabla C \cdot \eta = 0 \tag{4}$$

on regions 1 and 2. Also, the condition imposed on the bottom (region 7) $z_A = x_I = 0$ is

$$uC - \nabla C \cdot \eta = 0 \tag{5}$$

Because of the no-flow condition used for the flow problem equation 5 reduces to equation 4 since $u = 0$ at this part of the boundary. All other regions use the homogeneous Dirichlet condition as in equation 3. The specification is as follows:

```
BOUND_TYPE_D(1 TO 2) = 0
BOUND_TYPE_D(3 TO 6) = 2
BOUND_TYPE_D(7) = 0


TRBOUND1(3) Block $ CONC1
  Interpolation Linear
  Extrapolation Constant
  Data  0.   0.
EndBlock
```

Pure transport well. Here we consider the wells that are source terms for the transport but do not influence the flow at all. This is exactly the source term in ANDRA case.

The usage for pure transport well is as follows.

- Define the wells as usual but let KINDWELL(i) = -1 where i is the well number, so that flow solver does not "see" the wells.

- Specify the source term by TRXWELL1(i) keyword: TRXWELL1(well index) – input the table of time and source rate by "Block"

- default unit for the source rate: $[lbmol/(ft^3 * day)]$

Example for Iodine case:

```
NUMWELL = 1
WELLNAME(1) = "I REPOSITORY"
WELLTOP(1 TO 3,1,1) =     247.[m]    18440.[m] 1.[m]
WELLBOTTOM(1 TO 3,1,1) = 247.[m]    21680.[m] 1.[m]
KINDWELL(1) = -1
TRXWELL1(1) Block
  Interpolation Linear
  Extrapolation Constant
  Data
   3.6500000E05    6.3506168E-56
   3.6865000E05    6.3506168E-56
   3.7230000E05    6.3506168E-56
   3.7595000E05    2.3972747E-11
   3.7960000E05    1.4529945E-07
   ...
EndBlock
```

Note for conversion of the source term between IPARS and ANDRA:

The file source.dat (from ANDRA) contains 212 lines, with three numbers t, f1 and f2 on each line, where t is the time in years; f1 is the source for Iodine-129 in mole/year; f2 is the source for Plutonium-242 in mole/year. Thus (source rate in IPARS) = (source in ANDRA) / (AreaRepository * DZ), where, AreaRepository = (250-244)*(21680-18440) $meter^2$; DZ is the size of the (pseduo-) third dimension with only 1 grid (see section 1).

After that, we still need to convert the quantity from the ANDRA unit $mol/(m^3 * yr)$ to IPARS unit $lbmol/(ft^3 * day)$ if IPARS default unit is used.

4 Diffusion

Currently, we can handle only molecular diffusion with IPARS TRCHEM module.

The usage for diffusion term is as follows.

- Make sure keyword NO_DISPERSION is commented out (NO_DISPERSION will disable the whole diffusion/dispersion part)

- Specify the molecular effective diffusivity keyword:

  MOLECULAR_DIFFUSIVITY(rock type index, species index, phase index)

- The contribution to the diffusion/dispersion tensor from the molecular diffusion is (porosity)*(tortuosity)*(real molecular diffusivity). In IPARS, it is defined that

  MOLECULAR_DIFFUSIVITY = (tortuosity)*(real molecular diffusivity)

  But, de_1 and de_2 in the ANDRA case are defined as the whole thing, i.e. (porosity)*(tortuosity)*(real molecular diffusivity).

  Thus, MOLECULAR_DIFFUSIVITY (in IPARS) = $\frac{de_i(inANDRA)}{Porosity}$ Since porosity data is not given the ANDRA specification, We let porosity = 0.1 everywhere – note porosity doesn't influence the flow part of ANDRA, as long as we are consistent. Of course, we need to convert the unit from $[m^2/year]$ (in ANDRA) to $[ft^2/day]$ (in IPARS).

- The IPARS default units are $[ft^2/day]$, so they must be converted from $[m^2/yr]$ specified in ANDRA.

Example for Iodine:

```
MOLECULAR_DIFFUSIVITY(1 TO 4,1,1) = 1.474508E-4
MOLECULAR_DIFFUSIVITY(2,1,1) = 1.303465E-4
```

Tolerance for linear solver. The tolerance for linear solver used in the diffusion/dispersion step is critical here. The main reason is that solvers in IPARS are mainly rigged to solve systems arising from implicit models where Newtonian iteration is used to achieve convergence and ensure proper balances. In implicit models for efficiency reasons it is advisable to not oversolve the linear system and that's why the code currently uses only relative single precision tolerance rather than double precision absolute. Another issue is how to separate tolerance used for the pressure solution from the one used for diffusion equation. We use TMP_LSOL_* for diffusion tolerance as opposed to LSOL_* for flow tolerance.

The stairstep and the simplified files give very similar concentration profiles for both elements throughout the time scale of the simulation 10^7 years.
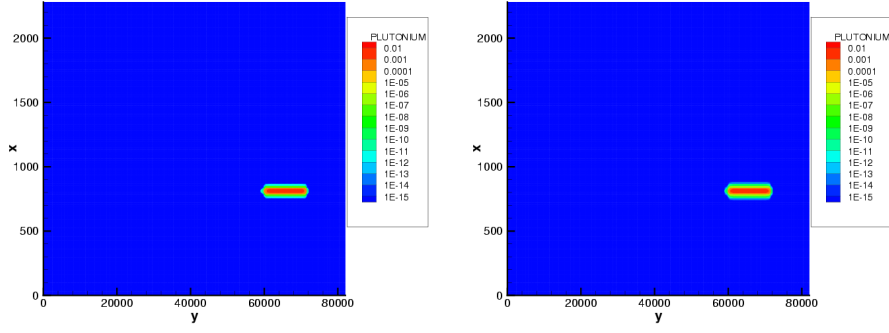
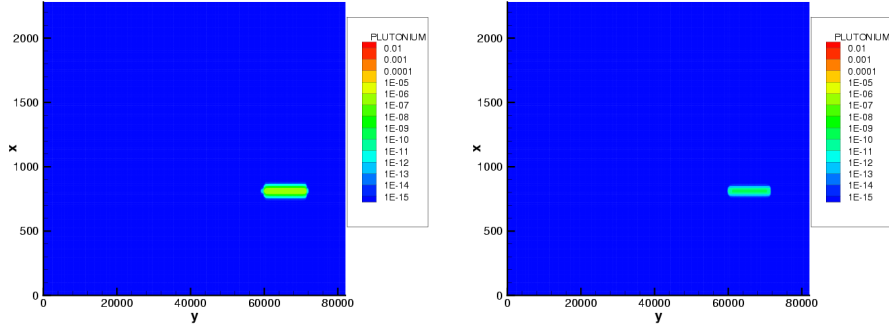Figure 6: Concentrations for Plutonium[$lbmol/ft^3$] at times $3*10^5$ years and 10^6 years

Figure 7: Concentrations for Plutonium[$lbmol/ft^3$] at times $5*10^6$ years and 10^7 years.

5 Linear equilibrium adsorption chemistry

ANDRA has a strong adsorption for Plutonium-242 in the clay rock. It is strongly recommended that linear equilibrium be solved by the efficient implementation (modifying the coefficent of the accumulation term by counting the contribution from adsorption), rather than using the general chemistry routine (performing flash calculation), specially for strong adsorption.

The usage for linear equilibrium adsorption chemistry is as follows.

- declare the flag USE_LINEAR_ADSORPTION in input file

- specify the effective adsorption capacity with keyword EFF_SORP_CAPACITY(rock index, species index). The unit for it is dimensionless.

Example:

```
USE_LINEAR_ADSORPTION
$ EFF_SORP_CAPACITY for each (rocktype,species)
$ assume we choose porosity = 0.1 everywhere
EFF_SORP_CAPACITY(1,1) = 0.0          $ for Plutonium-242 in dogger
EFF_SORP_CAPACITY(2,1) = 19999.9      $ for Plutonium-242 in clay
```

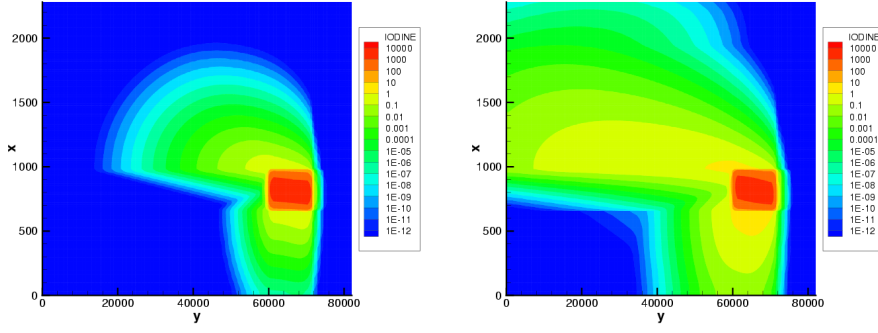Note for conversion between IPARS and ANDRA:

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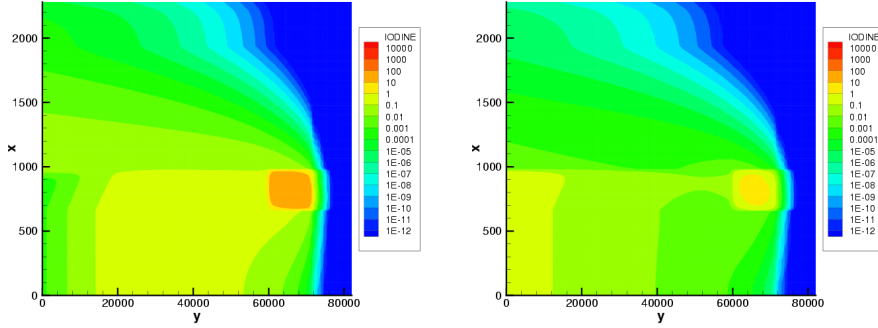Figure 8: Concentrations of Iodine$[lbmol/ft^3]$ at times $3*10^5$ years and 10^6 years for the simplified problem

Figure 9: Concentrations of Iodine$[lbmol/ft^3]$ at times $5*10^6$ years and 10^7 years for the simplified problem

The effective adsoprtion capacity (EFF_SORP_CAPACITY) in IPARS is defined to be the product of Henry's law constant and the adsorption capacity. Note that

$$dx * dy * dz * EFF\_SORP\_CAPACITY * concentration$$

means the amount (in lbmol) of the species adsorbed in the cell, where dx, dy, dz are cell size parameters.

ANDRA case use latency retardation factor R and effective porosity ω. We have the relation:

$$\Phi + \sigma = R\omega$$

where, Φ and σ in left hand side is porosity and effective adsoprtion capacity in IPARS, while R and ω are the latency Retardation factor and effective porosity in ANDRA.

6   First order decay chemistry

The only kinetic type reactions ANDRA case has is the radionuclide decay, which belongs to the family of first order decay chemical reactions. It is strongly recommended that first order decay chemical reaction be solved by the efficient implementation (solved implicitly by combining into
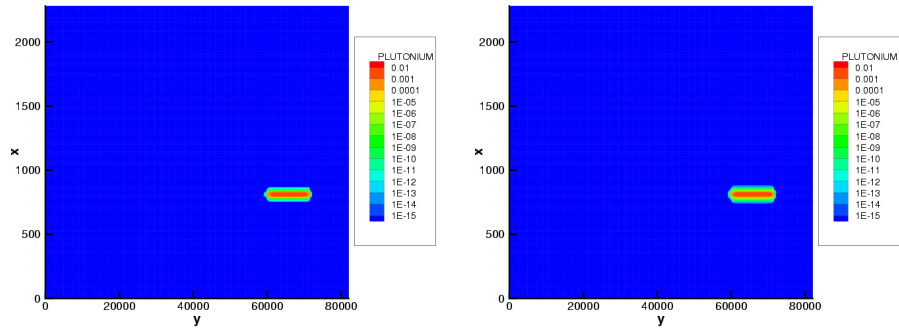
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Figure 10: Concentrations of Plutonium[$lbmol/ft^3$] at times $3*10^5$ years and 10^6 years for the stairstep problem
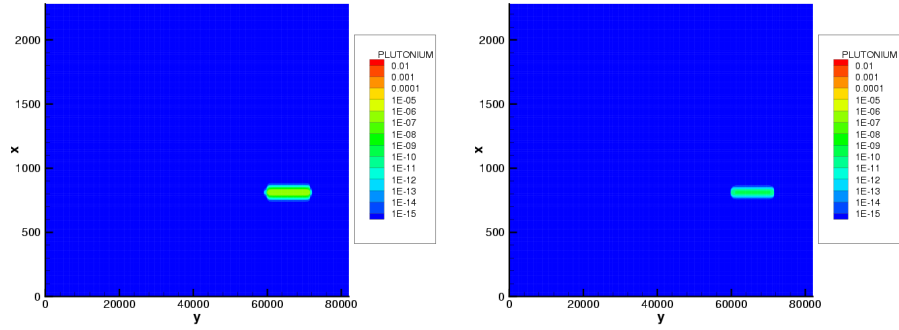
Figure 11: Concentrations of Plutonium[$lbmol/ft^3$] at times $5*10^6$ years and 10^7 years for the stairstep problem

the diffusion/dispersion part) rather than using the general chemistry routine (performing ODE solve).

The usage for first order decay chemistry is as follows.

- declare the flag USE_RADIODECAY in input file

- specify the parameter for first order decay chemistry – the half life time (HALF_LIFE_TIME) keyword: HALF_LIFE_TIME(species index) default unit: day

Example from Iodine case:

```
USE_RADIODECAY
HALF_LIFE_TIME(2) = 5.7305E9 $in days
```

Note for conversion between IPARS and ANDRA: Unit conversion from years (in ANDRA) into days (in IPARS) if IPARS default unit is used.

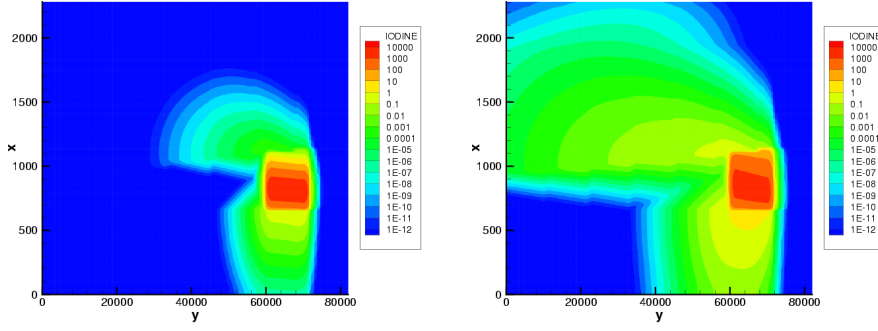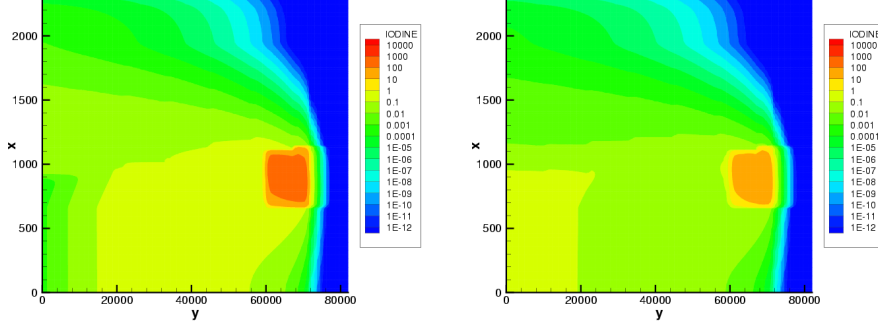Figure 12: Concentrations of Iodine$[lbmol/ft^3]$ at times $3*10^5$ years and 10^6 years for the stairstep problem

Figure 13: Concentrations of Iodine$[lbmol/ft^3]$ at times $5*10^6$ years and 10^7 years for the stairstep problem

7 Other control parameters

7.1 Disable the CFL check

The purpose is, for example, to experiment with a large time step. This is useful when for example the time step is restricted severely by CFL condition but we know a-priori that there is no advection locally in time in this part of the domain where the velocities are large. This is the case in Couplex1 in the limestone layer. The velocities there are large but neither Plutonium nor Iodine are present in that layer over a long initial time interval.

Usage: just declare the flag NO_CFL_CHECK in the input file. Example is as follows.

```
NO_CFL_CHECK
```

7.2 Report of the transport flux across boundary and of the rock subdomain balance for each species

If you declare the flag REPORT_BD_FLUX in input file, you will get a output file "transpBd-Flux.dat" after IPARS runs. The file TranspBdFlux.dat will contain information of the accumulated net amount of species flowing across boundary for each individual boundary region (unit in

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lbmol) and balance of species in each individual rock subdomain (unit in lbmol) at each flowing time step. Example is as follows.

```
REPORT_BD_FLUX
```

We used this option for Couplex1 to calculate the requested cumulative flux between the rock layers as well as the flux(es) across the left boundary of the domain.

7.3   General Chemistry Feature

IPARS-TRCHEM allows for quite general chemistry [9]. However, the chemistry present in Couplex1: adsorption and first order decay were both modeled directly as described above.

8   Acknowledgements

IPARS is a reservoir simulator framework developed at CSM [1, 2, 3]. Parts of the chemistry module in TRCHEM have been ported from ParSSim [4]. We thank Mary Wheeler and John Wheeler for helpful suggestions.

9   BIBLIOGRAPHY

References

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10 Appendix 1: Original ANDRA data file

COUPLEX1 Test Case
Nuclear Waste Disposal Far Field Simulation

January 25, 2001

Abstract

This first COUPLEX test case is to compute a simplified Far Field model used in nuclear waste management simulation. From the mathematical point of view the problem is of convection diffusion type but the parameters are highly varying from one layer to another. Another particularity is the very concentrated nature of the source, both in space and in time.

1 Introduction

The repository lies at a depth of 450m (meters) inside a clay layer which has above it a layer of limestone and a layer of marl and below it is a layer of dogger limestone. Water flows slowly (creeping flow) through these porous media and convects the radioactive materials once the containers leak; there is also a dilution effect which in mathematical terms is similar to diffusion. The problem has two main difficulties:

1. The radioactive elements leak from the containers, into the clay, over a period that is small compared with the millions of years over which convection and diffusion are active.

2. The convection and diffusion constants are very different from one layer to another; for instance, in the clay layer there is almost no convection while, in the other layers, diffusion and convection are both important.

2 The Geometry

In this first test case, the computation is restricted to a 2D section of the disposal site. Thus, the computational domain is in a rectangle $\mathcal{O} = (0, 25000) \times (0, 695)$ in meters. The layers of dogger, clay, limestone, and marl are located as follows (with the origin taken at the bottom left corner of the rectangle):

- dogger $0 < z < 200$

1

- clay lies between the horizontal line $z = 200$ and the line from $(0, 295)$ to $(25000, 350)$

- limestone lies between the line from $(0, 295)$ to $(25000, 350)$ and the horizontal line $z = 595$

- marl $595 < z < 695$.

The repository, denoted by R, is modeled by a uniform rectangular source in the clay layer:

$$R = \{(x, z) \in (18440, 21680) \times (244, 250)\}$$

The geometry is summarized on figure 1 below. For this domain the computation should be carried for $t \in (0, T)$ with $T = 10^7$ years.
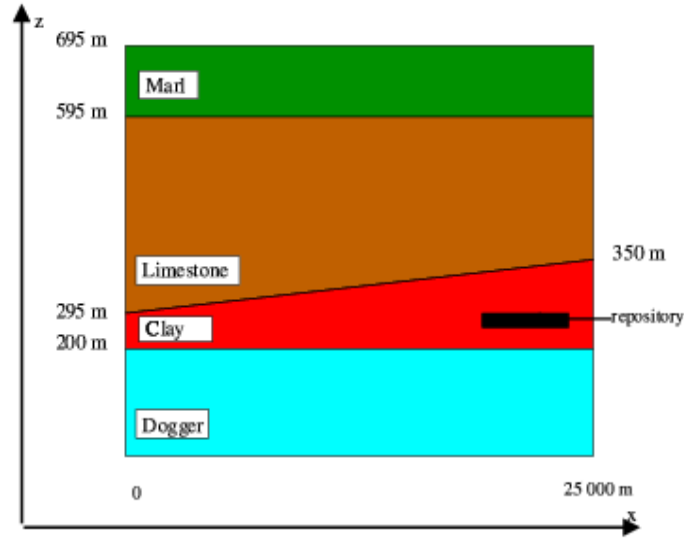

Figure 1: *Geometry of computational domain*

3 The Flow

It is assumed that all rock layers are saturated with water and that boundary loads are stationary so that the flow is independent of time. Darcy's law gives the velocity u in terms of the hydrodynamic load $H = P/\rho g + z$:

$$\mathbf{u} = -K \nabla H \tag{1}$$

2

where the permeability tensor K, assumed constant in each layer is given in Table 1, P is the pressure and g is Newton's constant. Conservation of mass ($\nabla \cdot (\rho u) = 0$, with the density ρ assumed constant) implies that

$$\nabla \cdot (K \nabla H) = 0 \quad \text{in } \mathcal{O} \tag{2}$$

	Marl	Limestone	Clay	Dogger
K (m/year)	3.1536e-5	6.3072	3.1536e-6	25.2288

Table 1: *Permeability tensor in the four rock layers*

On the boundary, conditions are:

$$\begin{aligned}
H &= 289 & &\text{on } \{25000\} \times (0, 200), \\
H &= 310 & &\text{on } \{25000\} \times (350, 595), \\
H &= 180 + 160x/25000 & &\text{on } (0, 25000) \times \{695\}, \\
H &= 200 & &\text{on } \{0\} \times (295, 595), \\
H &= 286 & &\text{on } \{0\} \times (0, 200), \\
\frac{\partial H}{\partial n} &= 0 & &\text{elsewhere.}
\end{aligned}$$

4 The Radioactive Elements

We are considering two species of particular interest, Iodine 129 and Plutonium 242. Both escape from the repository cave into the water and their concentrations $C_i, i = 1, 2$ is given by two independent convection-diffusion equations:

$$R_i \omega \left(\frac{\partial C_i}{\partial t} + \lambda_i C_i \right) - \nabla \cdot (\mathbf{D}_i \nabla C_i) + \mathbf{u} \cdot \nabla C_i = f_i \quad \text{in } \mathcal{O} \times (0, T) \quad i = 1, 2. \tag{3}$$

where

- R_i is the latency Retardation factor, with value 1 for ^{129}I, 10^5 for ^{242}Pu in the clay and 1 elsewhere for both Iodine and Plutonium;

- the effective porosity ω, is equal to 0.001 for ^{129}I, 0.2 for ^{242}Pu in the clay layer and 0.1 elsewhere for both;

- $\lambda_i = \log 2 / T_i$ with T_i being the half life time of the element : $1.57\,10^7$ for ^{129}I, $3.76\,10^5$ for ^{242}Pu (in years);

- The effective diffusion/dispersion tensors $\mathbf{D}_i$ for any species $i = 1, 2$ depend on the Darcy velocity as follows:

$$\mathbf{D}_i = d_{e_i} I + |\mathbf{u}| \left[\alpha_{l_i} E(\mathbf{u}) + \alpha_{t_i} (I - E(\mathbf{u})) \right]$$

3

with

$$E_{kj}(\mathbf{u}) = \frac{u_k u_j}{|\mathbf{u}|^2}.$$

and with the coefficients, assumed constant in each layer, given in Table 2 below.

	^{129}I			^{242}Pu		
	de_1(m²/year)	a_L(m)	a_T(m)	de_2(m²/year)	a_L(m)	a_T(m)
Dogger	5.0e-4	50	1	5.0e-4	50	1
Clay	9.48e-7	0	0	4.42e-4	0	0
Limestone	5.0e-4	50	1	5.0e-4	50	1
Marl	5.0e-4	0	0	5.0e-4	0	0

Table 2: *Diffusion/dispersion coefficients for the radioactive elements in the 4 layers*

In this test case, the values of the source terms f_i, $(i = 1, 2)$ in the repository R are given in tabulated form in separately provided data files. The source terms are assumed to be spatially uniformly spread out in all the repository R. It is assumed that there is no source outside the repository (f_i, $(i = 1, 2)$ in $\mathcal{O} \backslash \bar{\mathcal{R}}$). The dependence in time is shown on figure 2, for illustrative purposes. The structure of the data file is described in appendix A.
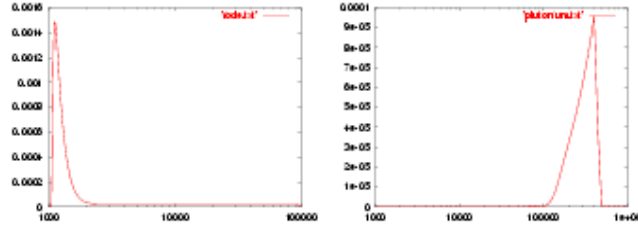

Figure 2: *Release of Iodine and Plutonium as a function of time*

4.1 Initial and Boundary Conditions

We call time zero the time when the containers begin to leak and the radioactive elements to spread, hence the initial values of the concentration C_i are zero at time zero.

4

Boundary conditions for the transport of any nuclide $i = 1, 2$ are

$$\frac{\partial C_i}{\partial n} = 0 \qquad \text{on } \{0\} \times (295, 595)$$

$$\frac{\partial C_i}{\partial n} = 0 \qquad \text{on } \{0\} \times (0, 200)$$

$$\mathbf{D}_i \nabla C_i \cdot \mathbf{n} - C_i \mathbf{u} \cdot \mathbf{n} = 0 \qquad \text{on } (0, 25000) \times \{0\}$$

$$C_i = 0 \qquad \text{elsewhere on the boundary.}$$

where $\mathbf{n}$ is the outward normal to the vertical line $\{0\} \times \{0, 695\}$

5 Output requirements

The following output quantities are expected from the simulations(both tables and graphical representations):

- Contour levels of C_i at times $200, 10110, 50110, 10^6, 10^7$ years (the following level values should be used: $10^{-12}, 10^{-10}, 10^{-8}, 10^{-6}, 10^{-4}$);

- Pressure field (10 values uniformly distributed between 180 and 340;

- Darcy velocity field, along the 3 vertical lines given by $x = 50, x = 12500, x = 20000$, using 100 points along each line;

- Places where the Darcy velocity is zero;

- Cumulative total flux through the top and the bottom clay layer boundaries, as a function of time;

- Cumulative total fluxes through the left boundaries of the dogger and limestone layers;

- The discretization grid of the domains and the time stepping used in the simulations should also be given.

A Descritpion of the data file

The file source.dat contains data needed to compute the source term f_i in eq. (3). These data come from a Near Field computation. The file has 212 lines, and each line contains three numbers $t^p, \bar{f}_1^p, \bar{f}_2^p$, $p = 1, \ldots 212$, where t^p is the time, and the source term $f_i(t^p)$ is related to $\bar{f}_i^p$ by: $f_i(t^p) = \bar{f}_i^p / S$, where S is the surface of the repository.

The times t^p are in years, and the numbers $\bar{f}_i^p$ are in units of mole /year.

5

11 Appendix 2: Simplified data input file

This input file is in CVS repository /IPARSv2/datatr_andra.dat.

```
TITLE(2)="SINGLE PHASE 1D BOUNDARY CONDITION EXAMPLE"

DESCRIPTION()=

"BLOCK     LENGTH (FT)   WIDTH (FT)    HEIGHT (FT)    SIZE      CORNER"
" 1          80            20            100          1x4x1      0,0,0"

"DATE : 3/01"

TRANSPORT_CHEMISTRY

$$$$$$$$$$ mpesz
$ this is what Couplex1 is set for: million(s) of years
$ I ran the case only up to $TIMEEND = 36500.0

TIMEEND = 1.0E+7[yr]

$ I/O OPTIONS

OUTLEVEL = 2

$NO_CFL_CHECK
$REPORT_BD_FLUX

$$$$$$$$$$$$$$$$$$$$$$$$$
$ FAULT BLOCK AND MESH DATA

BLOCKNAME(1) = "BLOCK1"
DOWN(1 TO 3,1) = -1 0 0

NX(1) = 109
DX(,1) = 20.[ft]*10.[m] 19.[ft]*5.[m] 60.[ft]*5.[m] 10.[ft]*10.[m]

NY(1) = 101
DY(,1) = 73*250.[m] 1[ft]*190.[m]
6[ft]*250.[m]  1[ft]*240.[m] 6[ft]*250.[m]
2[ft]*160.[m]  12[ft]*250.[m]

NZ(1) = 1
DZ(,1) = 10.[m]

XYZ111(,1) = 0. 0. 0.

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$ porosity / permeability data

POROSITY1() = .1

$$$$$$$$ mpesz
$ these values are of correct order but values need to be
$ carefully checked (see report).
$ Must convert carefully from hydr. conductivities
$ [m/year]->[ft/year] to [md]

$ PERMEABILITIES:

XPERM1(1 TO 20,,) = 7.62            $ dogger:    25.[m/year]
XPERM1(21 TO 40,,) = .9E-6          $ clay:      3.E-6[m/year]
XPERM1(41 TO 99,,) = 1.92           $ limestone: 6.3[m/year]
XPERM1(100 TO 109,,) = .9E-5        $ marl:      3.E-5[m/year]

PERM_HTOV_RATIO = 1.

ZPERM1(,,)=1.E-8

NROCKTYPE = 4
ROCK1(1 TO 20,,) = 1
ROCK1(21 TO 40,,) = 2
ROCK1(41 TO 99,,) = 3
ROCK1(100 TO 109,,) = 4

$$$$$$$ mpesz
$ if you want to visualize the perms ... note that Tecplot
$ will need some tweaking after you use VISFLAG = 2 in 2D.
$ Could also use FLAG 3 and do average cell in Tecplot.
$
VIS_SCL = 2
VIS_SCL_NAMES(1) = "TCOFX"
VIS_SCL_NAMES(2) = "DEPTHG"
VIS_NVEC = 1
VIS_VEC_NAMES(1)="TRVEL"
PERMOUT
VIS_FNAME = "ANPERM"
VISFLAG = 2
$$$$$$$

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
```

```
FLOW_MODEL = "SINGLE_PHASE_IMPLICIT"


FLCOMP = 0.
STFLDEN = 1000.[k/cu-m]    $ 62.428 [lb/cu-ft]
PINIT =   100.             $ linear solver has to start from something
FLVIS =   1.0


$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ boundary conditions: geometry

NBND_REG = 7
NBND_SUBREG = 10


$              nreg nblk  x1 y1 z1      x2 y2 z2
BND_VOL(1 TO 2,1) = 1[ft]      1
BND_VOL(3 TO 8,1) =       0. 0. 0.     200.[m] 0.  10.
BND_VOL(1 TO 2,2) = 2[ft]      1
BND_VOL(3 TO 8,2) =      300.[m] 0. 0.   595. 0.  10.
BND_VOL(1 TO 2,3) = 3[ft]      1
BND_VOL(3 TO 8,3) =        0.[m] 25000. 0.   200. 25000.  10.
BND_VOL(1 TO 2,4) = 4[ft]      1
BND_VOL(3 TO 8,4) =      300.[m] 25000. 0.  595. 25000.  10.
BND_VOL(1 TO 2,5) = 5[ft]      1
BND_VOL(3 TO 8,5) =      695.[m] 0. 0.   695. 25000. 10.


BND_VOL(,6) = 6[ft]      1,   200.[m] 0. 0.    300. 0.  10.
BND_VOL(,7) = 6[ft]      1,   595.[m] 0. 0.    695. 0.  10.
BND_VOL(,8) = 6[ft]      1,   200.[m] 25000. 0.   300. 25000.  10.
BND_VOL(,9) = 6[ft]      1,   595.[m] 25000. 0.   695. 25000.  10.

BND_VOL(,10) = 7[ft]      1,   0.[m] 0. 0.  0. 25000. 10.

BOUND_TYPE(1) = 3
TBDMOD(1) Block
   EXTERNAL XB,YB,ZB,VALB
   VALB = 62.428*.006944445* ( 286./.3048 - XB)
EndBlock

BOUND_TYPE(2) = 3
TBDMOD(2) Block
   EXTERNAL XB,YB,ZB,VALB
   VALB = 62.428*.006944445* ( 200./.3048 - XB)
EndBlock

BOUND_TYPE(3) = 3
TBDMOD(3) Block
   EXTERNAL XB,YB,ZB,VALB
   VALB = 62.428*.006944445* ( 289./.3048 - XB)
EndBlock

BOUND_TYPE(4) = 3
TBDMOD(4) Block
   EXTERNAL XB,YB,ZB,VALB
   VALB = 62.428*.006944445* ( 310./.3048 - XB)
EndBlock

$ top value is (left corner at y=0): 180, (right corner at y=25000): 340.
BOUND_TYPE(5) = 3
TBDMOD(5) Block
   EXTERNAL XB,YB,ZB,VALB
   VALB = 62.428*.006944445* ( 180./.3048 - XB + 160.*YB/25000. )
EndBlock

$ flow boundaries on these regions are no-flow
BOUND_TYPE(6 TO 7) = 0

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$ TRANSPORT-CHEMISTRY PART
NSPECIES = 2
N_COMPONENTS = 2
N_CONC_STEPS = 1

USE_RADIODECAY
HALF_LIFE_TIME(1) = 1.3724E8 $in days
HALF_LIFE_TIME(2) = 5.7305E9 $in days


USE_LINEAR_ADSORPTION
$EFF_SORP_CAPACITY(rock,species) = R(rock,species)*omega(rock,species)-porosity
$EFF_SORP_CAPACITY(1,1) = 1*.1 - .1
EFF_SORP_CAPACITY(1,1) = 0
EFF_SORP_CAPACITY(2,1) = 19999.9   $10.E5*.2 - .1
EFF_SORP_CAPACITY(3,1) = 0
EFF_SORP_CAPACITY(4,1) = 0

EFF_SORP_CAPACITY(1,2) = 0
EFF_SORP_CAPACITY(2,2) = -.099
EFF_SORP_CAPACITY(3,2) = 0
EFF_SORP_CAPACITY(4,2) = 0


$------------------------------$
```

```
$           COMPONENT 1           $
$-------------------------------$
NAME_SPECIES(1) = "PLUTONIUM"
MOLECULAR_WEIGHT(1) = 242
PHASE_TYPE(1) = "FLOWING"


PLUTONIUM1(,,) = 0.


$-------------------------------$
$           COMPONENT 2           $
$-------------------------------$
NAME_SPECIES(2) = "IODINE"
MOLECULAR_WEIGHT(2) = 129
PHASE_TYPE(2) = "FLOWING"


IODINE1(,,) = 0

$$$$$$$$ mpesz
$ these linear solver parameters apply to yGMRES.
$ if using GMRES, use N_GS_STEP instead of GMRES_PREC.
$ GMRES_PREC = 16 is faster but gives less "accurate" balances
$ in diff. /disp. equation. CVTOL does not need to be so small.
$$$$$$
LSOL_TOL = 1.E-4
$FORCING = 1.0
GMRES_PREC = 16
$N_GS_STEP = 5
MAXNEWT = 20


$$$$$$$$ mpesz
SKIP_FLOW        $ use this or do not skip flow but .....
FACTOR_RATE = 0.$ .... turn off extrapolation


$$$$$$ mpesz
$ initial conditions for all species are 0.
$ use advection if you want the source term to work !
$NO_ADVECTION $ can't use this or else there will be no species


$$$$$$ boundary conditions for transport-diffu/dispersion (see report)
BOUND_TYPE_D(1 TO 2) = 0
BOUND_TYPE_D(3 TO 6) = 2
BOUND_TYPE_D(7) = 0



TRBOUND1(3) Block $ PLUTONIUM
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock


TRBOUND1(4) Block $ PLUTONIUM
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock


TRBOUND1(5) Block $ PLUTONIUM
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock


TRBOUND1(6) Block $ PLUTONIUM
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock



TRBOUND2(3) Block $ IODINE
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock


TRBOUND2(4) Block $ IODINE
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock


TRBOUND2(5) Block $ IODINE
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock


TRBOUND2(6) Block $ IODINE
  Interpolation Linear
  Extrapolation Constant
  Data  0.  0.
EndBlock
```

```
$$$$$$$$$$$$$$$ if dispersion ...
$ NO_DISPERSION

$$$$$$$$$ mpesz
$ use these to force linear solver in diff. step to perform
$ a couple of iterations. Unfortunately, this requires that
$$$$ TMP_LSOL_TOL etc. are read with GETVAL ( 'R8' ).

TMP_LSOL_ATOL = 1.E-20
TMP_LSOL_ABSFLAG = 1

MOLECULAR_DIFFUSIVITY(1 TO 4,1,1) = 1.474508E-4
MOLECULAR_DIFFUSIVITY(2,1,1) = 1.303465E-4

MOLECULAR_DIFFUSIVITY(1 TO 4,2,1) = 1.474508E-4
MOLECULAR_DIFFUSIVITY(2,2,1) = 1.795668E-7


$ For reference, repository is positioned:
$PLUTONIUM1(39,75 TO 87,1) = 1000. $ one cell spreading

NUMWELL = 1
WELLNAME(1) = "PU AND I REPOSITORY"
WELLTOP(1 TO 3,1,1) =     247.[m]   18440.[m] 1.[m]
WELLBOTTOM(1 TO 3,1,1) = 247.[m]   21680.[m] 1.[m]
$
KINDWELL(1) = -1  $ this is not a flow model well !
TRXWELL1(1) Block
  Interpolation Linear
  Extrapolation Constant
  Data
  3.6500000E05   1.2667984E-55
  3.6865000E05   1.2667984E-55
   $ ...... the rest of well data for is skipped in this report
EndBlock

TRXWELL2(1) Block
  Interpolation Linear
  Extrapolation Constant
  Data
  3.6500000E05   6.3506168E-56
  3.6865000E05   6.3506168E-56
   $ ...... the rest of well data for is skipped in this report
EndBlock


$$$ this is if you want to check on the total input
WELLOUTKEY = 3  WELLFILE = "ANDRAW.WEL"
EndInitial

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ TRANSIENT DATA INPUT BLOCKS

BeginTime    0.
DELTIM = 1.  DTIMMUL = 1.
DTIMMAX = 100.[yr]  DTIMMIN = 100.[yr]
CVTOL = 1.E-8   $ use if deltim =100[yr]
TIMOUT = 100.[yr]  DTIMOUT = 100.[yr]

$ these must be set for visualization to be active
VISOUT = 100.[yr] DVISOUT = 100.[yr]
VIS_SCL = 3
VIS_SCL_NAMES(1) = "PRES"
VIS_SCL_NAMES(2) = "PRESHEAD"
VIS_SCL_NAMES(3) = "DEPTHG"
VIS_NVEC = 2
VIS_VEC_NAMES(1)="VEL"
VIS_VEC_NAMES(2)="TRVEL"
$VIS_VEC_NAMES(3)="TRV"
VIS_FNAME = "FLOW"
VISFLAG = 3

EndTime

BeginTime    36500
DELTIM = 100.[yr]  DTIMMUL = 1. DTIMMAX = 100.[yr] DTIMMIN = 100.[yr]
TIMOUT = 1000.[yr]  DTIMOUT = 100000.[yr]
VISOUT = 200.[yr]  DVISOUT = 300000.[yr]

VIS_SCL = 2
VIS_SCL_NAMES(1) = "PLUTONIUM"
VIS_SCL_NAMES(2) = "IODINE"
VIS_FNAME = "TRANS"
VIS_NVEC = 0
VISFLAG = 3

EndTime
```