

Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Report for AP-100 Tasks 4-6:
Extraction of Flow Field Values for SECOTP2D,
Scaling of Flow Field for Climate Change, and
Radionuclide Transport Calculations

AP-100
Analysis Plan for Calculations of Culebra Flow and Transport:
Compliance Recertification Application

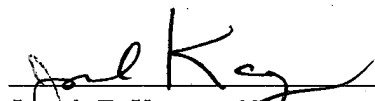
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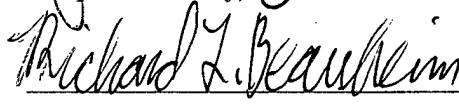
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Author:


Joseph F. Kanney, 6821

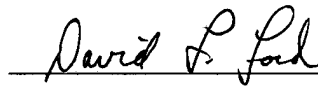
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Technical Review:


Richard L. Beauheim, 6822

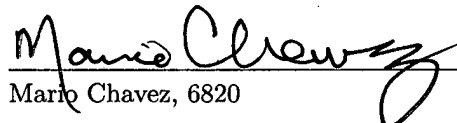
Date: 11/19/03

Technical Review:


David L. Lord, 6821

Date: 11/14/03

QA Review:


Mario Chavez, 6820

Date: 11/18/03

Management Review:


David Kessel, Manager 6821

Date: 11/14/03

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1 Introduction

1.1 Background

The Waste Isolation Pilot Plant (WIPP) is located in southeastern New Mexico and has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations, Parts 191 and 194. The DOE demonstrates compliance with the containment requirements in the regulations by means of a performance assessment (PA), which estimates releases from the repository for the regulatory period of 10,000 years after closure.

In October 1996, DOE submitted the Compliance Certification Application (CCA) to the EPA, which included the results of extensive PA analysis and modeling. After an extensive review, in May 1998 the EPA certified that the WIPP met the criteria in the regulations and was approved for disposal of transuranic waste. The first shipment of waste arrived at the site in March 1999.

The results of the PA conducted for the CCA were subsequently summarized in a Sandia National Laboratories (SNL) report [13] and in refereed journal articles [14].

The DOE is required to submit an application for re-certification every five years after the initial receipt of waste. The re-certification applications take into account any information or conditions that have changed since the original certification decision. Accordingly, the DOE is conducting a new PA in support of the Compliance Recertification Application (CRA). Analysis Plan AP-105 [19] presents the full set of PA calculations required for the CRA and lists the analysis plans that describe each component of the calculations.

One component of the CRA-PA is the calculation of the complementary cumulative distribution function (CCDF) of the normalized cumulative radionuclide release to the accessible environment. Groundwater flow and radionuclide transport in the Culebra Dolomite Member of the Rustler Formation are simulated using numerical models as part of this calculation.

The WIPP repository is located 26 miles (42 kilometers) southeast of Carlsbad, New Mexico. The disposal horizon of the WIPP is approximately 2,150 feet (655 meters) below the ground surface in the Salado Formation of the Delaware Basin. The Salado is regionally extensive, consisting predominantly of halite, a low permeability evaporite [39].

The Rustler Formation is located above the Salado and is of particular importance to the CRA because it contains the most transmissive units above the repository. In the vicinity of the WIPP, the Rustler consists of evaporite units interbedded with carbonates and siliciclastic units [17, 50]. The Culebra Dolomite Member has been identified as the most transmissive unit in the Rustler and consequently the most likely pathway for subsurface transport of radionuclides.

1.2 Analysis Overview

The cumulative release of radionuclides through the Culebra to the accessible environment is estimated using a public domain single phase flow code (MODFLOW) and single-phase transport codes (the SECOTP2D suite) developed by Sandia National Laboratories (SNL). The estimation procedure may be divided into three major parts, namely, generation of the transmissivity fields, groundwater flow calculations and radionuclide transport calculations. The results of the Culebra flow and transport calculations are combined with the results of other calculations during the construction of the complementary cumulative distribution function (CCDF) of the normalized cumulative radionuclide release to the accessible environment.

Calculation of groundwater flow and radionuclide transport in the Culebra is carried out under Analysis Plans AP-088 [2] and AP-100 [20] (see Figure 1). AP-088 addresses the calculation of a set of possible Culebra transmissivity fields (T fields) in the vicinity of the repository. AP-100 describes the process of selecting 100 T fields from the set produced in AP-088, and the set of calculations that are run to simulate Culebra flow and transport in the vicinity of the WIPP site.

This report documents the methods, software, input files, and output files used to complete Tasks 4-6 of the Analysis Plan for Calculation of Culebra Flow and Transport for the CRA (AP-100) [20] and summarizes the results obtained. The specific tasks covered in this report are:

Task 4 Extraction of flow field values from the regional flow field computed using modflow and preparation of these flow fields for use in transport modeling with secotp2d.

Task 6 Scaling of the flow field for climate change.

Task 5 Culebra radionuclide transport calculations using secotp2d.

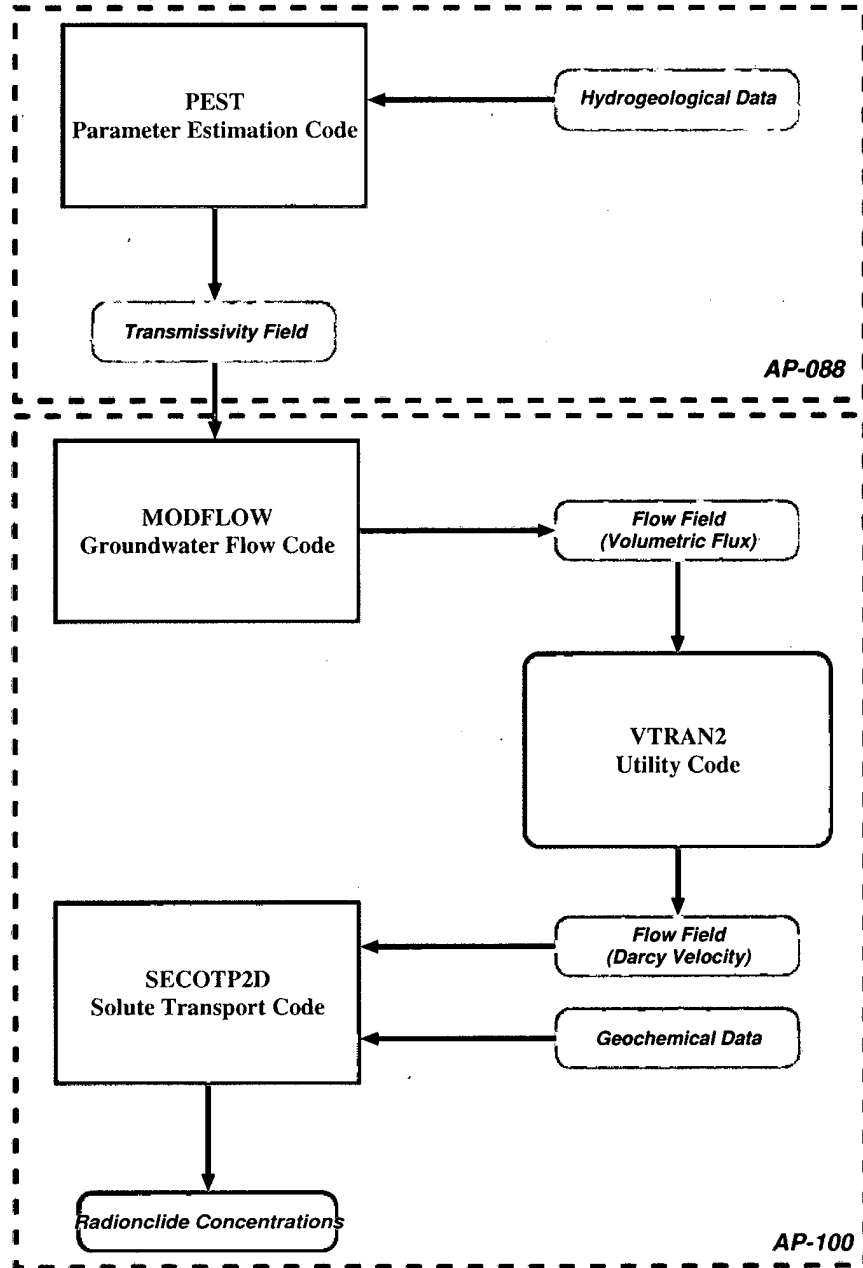


Figure 1: Analysis Overview (AP-88 and AP-100)

2 Flow Field Extraction (Task 4)

2.1 Objective

The objective of Task 4 is to develop and implement a procedure for extracting the groundwater flow field from the output of the `modflow` groundwater flow model and to put it into the format which the `secotp2d` code suite expects.

2.2 Background

Several issues need to be addressed when using the results of the groundwater flow calculations computed using `modflow` as input to the Culebra transport calculations: 1) the `modflow` code outputs the volumetric flux across the face of each cell in the computational mesh, while the `secotp2d` code suite expects the flow field in terms of the specific discharge at cell faces; 2) the computational domain used in the transport calculations is a subregion of that used in the groundwater flow calculations; 3) the origin of the two-dimensional `modflow` computational mesh corresponds to the northwest corner of the groundwater flow modeling domain while the `secotp2d` computational mesh locates its origin at the southwest corner of the transport model domain; 4) the coordinate system used by `modflow` also differs from that used by `secotp2d` in that the positive y-direction in `modflow` is opposite that of `secotp2d` and thus the flux in the y-direction has different sense in the two systems; and 5) `modflow` defines the x-direction flux for a given cell index as the flux through that cell's right face while `secotp2d` defines it as the flux through the left cell face.

The specific discharge or Darcy velocity across the cell face is computed by dividing the volumetric flux across the cell face by its area (See Figure 2).

$$u = \frac{Q_x}{A_x} = \frac{Q_x}{\Delta y \Delta z} \quad (1)$$

$$v = \frac{Q_y}{A_y} = \frac{Q_y}{\Delta x \Delta z} \quad (2)$$

where u, v are the specific discharge (Darcy velocity) across the cell face in the x- and y-direction, respectively; Q_x, Q_y are the volumetric flux across the cell faces; and A_x, A_y are areas of the cell face perpendicular to the x- and y-directions, respectively.

The remaining issues can be dealt with as outlined below and illustrated in Figure 3. Let (j, i) be the x-direction and y-direction indices of a cell in the `modflow` mesh with $j \in [1, N_{cols}]$ and $i \in [1, N_{rows}]$. Let (l, m) be the indices of the *same cell* referenced to the `secotp2d` mesh with $l \in [0, N_{cx} + 1]$ and $m \in [0, N_{cy} + 1]$. Note that the `secotp2d` mesh uses a band of ghost cells which extend beyond the boundaries of the transport domain in order to implement boundary conditions.

Since the positive y-direction of the two meshes are opposite in sense, we must have

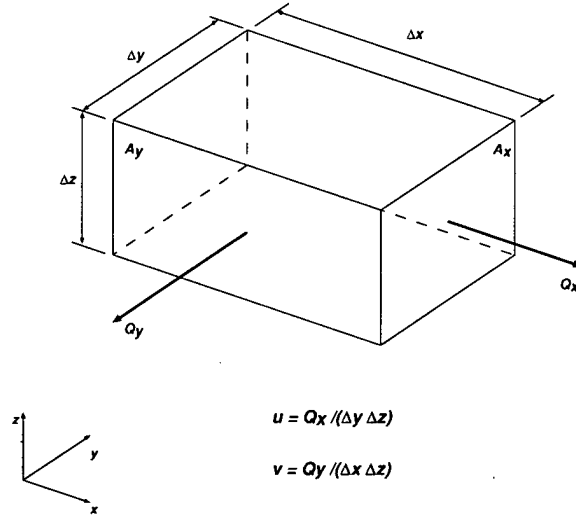


Figure 2: modflow Volumetric Flux and Darcy Velocity

$$v_{i,m}^S = -v_{j,i}^M \quad (3)$$

where the S superscript denotes the `secotp2d` velocity and M denotes the `modflow` velocity. The difference in conventions regarding which face to associate with a given cell can be written as

$$u_{i,m}^S = u_{j-1,i}^M \quad (4)$$

Let X_{shift} be the x-direction distance (in number of cells) between the origin of the `modflow` mesh and the `secotp2d` mesh. Let Y_{shift} represent the corresponding distance in the y-direction. Then the `modflow` cell indices corresponding to the cell (l, m) in the `secotp2d` mesh are given by

$$j = l + X_{shift} \quad (5)$$

$$i = Y_{shift} + 1 - m \quad (6)$$

The preceding set of rules may be summarized by Algorithm 1.

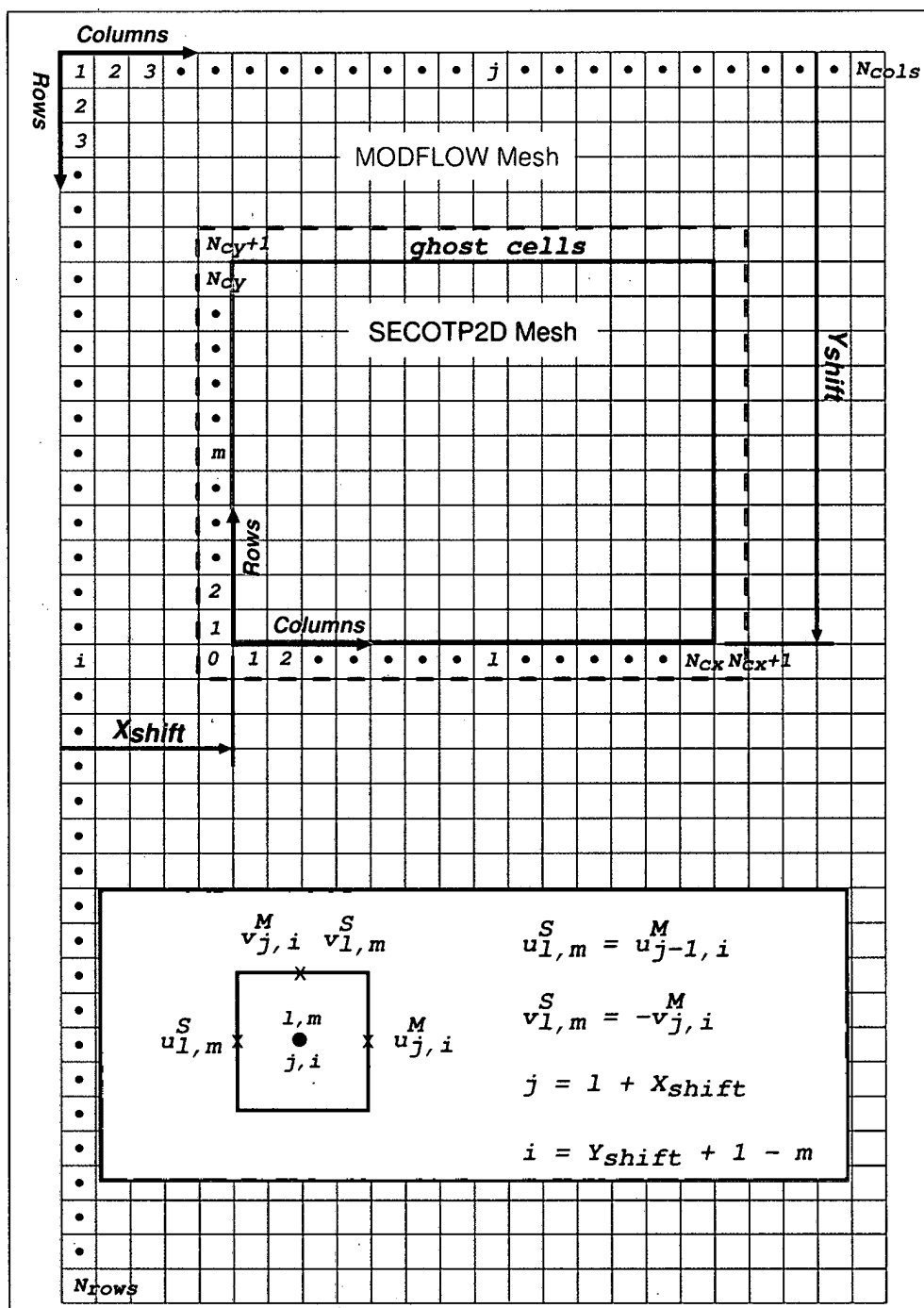


Figure 3: Transferring Velocities Between modflow and secotp2d Meshes

Algorithm 1 Velocity Extraction Algorithm

```
for  $l = 0$  to  $N_{cx}$  do
  for  $m = 0$  to  $N_{cy}$  do
     $j \leftarrow l + X_{shift}$ 
     $i \leftarrow Y_{shift} + 1 - m$ 
     $u_{l,m}^S \leftarrow u_{j-1,i}^M$ 
     $v_{l,m}^S \leftarrow -v_{j,i}^M$ 
  end for
end for
```

2.3 Approach

The rules for converting the modflow output data (volumetric flux) to secotpd input data (Darcy velocity) described above were implemented in the Fortran code `vtran2`. `vtran2` neither models physical phenomena nor solves differential equations that model physical phenomena. Rather, it is a utility code that processes the output data produced by a modeling code and formats that data for use in another modeling code.

The `vtran2` code takes five command line arguments, four required and one optional. All arguments are the names of input or output files, descriptions of which follow:

- File 1 (`cmd_file`) is an input ASCII format `vtran2` command file. The command file describes the modflow mesh, the secotpd mesh, the x- and y-direction offsets between the two meshes, and the format used in AP-100 Task 3 [23] to write the modflow velocities.
- File 2 (`bud_file`) is an input ASCII format modflow budget file containing the volumetric flux values for each cell in the groundwater flow modeling mesh.
- File 3 (`trn_file`) is an output binary format output file containing the groundwater flow velocities for the transport domain (including the ghost cells) in the format required by the secotpd transport code.
- File 4 (`dbg_file`) is an output ASCII format diagnostic/debug file containing information about the `vtran2` run.
- File 5 (`txt_file`) is an optional output ASCII format file containing the same data as the `trn_file`.

A sample command line procedure that executes `vtran2` could be:

```
$ vtran2 test.cmd test.bud test.trn test.dbg test.txt
```

The source listing for `vtran2`, along with sample command and diagnostic output files, is given in Appendix A. Also included in Appendix A is a description of the test cases used to verify this utility code.

Because of the large number of velocity files to process (three replicates with 100 vectors per replicate and two mining scenarios per vector) a Digital Command Language (DCL) script (`vtran2_run.com`) was written to run `vtran2` for all the elements in a given replicate. The source listing for this script is provided in Appendix A.

The `vtran2_run.com` script is run from the VMS command line:

```
$ @vtran2_run analysis replicate
```

where `analysis` is the name of the analysis (e.g., `CRA1`), and `replicate` identifies the replicate (e.g., `R1`, `R2`, or `R3`). (The location of the `vtran2` executable is hardwired into the `vtran2_run` script.)

When executed, the `vtran2_run` script looks for an input file with the name `vtran2_run.analysis.replicate.inp` (e.g. `vtran2_run.cra1.r1.inp`). This input file should contain data in two columns. The first column lists flow field names according to the convention used for the modflow runs in the Task 3/AP-100 [23]. This name is passed to `vtran2` in its `bud_file` argument. For each item in the first column, the second column gives the name for that flow field used in the Run Control System (RCS) that executes the transport calculations on the VMS cluster [21]. This name is passed to `vtran2` in its `trn_file` argument.

In order to process the velocity files, `vtran2_run` assumes a particular (relative) directory structure. If `[cwd]` is the current working directory, then

1. The `vtran2_run` script, as well as the `vtran2_run` input file and `vtran2` command file must reside in `[cwd]`.
2. When `vtran2_run` executes, it will place its log file in `[cwd]`.
3. The modflow output files are located in `[cwd.bud_files.Rx]` where x is the replicate number.
4. The `vtran2` output files are placed in `[cwd.trn_files.Rx]` where x is the replicate number.
5. The `vtran2` diagnostic files are placed in `[cwd.dbg_files.Rx]` where x is the replicate number.

Examples of the directory structure, input files, and output files are shown in Figure 4 and Table 1.

2.4 Results

The velocity extraction process was executed on the WIPP Alpha Cluster. The DCL script `vtran2_run.com` was run once for each replicate. Each run of the script executed the `vtran2` code for both full and partial mining scenarios for all 100 vectors in the replicate. A `vtran2` command file and a `VTRAN2_RUN` input file were prepared for each replicate. These files, along with the log file from each run are included in Appendix B.

Source code, executables, scripts, input and output files
stored in CMS library

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LIBCRA1-MF2K

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Table 1: vtran2.run script, input and output files

Directory	File	Description
[flow_fields]	vtran2.run.com	DCL script to run vtran2
	vtran2.run_cra1_r1.inp	vtran2.run input file for replicate 1
	vtran2.run_cra1_r2.inp	vtran2.run input file for replicate 2
	vtran2.run_cra1_r3.inp	vtran2.run input file for replicate 3
	vtran2.run_cra1_r1.log	vtran2.run log file for replicate 1
	vtran2.run_cra1_r2.log	vtran2.run log file for replicate 2
	vtran2.run_cra1_r3.log	vtran2.run log file for replicate 3
	vtran2_cra1_r1.cmd	vtran2 command file for replicate 1
	vtran2_cra1_r2.cmd	vtran2 command file for replicate 2
	vtran2_cra1_r3.cmd	vtran2 command file for replicate 3
[flow_fields.bud_files.r1]	dddrmmr1.out	
[flow_fields.bud_files.r2]	dddrmmr2.out	
[flow_fields.bud_files.r3]	dddrmmr3.out	
[flow_fields.trn_files.r1]	mf2k_cra1_r1.fff_mm.trn	
[flow_fields.trn_files.r2]	mf2k_cra1_r2.fff_mm.trn	
[flow_fields.trn_files.r3]	mf2k_cra1_r3.fff_mm.trn	
[flow_fields.bud_files.r1]	mf2k_cra1_r1.fff_mm.trn	
[flow_fields.bud_files.r2]	mf2k_cra1_r2.fff_mm.trn	
[flow_fields.bud_files.r3]	mf2k_cra1_r3.fff_mm.trn	

Note 1: $dd \in [01, 22]$, $rr \in [01, 10]$ as described in Analysis Report for tasks 2 & 3 of AP-100 [23]

Note 2: $fff \in [001, 100]$

Note 3: $m \in [f, p]$

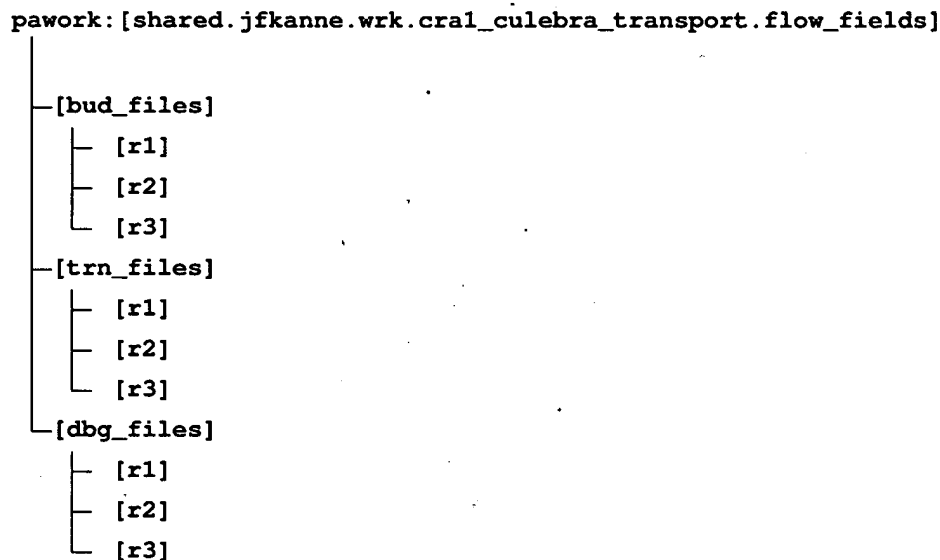


Figure 4: Directory tree for vtran2_run

3 Scaling For Climate Change (Task 5)

3.1 Objective

The objective of Task 5 is to incorporate effects of potential future climate change into the modeling of radionuclide transport in the Culebra.

3.2 Background

The 1996 WIPP Compliance Certification Application (CCA) [11] discusses the effect of potential future climate change on groundwater flow and radionuclide within the Culebra formation. In summary, it concludes that the regional effects of climate change may be reasonably approximated through the direct scaling of the two-dimensional, steady state groundwater velocity field used in the Culebra transport modeling. The scaling factor is treated as an uncertain parameter in the probabilistic modeling of the repository performance.

3.3 Approach

Since the climate index is an uncertain parameter, a sampled value is assigned to each vector and replicate by the LHS suite of codes (See Figure 5 and Table 2 for a summary of the codes and data flow for the transport calculations). The value of the climate index is stored in the CAMDAT database variable CLIMTIDX. This CAMDAT variable name is made known to the secotp2d suite of codes through the presecotp2d run control parameter CLIMATE, specified in the

presecotp2d input file (A sample presecotp2d input file is provided in Appendix C).

The presecotp2d code reads the value of CLIMTIDX from the input CAM-DAT database file, performs the scaling, and writes the scaled velocities to an output velocity file. The velocity file is then used as input to the secotp2d code which performs the actual transport calculations.

3.4 Results

Because scaling the flow field for climate change is incorporated into the secotp2d code suite, no separate results need to be discussed here.

Table 2: Primary Codes used in Culebra Transport Calculations

Code Name	Purpose	Input File(s)	Primary Output File(s)
genmesh	Creates grid. Run once.	gm_st2d_cra1.inp	gm_st2d_cra1.cdb
matset	Sets material regions and extracts constant parameters from secondary database. Run once.	ms_st2d_cra1.inp gm_st2d_cra1.cdb	ms_st2d_cra1.cdb
prelhs	Creates lhs input file. Run once per replicate	lhs1_st2d_cra1_Rx.inp	lhs1_st2d_cra1_trn_Rx.out lhs1_st2d_cra1_Rx.out
lhs	Performs Latin hypercube sampling of uncertain parameters. Run once per replicate.	lhs1_st2d_cra1_trn_Rx.out	lhs2_st2d_cra1_trn_Rx.out
postlhs	Distributes lhs sampled values to individual CAMDAT data base (CDB) files. Run once per replicate.	lhs3_st2d_cra1.inp lhs2_st2d_cra1_trn_Rx.out ms_st2d_cra1.cdb	lhs3_st2d_cra1_Ax_Rnnn.cdb
algebracdb	Run 100 times per replicate	alg_st2d_cra1.inp lhs3_st2d_cra1_Ax_Rnnn.cdb	alg_st2d_cra1_Rx_Vnnn.cdb
relate	Consolidates all parameters into single material block. Run 100 times per replicate	rel_st2d_cra1.inp gm_st2d_cra1.cdb alg_st2d_cra1_Rx_Vnnn.cdb	rel_st2d_cra1_Rx_Vnnn.cdb
presecotp2d	Configures transport simulation, scales velocities, assigns parameters, sets boundary conditions, and defines sources. Run 100 times per replicate/mining type combination	st2d_cra1.inp mf2k_cra1_Fff_mM.trn rel_st2d_cra1_Rx_Vnnn.cdb	st2d2_cra1_Rx_Vnnn_mM.inp st2d1_cra1_Rx_Vnnn_mM.prp st2d1_cra1_Rx_Vnnn_mM.vel
secotp2d	Performs transport simulation. Run 100 times per replicate/mining type combination	st2d2_cra1_Rx_Vnnn_mM.inp st2d1_cra1_Rx_Vnnn_mM.prp st2d1_cra1_Rx_Vnnn_mM.vel	st2d3_cra1_Rx_Vnnn_mM.bin
postsecotp2d	Translates secotp2d output to CDB format. Run 100 times per replicate/mining type combination	st2d3_cra1_Rx_Vnnn_mM.bin rel_st2d_cra1_Rx_Vnnn.cdb	st2d3_cra1_Rx_Vnnn_mM.cdb

Note: $x = 1, 2, 3$; $nnn = 1$ to 100; $m = P, F$

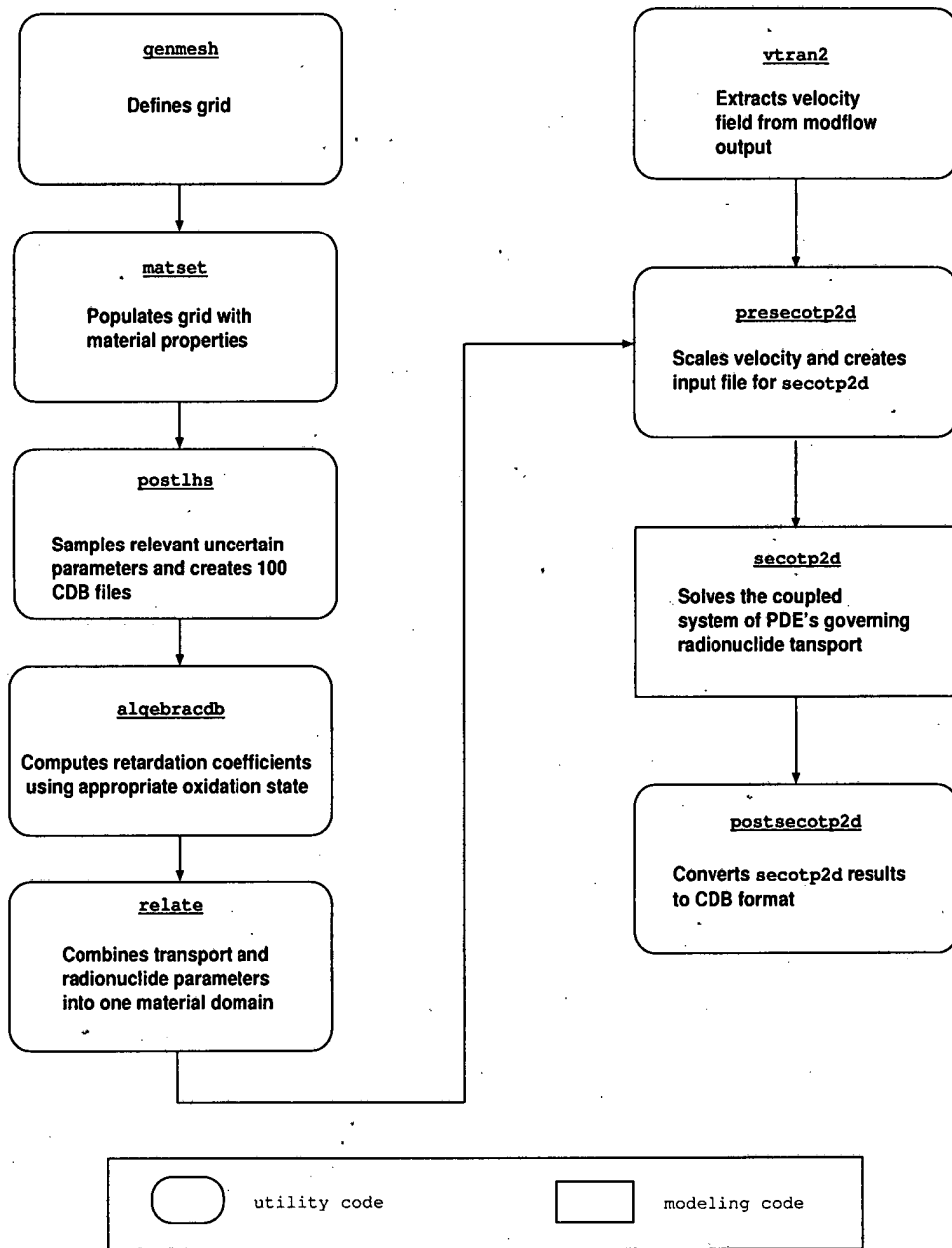


Figure 5: Flow Chart for Culebra Transport Calculations

4 Radionuclide Transport Calculations (Task 6)

4.1 Objective

The objective of Task 6 is to calculate radionuclide transport through the Culebra using the flow fields obtained in Task 5, along with the appropriate physicochemical data obtained from the WIPP parameter database.

4.2 Background

The Culebra is a 7.75 meter thick fractured dolomite with nonuniform properties in both the horizontal and vertical directions [16]. There are multiple scales of porosity and permeability within the Culebra ranging from microfractures to potentially large vuggy zones. Flow occurs through fractures, vugs and, to some extent, through intergranular pores. The large permeability contrast between the different scales of inter-connected porosity suggests a dual porosity conceptualization consisting of advective porosity (also referred to as fracture porosity) and diffusional porosity (also known as matrix porosity). The advective porosity is thought to consist of the void space contained in the highly transmissive portions of the rock such as large open fractures and/or interconnected vugs. The diffusional porosity represents the inter- and intragranular porosity and may also include microfractures and/or vugs. Tracer tests conducted at the WIPP site demonstrate both advective transport and matrix diffusion [36].

Although the Culebra properties vary in the vertical direction, the error introduced by modeling the Culebra in two rather than three dimensions has been determined to be negligible for the objective of these calculations [9].

4.3 Approach

The Culebra radionuclide transport calculations are performed using `secotp2d`, a two-dimensional dual porosity transport code developed to simulate radionuclide transport through fractured porous media [42, 43]. The `secotp2d` code assumes a parallel plate type fracturing where fluid flow is restricted to the advective continuum (fractures) and mass is transferred between the advective and diffusive (matrix) continua via molecular diffusion. The dual porosity conceptualization is illustrated in Figure 6. Retardation is permitted in both the advective and diffusive domains assuming linear equilibrium isotherms. Radioactive decay is accounted for through the use of multiple straight decay chains.

4.4 Road map of the Transport Calculations

The `secotp2d` solute transport code is used in conjunction with a preprocessor (`presecotp2d`) and a postprocessor (`postsecotp2d`). In addition, a set of utility codes is required to define the mesh, set material properties and deterministic parameters, and sample the distributions for uncertain parameters. These codes are described in Table 2, and the flowchart in Figure 5. All of these codes are

located in the WIPP Software Configuration Management System (SCMS) and are run on the WIPP Alpha Cluster.

All codes used in the analysis, with the exception of `vtran2`, are qualified per NP 19-1. As required by NP 9-1, a listing of the source code and code verification are included in Appendix A of this document.

4.4.1 Governing Equation for Advective Continuum

The `secotp2d` code solves the following partial differential equation (PDE) for radionuclide transport in the advective continuum

$$\begin{aligned} \phi R_k \frac{\partial C_k}{\partial t} = & -\nabla \cdot (\mathbf{v} C_k) + \nabla \cdot (\phi \mathbf{D}_k \nabla C_k) \\ & - \phi R_k \lambda_k C_k + \phi R_{k-1} \lambda_{k-1} C_{k-1} \\ & + Q_k + \Gamma_k \end{aligned} \quad (7)$$

where k is a species index, C_k is the unknown concentration of the k th radionuclide in the advective continuum (kg/m^3), \mathbf{v} is the specific discharge vector (m/s), \mathbf{D}_k is the hydrodynamic dispersion tensor (m^2/s), ϕ is the advective porosity (dimensionless), R_k is the retardation coefficient (dimensionless), λ_k is the radioactive decay rate constant (s^{-1}), Q_k is the specific injection rate ($kg/m^3/s$), and Γ_k denotes rate of mass transfer to the advective continuum from the diffusive continuum, per unit volume ($kg/m^3/s$).

The concentration C_k is defined as the mass of the k th radionuclide per unit volume of pore fluid. The advective porosity, ϕ , is defined as the ratio of the advective pore volume to the total or bulk volume. Similarly, the specific injection rate is defined as the rate of mass injected per unit bulk volume. Terms involving $k-1$ are omitted for the parent of the decay chain ($k=1$). Eq. (7) is linear in C_k and is solved simultaneously for all species in a given decay chain ($k=1, 2, \dots, N$), where N is the number of species in the decay chain.

The flow field given by \mathbf{v} is assumed to be independent of the solute concentration. In practice, the flow field is obtained from a groundwater flow code (`modflow` in this analysis).

The product $\phi \mathbf{D}_k$ in Eq. (7) is defined as

$$\phi \mathbf{D}_k = \frac{1}{|\mathbf{v}|} \begin{bmatrix} u & -v \\ v & u \end{bmatrix} \begin{bmatrix} \alpha_L & 0 \\ 0 & \alpha_T \end{bmatrix} \begin{bmatrix} u & v \\ -v & u \end{bmatrix} + \phi \tau D_k^* \quad (8)$$

where α_L is the longitudinal dispersivity of the advective continuum (m), α_T is the transverse dispersivity (m), u and v are the x- and y-components of the specific discharge vector (m/s), D_k^* is the free water molecular diffusion coefficient (m^2/s), and τ is the advective tortuosity defined as the ratio of the fluid particle flow path length to the length of the porous medium (dimensionless).

The retardation coefficient R_k is defined by

$$R_k = 1 + \frac{\rho_s (1 - \phi) (k_d)_k}{\phi} \quad (9)$$

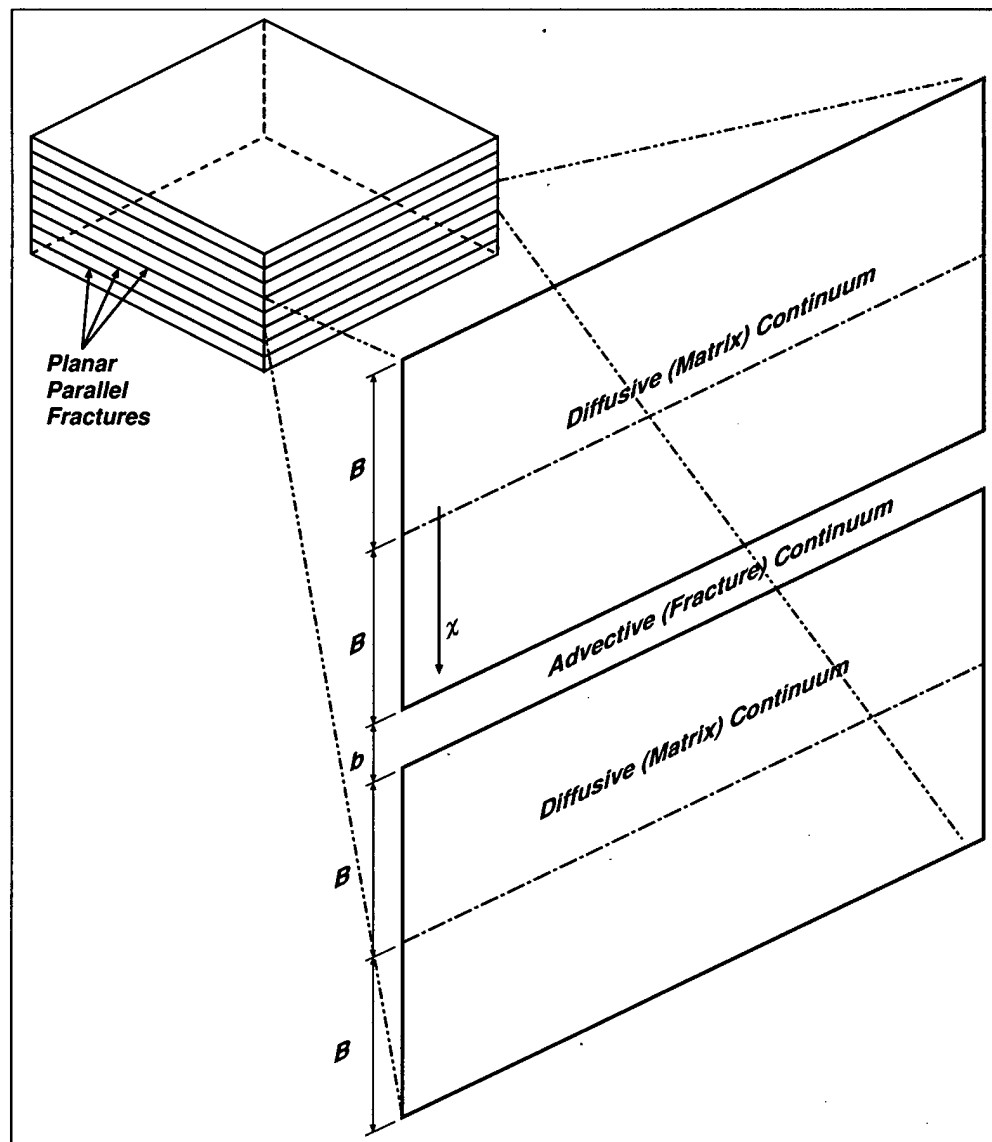


Figure 6: Parallel Plate Dual Porosity Conceptualization

where ρ_s is the Culebra Dolomite grain density (kg/m^3) and $(k_d)_k$ is the distribution coefficient ($/m^3/kg$) which completely describes the linear isotherm for radionuclide sorption to the Culebra.

4.4.2 Governing Equation for Diffusive Continuum

The `secotp2d` code also solves the following one-dimensional PDE for radionuclide transport in the diffusive continuum

$$\phi' \frac{\partial C'_k}{\partial t} = \frac{\partial}{\partial \chi} \left(\phi' D'_k \frac{\partial C'_k}{\partial \chi} \right) - \phi' R'_k \lambda'_k C'_k + \phi' R'_{k-1} \lambda'_{k-1} C'_{k-1} \quad (10)$$

C_k is the unknown concentration of the k th radionuclide in the diffusive continuum (kg/m^3), χ is the spatial coordinate as shown in Figure 6, and D'_k is the matrix diffusion coefficient. The matrix diffusion coefficient is defined as

$$D'_k = \tau' D_k^* \quad (11)$$

where τ' is the matrix tortuosity. All other symbols in Eq. (10) have the same meaning as those in Eq.(7) except that the prime denotes diffusive continuum properties.

4.4.3 Coupling between the Advective and Diffusive Continua

The governing equations for the advective and diffusive continua are coupled through the mass transfer term, Γ_k . Applying Fick's law at the interface between the two continua results in the following equation for mass transfer:

$$\Gamma_k = -\frac{2\phi}{b} \left(\phi' D'_k \frac{\partial C'_k}{\partial \chi} \Big|_{\chi=B} \right) \quad (12)$$

where B is the matrix half-block length (m), b is the fracture aperture (m), the terms in parentheses represent the mass flux per unit area of contact between the advective and diffusive continua and the term $2\phi/b$ represents the specific surface area (ratio of surface area to bulk volume) of the coupled system. In the parallel plate formulation, the fracture aperture b is defined by

$$b = \frac{\phi B}{1 - \phi} \quad (13)$$

4.4.4 Parameters and Data Sources

Tables 3 and 4 list the deterministic parameters and uncertain parameters, respectively, used in this analysis, along with the sources for their values/distributions.

4.4.5 Sources

In this analysis, we calculate the transport of each radionuclide over a 10,000 year interval due to the action of a source which injects a total of 1 kg at the center of the transport domain over the first 50 years of the simulation.

Table 3: Constant Parameters Used in Culebra Transport Calculations

Material	Property	Description	Units	Value	Reference
CULEBRA	DISP.L	Longitudinal Dispersivity	<i>m</i>	0.000000e+00	[24, 29, 31, 30]
CULEBRA	DISPT.L	Transverse Dispersivity	<i>m</i>	0.000000e+00	[24, 28, 29, 31, 30, 41]
CULEBRA	FTORT	Fracture Tortuosity	-	1.000000e+00	[52]
CULEBRA	DTORT	Diffusive tortuosity	-	1.100000e-01	[32, 35]
CULEBRA	SKIN.RES	Skin resistance	-	0.000000e+00	[53, 54]
CULEBRA	DNSGRAIN	Material grain density	<i>kg/mole</i>	2.820000e+03	[1, 7, 24, 27]
REFCON	YRSEC	Seconds per year	<i>s</i>	3.155693e+07	[25, 51]
AM241	ATWEIGHT	Atomic weight of ²⁴¹ Am	<i>kg/mole</i>	2.410570e-01	[15, 25, 47]
AM241	HALFLIFE	Half-life of ²⁴¹ Am	<i>s</i>	1.364000e+10	[24, 44, 47]
PU239	ATWEIGHT	Atomic weight of ²³⁹ Pu	<i>kg/mole</i>	2.390520e-01	[15, 25, 47]
PU239	HALFLIFE	Half-life of Pu	<i>s</i>	7.594000e+11	[24, 44, 47]
TH230	ATWEIGHT	Atomic weight of ²³⁰ Th	<i>kg/mole</i>	2.300330e-01	[15, 25, 47]
TH230	HALFLIFE	Half-life of Th	<i>s</i>	2.430000e+12	[24, 44, 47]
U234	ATWEIGHT	Atomic weight of ²³⁴ U	<i>kg/mole</i>	2.340410e-01	[15, 25, 47]
U234	HALFLIFE	Half-life of ²³⁴ U	<i>s</i>	7.716000e+12	[24, 44, 47]
AM+3	MD0	Pure liquid diffusion coefficient	<i>m²/s</i>	3.000000e-10	[5]
PU+3	MD0	Pure liquid diffusion coefficient	<i>m²/s</i>	3.000000e-10	[5]
PU+4	MD0	Pure liquid diffusion coefficient	<i>m²/s</i>	1.530000e-10	[5]
TH+4	MD0	Pure liquid diffusion coefficient	<i>m²/s</i>	1.530000e-10	[5]
U+4	MD0	Pure liquid diffusion coefficient	<i>m²/s</i>	1.530000e-10	[5]
U+6	MD0	Pure liquid diffusion coefficient	<i>m²/s</i>	4.260000e-10	[5]

Table 4: Sampled Parameters Used in Culebra Transport Calculations

Material	Property	Description	Units	Distribution	Range	Median	Reference
CULEBRA	APOROS	Advective Porosity	-	loguniform	[1.00e-04, 1.00e-02]	1.00e-03	[27, 37, 38, 48]
CULEBRA	DPOROS	Diffusive Porosity	-	cumulative	[1.00e-01, 2.50e-01]	1.60e-01	[27, 34, 48]
CULEBRA	HMBLKLT	Half-matrix block length	m	uniform	[5.00e-02, 5.00e-01]	2.75e-01	[27, 33, 37, 38, 48]
GLOBAL	OXSTAT	Oxidation state index	-	uniform	[0.00e+00, 1.00e+00]	5.00e-01	[8, 18, 45, 46, 55, 48]
GLOBAL	CLIMTIDX	Climate index	-	cumulative	[1.00e+00, 2.25e+00]	1.17e+00	[10, 27, 48]
AM+3	MKD_AM	Matrix K_d of ^{241}Am	m^3/kg	loguniform	[2.00e-02, 4.00e-01]	9.00e-02	[4, 3, 6, 26, 40, 48, 49]
PU+3	MKD_PU	Matrix K_d of ^{239}Pu	m^3/kg	loguniform	[2.00e-02, 4.00e-01]	9.00e-02	[4, 3, 6, 26, 40, 48]
PU+4	MKD_PU	Matrix K_d of ^{239}Pu	m^3/kg	loguniform	[7.00e-01, 1.00e+01]	2.60e+00	[4, 3, 6, 12, 26, 40, 48, 49]
TH+4	MKD_TH	Matrix K_d of ^{230}Th	m^3/kg	loguniform	[7.00e-01, 1.00e+01]	2.60e+00	[4, 3, 6, 12, 26, 40, 48, 49]
U+4	MKD_U	Matrix K_d of ^{234}U	m^3/kg	loguniform	[7.00e-01, 1.00e+01]	2.60e+00	[4, 3, 6, 12, 26, 40, 48, 49]
U+6	MKD_U	Matrix K_d of ^{234}U	m^3/kg	loguniform	[3.00e-05, 2.00e-002]	7.70e-04	[4, 3, 6, 12, 26, 40, 48, 49]

4.4.6 Initial Conditions and Boundary Conditions

Initial Conditions. In this analysis, the initial condition for both continua is that of zero radionuclide concentrations throughout their respective domains:

$$C_k(x, y, 0) = 0 \quad \forall (x, y) \in \Omega \quad (14)$$

$$C'_k(\chi, 0) = 0 \quad \forall \chi \in \Omega' \quad (15)$$

where Ω and Ω' are the spatial domains of the advective and diffusive continua, respectively.

Matrix Boundary Conditions. The center of matrix blocks is a symmetry boundary, so we must have

$$\left. \frac{\partial C'_k}{\partial \chi} \right|_{\chi=0} = 0 \quad \forall t > 0 \quad (16)$$

At the interface between a matrix block and a fracture, the concentration in the diffusive domain must be equal to that of the advective domain:

$$C'_k(B, t)|_{(x,y)} = C_k(x, y, t) \quad \forall t > 0 \quad (17)$$

where B is the matrix half-block length (m) as defined in Figure 6.

Fracture Boundary Conditions. In this analysis, the boundary conditions for the advective domain are set automatically by `secotp2d`, using the direction of the flow field to set the boundary condition type. At boundary locations where the flow direction is outward and therefore leaving the computational domain, a zero concentration gradient Neumann boundary condition is imposed. At boundary locations where the flow is inward, a zero concentration Dirichlet boundary condition is used.

4.5 Spatial Domain and Discretization

The spatial domain used for the transport calculations is shown in Figure 7 in relation to the groundwater modeling domain and the WIPP land withdrawal boundary (LWB). The UTM coordinates for these entities are given in Table 5.

The physical domain used in the transport calculations is a subregion of that used for the groundwater flow calculations. This subregion is approximately 7.5 km by 5.4 km, aligned with the principle directions of the groundwater flow domain. The transport domain extends beyond the boundaries of the WIPP in the east-west direction (approximately 250 m in the west and approximately 750 m in the east). Since the undisturbed groundwater flow direction is generally north to south, the transport domain is shifted so that it extends from a point midway between the waste panel and the northern LWB to approximately 1000

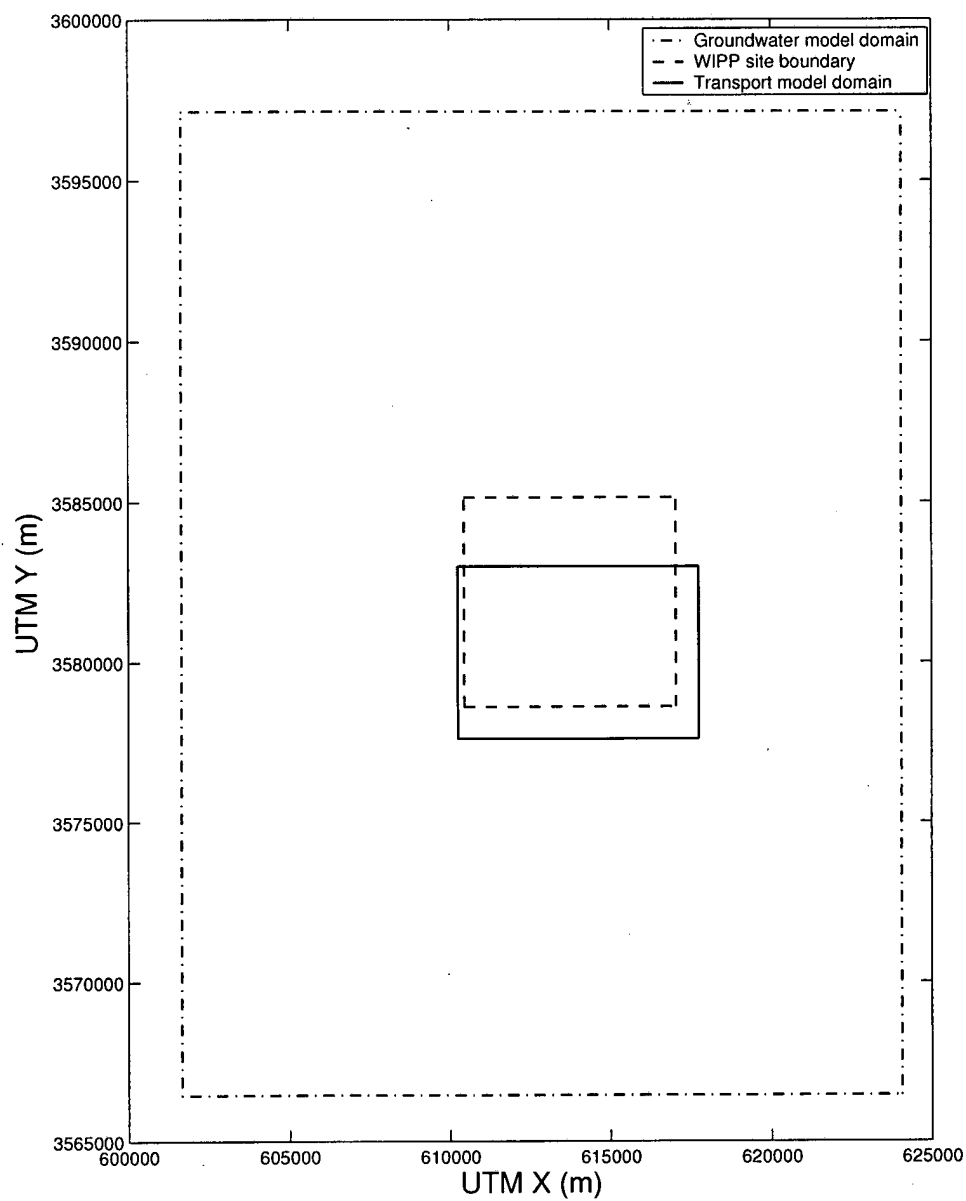


Figure 7: Culebra Groundwater Flow and Transport Modeling Domains

Table 5: UTM Coordinates of Spatial Domain Features
Groundwater Modeling Domain

	UTM X (m)	UTM Y (m)
SW Corner	601650	3566450
SE Corner	624050	3566450
NE Corner	624050	3597150
NW Corner	601650	3597150

WIPP Land Withdrawal Boundary

	UTM X (m)	UTM Y (m)
SW Corner	610567	3578623
SE Corner	617015	3578681
NE Corner	616941	3585109
NW Corner	610495	3585068

Transport Domain

	UTM X (m)	UTM Y (m)
SW Corner	610250	3577600
SE Corner	617750	3577600
NE Corner	617750	3583000
NW Corner	610250	3583000

m beyond the LWB in the south. The transport calculations use a uniform computational grid composed of 50m by 50m cells.

Spatial discretization of the diffusive (matrix) continuum is accomplished using the grid stretching algorithm in `preseco2d`. The equation used to discretize the matrix is

$$\Delta l_i = \Delta l_0(1 + \epsilon)^i \text{ for } i = 1, n - 2 \quad (18)$$

where $\Delta l_i = \Delta l_i/B$. The total number of nodes, n , and the size of the first grid block, Δl_0 , are supplied to `preseco2d`, which then computes ϵ such that

$$\Delta l_0 + \sum_{i=1}^{n-2} \Delta l_i = 1 \quad (19)$$

In this analysis, n was set to 20 and Δl_0 was chosen to be 1e-03.

4.6 Temporal Discretization

A constant time step size of 0.5 years was used in this analysis. Thus, the 10,000 year simulation was computed in 20,000 time steps.

4.7 Results

Radionuclide transport calculations for the Culebra were performed with the `seco2d` code as summarized in the preceding sections. All calculations were

performed on the WIPP Alpha Cluster. The input files used in the transport calculations are included in Appendix C.

The specific quantity of interest in the Culebra transport calculations is the cumulative release of radionuclides at the LWB during the time-span of 10,000 years in response to unit releases from a point source located at the center of the waste panel area (WPA) during the first 50 years after repository closure. The radionuclides transported in the Culebra are ^{241}Am , ^{234}U , ^{230}Th and ^{239}Pu . ^{234}U may be present in either the U(III) or U(IV) oxidation state. ^{239}Pu may be present as Pu(IV) or Pu(VI).

Transport calculations were performed for both partial mining and full mining scenarios. The partial mining scenario assumes the extraction of all potash reserves outside the LWB while full mining assumes that all reserves both inside and outside the LWB are exploited. The effect of mining enters the transport calculations through the Culebra flow field computed using the modflow 2000 program [23, 22].

Since the 2003 WIPP PA used a total of 300 sample elements (three replicates of 100 vectors each) and calculations were required for both full and partial mining conditions, 600 Culebra transport simulations were required. Along with the input files referenced above, the output (CASMDAT database) files from these simulation are stored in the CMS library LIBCRA1.ST2D. The naming convention for the CAMDAT database files is: ST2D3_CRA1_Rx_Vnnn_mM.CDB where $x \in [1, 3]$, $nnn \in [001, 100]$, and $m \in [F, P]$.

4.7.1 Partial Mining Results

Under partial mining conditions, only the ^{234}U species was transported beyond the LWB in any significant amount during the course of the 10,000 year simulation. Eight to ten vectors in each replicate showed releases of ^{234}U greater than $1\text{e-}38\text{ kg}$. Only the eight vectors shown in Table 6 had releases greater than $1\text{e-}9\text{ kg}$. Sensitivity analysis indicates that releases of ^{234}U are associated with the U(IV) oxidation state. This result makes sense because the distribution coefficients for Uranium in the (IV) state are much lower than for the (III) state.

Each vector that showed release of ^{234}U also showed a release of the ^{230}Th daughter product. As the ^{230}Th daughter product releases observed were due to decay of ^{234}U , they were typically six to eight orders of magnitude less than the ^{234}U release.

Only one instance of ^{230}Th release not associated with the decay of ^{234}U transported to the boundary (i.e., due to the 1 kg ^{230}Th source injected at the center of the WPA over the first 50 years) was observed ($4.34\text{e-}20\text{ kg}$ for Replicate R1, Vector V068).

Only one release of ^{239}Pu was observed ($2.33\text{e-}36\text{ kg}$, for Replicate R1, Vector V052). No releases of ^{241}Am greater than $1\text{e-}38\text{ kg}$ were observed.

Table 6: Partial Mining ^{234}U releases at LWB greater than $1\text{e-}9\text{ kg}$

^{234}U Release (kg)	Replicate	Vector
4.79e-01	R3	V054
1.77e-01	R3	V084
8.15e-02	R3	V038
7.11e-02	R2	V010
5.41e-02	R1	V058
1.40e-03	R3	V023
2.36e-04	R1	V008
7.12e-08	R3	V071

4.7.2 Full Mining Results

Under full mining conditions, only the ^{234}U species was transported beyond the LWB in significant amounts during the course of the 10,000 year simulation. Twenty-one to twenty-three vectors in each replicate showed releases of ^{234}U greater than $1\text{e-}38\text{ kg}$. Only the eighteen elements shown in Table 7 had releases greater than $1\text{e-}9\text{ kg}$. As for the partial mining results, sensitivity analysis indicates that releases of ^{234}U are associated with the U(IV) oxidation state.

Most elements which showed release of ^{234}U also showed a release of the ^{230}Th daughter product. As the ^{230}Th daughter product releases observed were due to decay of ^{234}U , they were typically six to eight orders of magnitude less than the ^{234}U release.

Seven to fourteen vectors in each replicate showed very small releases of ^{230}Th due to the 1 kg source injected at the center of the WPA over the first 50 years. No releases were greater than $1\text{e-}9\text{ kg}$. The largest releases were $1.42\text{e-}10\text{ kg}$ (Replicate R2, Vector V071), $3.97\text{e-}11\text{ kg}$ (Replicate R3, Vector V065), $4.20\text{e-}12\text{ kg}$ (Replicate R1, Vector V065), $3.16\text{e-}14\text{ kg}$ (Replicate R2, Vector V098), $1.73\text{e-}15\text{ kg}$ (Replicate R3, Vector V059), and $3.49\text{e-}15\text{ kg}$ (Replicate R1, Vector V058). All other releases were smaller than $1\text{e-}17\text{ kg}$.

Eight to fifteen vectors in each replicate showed small releases of ^{239}Pu greater than $1\text{e-}38\text{ kg}$. Only two releases were greater than $1\text{e-}9\text{ kg}$. The largest releases were $6.15\text{e-}6\text{ kg}$ (Replicate R2, Vector V071), $2.03\text{e-}9\text{ kg}$ (Replicate R1, Vector V092), $5.12\text{e-}11\text{ kg}$ (Replicate R3, Vector V065), $1.19\text{e-}14\text{ kg}$ (Replicate R3, Vector V075), $2.97\text{e-}16\text{ kg}$ (Replicate R3, Vector V059), and $1.13\text{e-}16\text{ kg}$ (Replicate 3, Vector V024). All other releases were smaller than $1\text{e-}18\text{ kg}$.

Eleven to fourteen vectors in each replicate showed releases of ^{241}Am greater than $1\text{e-}38\text{ kg}$. No releases were larger than $1\text{e-}9\text{ kg}$. The largest releases were $1.77\text{e-}10\text{ kg}$, (Replicate 1, Vector 92), $1.93\text{e-}11\text{ kg}$ (Replicate 3, Vector 65), $2.99\text{e-}12\text{ kg}$ (Replicate 2, Vector 71), $5.32\text{e-}14\text{ kg}$ (Replicate 1, Vector 65) and $91.9\text{e-}15$ (Replicate 3, Vector 75). All other releases were smaller than $1\text{e-}18\text{ kg}$.

Table 7: Full Mining ^{234}U releases at LWB greater than $1\text{e-}9\text{ kg}$

^{234}U Release at (kg)	Replicate	Vector
9.87e-01	R2	V015
9.87e-01	R3	V038
8.89e-01	R1	V058
7.66e-01	R1	V065
7.12e-01	R3	V054
2.09e-01	R2	V010
2.69e-02	R3	V027
1.27e-02	R1	V090
1.23e-02	R2	V030
6.18e-03	R1	V031
4.72e-03	R3	V065
1.80e-04	R3	V066
1.66e-05	R2	V053
1.59e-07	R3	V067
1.03e-08	R1	V067
4.53e-09	R3	V042
1.98e-09	R2	V033
1.61e-09	R2	V024

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Appendix A: vtran2 Utility Code Description

A.1 vtran2.f Source listing

```

PROGRAM VTRAN

C
C
C      nrowmf - number of rows cells in the mf2k grid
C      ncolmf - number of columns in the mf2k grid
C
C      ncx - number of cells in x-direction in the st2d grid
C      ncy - number of cells in y-direction in the st2d grid
C
C      jshiftx - x offset of transport domain (# of cells in col direction)
C      ishity - y offset of transport domain (# of cells in row direction)
C
C
C      PARAMETER (nfsat = 2, mxfile=5)

C      CHARACTER*80 author, date, title
C      CHARACTER*80 filename(mxfile)
C      CHARACTER*80 fmat(nfsat),rdfmat
C      CHARACTER*80 fmcmd, fmbud, fmtrn, fmdbg, fmvsl

C      INTEGER ierr
C      INTEGER iunscr, iuncmd, iunbud, iuntrn, iundbg, iunvel
C      INTEGER nfiles, nfile
C      INTEGER nrowmf, ncolmf, ncx, ncy
C      INTEGER istart, ishift, jstart, jshift
C      INTEGER match, irdfmt
C      DOUBLE PRECISION time
C      DOUBLE PRECISION xyz_inv, xyz_inv, dx, dy, dz
C      DOUBLE PRECISION, ALLOCATABLE :: qx(:,,:), qy(:,,:)
C      DOUBLE PRECISION, ALLOCATABLE :: qxout(:,,:), qyout(:,,:)

C      LOGICAL vrtvel

C-----
C.....Setup
C-----

C.....Assign file unit numbers

      nfiles = 5

      iunscr = 6
      iuncmd = 11
      iunbud = 12
      iuntrn = 13
      iundbg = 14
      iunvel = 15

C.....Valid budget file input formats

      fmat(1) = '(448e16.8)'
      fmat(2) = '(448(e23.16,ix))'

C-----
C.....Process command line (get file names)
C-----

C      WRITE(iunscr,*) 'VTRAN >> Processing command line'

C.....Required args (1-4) are fmcmd, fmbud, fmtrn, fmdbg
C.....Optional arg (5) is fmvsl

      CALL filemdlin( nfiles, nfile, filename )

C      write(iunscr,*) 'nfile = ', nfile

      IF ( nfile .GT. nfiles ) THEN
        CALL QAABORT( 'VTRAN>> Too many command line arguments' )
      ELSE
        IF ( nfile .LT. nfiles-1 ) THEN
          CALL QAABORT( 'VTRAN>> Too few command line arguments' )
        ENDIF
      ENDIF

      fmcmd = filename(1)
      fmbud = filename(2)
      fmtrn = filename(3)
      fmdbg = filename(4)

      IF (nfile .eq. nfiles ) THEN
        vrtvel = .true.
      
```

```

      fmvvel = filemm(5)
    ELSE
      wrtvel = .false.
      fmvvel = 'None'
    ENDIF

C      write(iunscr,*) 'fmcmd is ', fmcmd
C      write(iunscr,*) 'fmbud is ', fmbud
C      write(iunscr,*) 'fmtrn is ', fmtrn
C      write(iunscr,*) 'fmdbg is ', fmdbg
C      write(iunscr,*) 'fmvel is ', fmvvel

C.....Open Diagnostics/Debug file

      OPEN (UNIT=iundbg, FILE=fmdbg, STATUS='UNKNOWN', IOSTAT=ierr)
      IF ( ierr .NE. 0 ) THEN
        CALL QAABORT ('Error opening command file')
      ENDIF

C-----
C.....Process command file
C-----

C      WRITE(iunscr,*) 'VTRAN >> Processing command file'

C.....Open command file

      OPEN (UNIT=iuncmd, FILE=fmcmd, STATUS='OLD',
+        READONLY, IOSTAT=ierr)
      IF ( ierr .NE. 0 ) THEN
        WRITE(iundbg,*) 'Error opening command file'
        CALL QAABORT ('Error opening command file')
      ENDIF

C.....Read from command file

      READ (iuncmd,*)
      READ (iuncmd,10) author
      READ (iuncmd,*)
      READ (iuncmd,10) date
      READ (iuncmd,*)
      READ (iuncmd,10) title
      READ (iuncmd,*)
      READ (iuncmd,10) rdfmat
      READ (iuncmd,*)
      READ (iuncmd,*) iscrn
      READ (iuncmd,*)
      READ (iuncmd,*) ncolmf, nrowmf
      READ (iuncmd,*)
      READ (iuncmd,*) jshftx, ishfty, ncx, ncy
      READ (iuncmd,*)
      READ (iuncmd,*) dx, dy, dz

10  FORMAT(A80)
11  FORMAT(3e01.3)
C.....Close command file

      CLOSE (UNIT=iuncmd, STATUS='KEEP')

C.....Send diagnostic ouput to screen or to debug file

      IF (iscrn .EQ. 0 ) THEN
        iunscr = iundbg
      ENDIF

C.....Echo input

      WRITE(iunscr,20) fmcmd, fmbud, fmtrn, fmdbg, fmvvel

20  FORMAT (1X, 'command file           = ',A80/
+        1X, 'budget file             = ',A80/
+        1X, '(binary) velocity transfer file = ',A80/
+        1X, 'diagnostic/debug file    = ',A80/
+        1X, '(ascii) velocity output file = ',A80/
+        )

      WRITE(iunscr,50) author, date, title, rdfmat
      WRITE(iunscr,100) iscrn, ncolmf, nrowmf,
+        jshftx, ishfty, ncx, ncy,
+        dx, dy, dz

50  FORMAT(1X, ' author = ',A80/
+        1X, ' date   = ',A80/
+        1X, ' title  = ',A80/
+        1X, ' format = ',A80/
+        )
100 FORMAT(1X, ' iscrn = ',15 /

```

```

+      1X,' ncolmf  = ',15 /
+      1X,' nrowmf  = ',15 /
+      1X,' jshftx  = ',15 /
+      1X,' ishfty  = ',15 /
+      1X,' ncr     = ',15 /
+      1X,' ncy     = ',15 /
+      1X,' dx      = ',10.4 /
+      1X,' dy      = ',10.4 /
+      1X,' dz      = ',10.4
+    )

C.....Assign correct format number

irdfmt = 0
match = 0
DO i=1,nfmat
  IF( LLE(rdfmat,fmat(i)) .AND. LLE(fmat(i),rdfmt)) THEN
    irdfmt = 1
    match = 1
  ENDIF
ENDDO

IF ( match .ne.1 ) THEN
  WRITE(iunscr,*) 'Invalid input format'
  CALL QAABORT ('Invalid input format')
ENDIF

WRITE(iunscr,150) irdfmt,rdfmt
150 FORMAT(1X,'Using input format (' ,12, ') = ',A80)

C.....Sanity check. Since ghost cells are added, we must have:
C.....jshftx >= 1 and ishfty >= ncy+1

IF ( jshftx .LT. 1 ) THEN
  WRITE(iunscr,*) 'Invalid jshftx value'
  CALL QAABORT ('Invalid jshftx value')
ENDIF

IF ( ishfty .LT. (ncy+1) ) THEN
  WRITE(iunscr,*) 'Invalid ishfty value'
  CALL QAABORT ('Invalid ishfty value')
ENDIF

C-----
C.....Allocate memory
C-----

C.....Mf2k grid is (1:ncolmf,1:nrowmf).
C.....Ghost cells placed around transport domain, so ST2D grid is
C.....(0:ncx,0:ncy). Thus qxout and qyout are padded to account for
C.....required ghost cells

ALLOCATE( qxin(1:ncolmf,1:nrowmf),
+         qyin(1:ncolmf,1:nrowmf),
+         qxout(0:ncx+1,0:ncy+1),
+         qyout(0:ncx+1,0:ncy+1),
+         STAT=ierr )

IF ( ierr .NE. 0 ) THEN
  WRITE(iunscr,*) 'Error allocating memory'
  CALL QAABORT ('Error allocating memory')
ENDIF

C-----
C.....Read budget file
C-----

WRITE(iunscr,*) 'VTRAN >> Reading budget file'

OPEN (UNIT=iunbud, FILE=fmbud, FORM='FORMATTED',
+      STATUS='OLD', IOSTAT=ierr)
IF ( ierr .NE. 0 ) THEN
  WRITE(iunscr,*) 'Error opening budget file'
  CALL QAABORT ('Error opening budget file')
ENDIF

DO i=1,nrowmf
  READ(iunbud,rdfmt) (qxin(j,i),j=1,ncolmf)
END DO
READ(iunbud,*)
DO i=1,nrowmf
  READ(iunbud,rdfmt) (qyin(j,i),j=1,ncolmf)
END DO

C.....Close budget file

```

```

CLOSE (UNIT=iunbud,STATUS='KEEP')

C.....Budget file contains volume fluxes, so must divide
C.....by area of cell face perpendicular to flow direction
C.....to get specific discharge (darcy velocity)

C.....X direction

      ayz_inv = 1.d0/(dy*dz)
      DO i=1,nrowmf
        DO j=1,ncolmf
          qxin(j,i) = qxin(j,i) * ayz_inv
        END DO
      END DO

C.....Y direction

      axz_inv = 1.d0/(dx*dz)
      DO i=1,nrowmf
        DO j=1,ncolmf
          qyin(j,i) = qyin(j,i) * axz_inv
        END DO
      END DO

C-----
C.....Process velocities
C-----

      WRITE(iunscr,*) 'VTRAN >> Processing velocities'

C.....Now grab velocities for internal cells and ghost cells.
C.....Let (l,m) be indices of the ST2D grid cells, ranging from 0:ncx+1
C.....and 0:ncy+1, respectively. We must compute the corresponding
C.....MF2K indices. The computed mf2k indices must account for:
C..... 1) The offset of the ST2D grid origin
C..... 2) The opposite sense of the y-coord in the two meshes
C..... 3) ST2D face-centered velocities of a given cell are defined
C.....    at the trailing edges of cells (defined according to sense of
C.....    the ST2D axes) while the MF2K face-centered velocities are
C.....    defined at the "right" and "front" faces of the cell.

      DO m=0,ncy+1
        DO l=0,ncx+1
          j = jshftx + 1
          i = ishfty + 1 - m
          qxout(l,m) = qxin(j-1,i)
          qyout(l,m) = qyin(j,i)
        END DO
      END DO

C..... For ST2D, face centered velocities defined at trailing edges
C of cells. Ghost cells are placed around the computational domain,
C but cells on left and bottom do not have defined velocities associated
C with them. Consider the x-dimension with limits [0,x1], with ncx
C regular cells and a ghost cell on each side of the domain. Then
C u(0,m) is not defined,
C u(1,m) = u at x=0, and
C u(ncx+1,m) = u at x1
C Similarly, Consider the y-dimension with limits [0,y1], with ncy
C regular cells and a ghost cell on each side of the domain. Then
C v(1,0) is not defined,
C v(1,1) = v at y=0, and
C v(1,ncy+1) = v at y1

C.....Zero out the undefined components

      DO m=0,ncy+1
        qxout(0,m) = 0.D0
      END DO

      DO l=0,ncx+1
        qyout(l,0) = 0.D0
      END DO

C.....Change sign of y-velocities. Modflow convention is that
C.....flow is positive in direction of increasing row numbers.
C.....But row numbers increase in negative y-direction.

      DO m=0,ncy+1
        DO l=0,ncx+1
          qyout(l,m) = -qyout(l,m)
        END DO
      END DO

C-----
C.....Write velocity transfer file
C-----

```

```

WRITE(iunscr,*) 'VTRAN >> Writing velocity transfer file'

C.....Open the file

OPEN (UNIT=iuntrn, FILE=fmtrn, FORM='UNFORMATTED',
+ STATUS='UNKNOWN', IOSTAT=ierr)
IF ( ierr .NE. 0 ) THEN
WRITE(iunscr,*) 'Error opening velocity transfer file'
CALL QABORT ('Error opening velocity transfer file')
ENDIF

C.....Write the following line because sf2d wrote it and
C.....st2d1 expects it (but does not use them)

time = 0.d0
WRITE(iuntrn) ncx, ncy, time

C.....Write velocities to output file. Include the undefined
C.....components, since ST2D1 expects them. (ST2D1 reads
C.....them in, but does not write them to the velocity file
C.....it passes to ST2D2)

WRITE(iuntrn) ( ( qkout(1,m), 1=0,ncx+1),m=0,ncy+1 )
WRITE(iuntrn) ( ( qkout(1,m), 1=0,ncx+1),m=0,ncy+1 )

C.....Close output file

CLOSE (UNIT=iuntrn,STATUS='KEEP')

C-----
C.....Write ascii velocity output file
C-----

IF ( wrtvel ) THEN

WRITE(iunscr,*) 'VTRAN >> Writing ascii velocity output file'

C.....Open the file

C OPEN (UNIT=iunvel, FILE=fmvel, FORM='FORMATTED',
C + STATUS='UNKNOWN', IOSTAT=ierr)

irecl = 448*(23+1)
OPEN (UNIT=iunvel, FILE=fmvel, FORM='FORMATTED',
+ STATUS='UNKNOWN', RECL=irecl, IOSTAT=ierr)

IF ( ierr .NE. 0 ) THEN
WRITE(iunscr,*) 'Error opening ascii velocity output file'
CALL QABORT ('Error opening ascii velocity output file')
ENDIF

C.....Write the following line because sf2d wrote it and
C.....st2d1 expects it (but does not use them)

time = 0.d0
WRITE(iunvel,200) ncx, ncy, time
200 FORMAT(1x,2(15,2x),e16.8)

C.....Write velocities to output file

WRITE(iunvel,rdfmt) ( ( qkout(1,m), 1=0,ncx+1),m=0,ncy+1 )
WRITE(iunvel,rdfmt) ( ( qkout(1,m), 1=0,ncx+1),m=0,ncy+1 )

C.....Close output file

CLOSE (UNIT=iunvel,STATUS='KEEP')

ENDIF

C-----
C.....Clean up
C-----

WRITE(iunscr,*) 'VTRAN >> Cleaning up'

DEALLOCATE(qxin,qkout,qyin,qyout)

WRITE(iunscr,*) 'VTRAN >> Normal Completion'
CLOSE (UNIT=iundbg,STATUS='KEEP')

```

C Signal normal completion
 STOP 'VTRAN >> Normal Completion'
 END

A.2 vtran2_run.com Source listing

```
#!/ Uncomment the next two lines and the "junk = " line near the end of
#!/ the script to turn on tracing
#
# saved_image = f$environment("VERIFY_IMAGE")
# saved_proc = f$verify("true")
#
# display = "write sys$output"
# ask      = "read sys$command /prompt="
#
#-----
#!/ Set foreign command for vtran
#-----
#
# vtran2_exe := "$ul:[jfkane.bin]vtran2.exe"
# show symbol veltrn_exe
#
#-----
#!/ Trap for incorrect usage
#-----
#
# if p1 .eqs. "" .or p2 .eqs. ""
# then
#     display "Usage: vtran2_run analysis replicate [debug]"
#     display "Example: vtran2_run cral R1 d"
#     exit
# endif
#
#
#-----
#!/ Set identifier
#-----
#
# analysis = f$edit(p1,"UPCASE")
# replicate = f$edit(p2,"UPCASE")
#
# case = analysis + "." + replicate
#
# debug = "F"
# if ( p3 .nes. "" ) then debug = "T"
#
#-----
#!/ Set subdirectory variables
#-----
#
# this_dir = f$trnlnm("sys$disk") + f$directory()
# str_len = f$length(this_dir)
# this_dir_c = f$extract( 0,str_len-1,this_dir)
#
# if ( debug)
# then
#     display "this_dir = ", this_dir
#     display "this_dir_c = ", this_dir_c
# endif
#
# bud_dir_name = "BUD_FILES"
# bud_dir      = "[" + bud_dir_name + "." + replicate + "]"
# bud_dir_spec = this_dir_c + "." + bud_dir_name + "]" + replicate + ".DIR"
# bud_dir_path = this_dir_c + "." + bud_dir_name + "." + replicate + "]"
#
# if ( debug)
# then
#     display " "
#     display "bud_dir      = ", bud_dir
#     display "bud_dir_spec = ", bud_dir_spec
#     display "bud_dir_path = ", bud_dir_path
# endif
#
# trn_dir_name = "TRN_FILES"
# trn_dir      = "[" + trn_dir_name + "." + replicate + "]"
# trn_dir_spec = this_dir_c + "." + trn_dir_name + "]" + replicate + ".DIR"
# trn_dir_path = this_dir_c + "." + trn_dir_name + "." + replicate + "]"
#
# if ( debug)
# then
#     display " "
#     display "trn_dir      = ", trn_dir
#     display "trn_dir_spec = ", trn_dir_spec
#     display "trn_dir_path = ", trn_dir_path
# endif
#
# dbg_dir_name = "DBG_FILES"
# dbg_dir      = "[" + dbg_dir_name + "." + replicate + "]"
# dbg_dir_spec = this_dir_c + "." + dbg_dir_name + "]" + replicate + ".DIR"
# dbg_dir_path = this_dir_c + "." + dbg_dir_name + "." + replicate + "]"
```

```

$
$ if ( debug)
$ then
$   display " "
$   display "dbg_dir      = ", dbg_dir
$   display "dbg_dir_spec = ", dbg_dir_spec
$   display "dbg_dir_path = ", dbg_dir_path
$ endif
$
$! Check that the required directories exist
$
$ if f$search(bud_dir_spec) .eqs. ""
$ then
$   display "directory ", bud_dir, " does not exist"
$   exit
$ endif
$ if f$search(trn_dir_spec) .eqs. ""
$ then
$   display "directory ", trn_dir, " does not exist"
$   exit
$ endif
$ if f$search(dbg_dir_spec) .eqs. ""
$ then
$   display "directory ", dbg_dir, " does not exist"
$   exit
$ endif
$
$
$!-----
$! Set file variables
$!-----
$
$! comment character in vtran2_run input file
$ vtran2_run_comment_char = "!"
$
$! vtran2_run input file
$ vtran2_run_inp = this_dir + "VTRAN2_RUN_" + case + ".INP"
$
$ if ( debug)
$ then
$   display " "
$   display "vtran2_run_inp = ", vtran2_run_inp
$ endif
$
$ if f$search(vtran2_run_inp) .eqs. ""
$ then
$   display "file ", vtran2_run_inp, " does not exist"
$   exit
$ endif
$
$
$! vtran2_run log file
$ vtran2_run_log_name = this_dir + "VTRAN2_RUN_" + case + ".LOG"
$
$ if ( debug)
$ then
$   display " "
$   display "vtran2_run_log_name = ", vtran2_run_log_name
$ endif
$
$
$! vtran2 command file
$ vtran2_cmd_name = "VTRAN2_" + case + ".CMD"
$ vtran2_cmd_path = this_dir + vtran2_cmd_name
$
$ if ( debug)
$ then
$   display " "
$   display "vtran2_cmd_path = ", vtran2_cmd_path
$ endif
$
$
$
$! base for transfer file names
$ fbase = "MF2K_" + case + "_"
$
$
$! exit
$
$!-----
$! Open log file, write time stamp and header
$!-----
$
$ open/write vtran2_run_log_file 'vtran2_run_log_name
$
$ write vtran2_run_log_file " "
$ write vtran2_run_log_file "Starting Time Stamp: ", f$time()
$ write vtran2_run_log_file " "
$
$ write vtran2_run_log_file "working dir      = ", this_dir

```

```

$ write vtran2_run_log_file "budget file dir      = ", bud_dir_path
$ write vtran2_run_log_file "trn file dir      = ", trn_dir_path
$ write vtran2_run_log_file "dbg file dir      = ", dbg_dir_path
$ write vtran2_run_log_file "vtran2_run input file = ", vtran2_run_inp
$ write vtran2_run_log_file "vtran2_run log file  = ", vtran2_run_log_name
$ write vtran2_run_log_file "vtran2_cmd_file    = ", vtran2_cmd_path
$
$!-----
$! Open vtran2_run input file, then loop
$! through the list of flow field pairs,
$! processing full and partial
$! mining cases for each pair
$!-----
$
$ write vtran2_run_log_file " "
$ write vtran2_run_log_file "Opening vtran2_run input file "
$ write vtran2_run_log_file " "
$
$ open/read vtran2_run_inp_file 'vtran2_run_inp
$
$ wr1 = "write vtran2_run_log_file"
$ wr1 "mf2k budget file    mf2k velocity transfer file"
$ wr1 "-----"
$
$10: read vtran2_run_inp_file line /error=30/end_of_file=20
$
$   if (debug ) then display line
$
$   if f$extract(0,1,line) .nes. vtran2_run_comment_char
$   then
$     gosub proc_line
$   else
$     if (debug) then display "this is a comment"
$     endif
$     goto 10
$
$20: if ( debug ) then display "reached end of vtran2_run input file "
$     goto 40
$30: display "error reading vtran2_run input file "
$     close vtran2_run_inp_file
$     close vtran2_run_log_file
$     exit
$40:
$
$!-----
$! Cleanup
$!-----
$
$ write vtran2_run_log_file " "
$ write vtran2_run_log_file "Closing vtran2_run input file"
$ write vtran2_run_log_file " "
$
$ close vtran2_run_inp_file
$
$ write vtran2_run_log_file " "
$ write vtran2_run_log_file "Ending Time Stamp: ", f$time()
$ write vtran2_run_log_file " "
$
$ close vtran2_run_log_file
$
$
$! junk = f$verify(saved_proc,saved_image)
$
$ display "vtran2_run normal completion"
$ exit
$
$
$!-----
$!-----
$
$proc_line:
$
$   if ( debug)
$   then
$     display "Entering proc_line"
$   endif
$
$   line_length = f$length(line)
$   blank_loc = f$locate(" ",line)
$   bud_length = blank_loc
$   ff_length = line_length-blank_loc
$
$   bud_name = f$extract(0,blank_loc,line)
$   bud_name = f$edit(bud_name,"TRIM,UPCASE")
$   ff_name = f$extract(blank_loc+1,ff_length,line)
$   ff_name = f$edit(ff_name,"TRIM,UPCASE")
$
$   if ( debug)
$   then

```

```

$   display "bud_name = ", bud_name, "."
$   display "ff_name = ", ff_name, "."
$   endif
$
$   cmd_fname = vtran2_cmd_name
$   cmd_fpath = vtran2_cmd_path
$   bud_fname = bud_name + ".OUT"
$   bud_fpath = bud_dir + bud_fname
$   trn_fname = fbase + ff_name + ".TRN"
$   trn_fpath = trn_dir + trn_fname
$   dbg_fname = "vtran2_" + case + "_" + ff_name + ".DBG"
$   dbg_fpath = dbg_dir + dbg_fname
$
$   if ( debug)
$   then
$       display "vtran2 cmd_file = ", cmd_fpath
$       display "vtran2 bud_file = ", bud_fpath
$       display "vtran2 trn_file = ", trn_fpath
$       display "vtran2 dbg_file = ", dbg_fpath
$   endif
$
$   vtran2_exe 'cmd_fpath' 'bud_fpath' 'trn_fpath' 'dbg_fpath'
$
$   write vtran2_run_log_file bud_fname, "      ", trn_fname
$
$   if ( debug)
$   then
$       read sys$command/prompt="press return" junk
$       display "Leaving proc_line"
$   endif
$
$   return

```

A.3 Sample vtran2 Command File

```
* author
Joseph F. Kanney
* date
2003 09 24
* title
CRAI_R1 Vtran2 command file
* input format type
(448e16.8)
* iscrn > 0 will print to screen, otherwise to dbg file
0
* ncol nrow
448 614
* jshftx ishfty ncx ncy
172 391 150 108
* dx dy dz
50 50 4
```

A.4 Sample vtran2_run.com Diagnostic File

```
command file          = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN_CRA1_R1.CMD
budget file           = [.BUD_FILES.R1]D01R02PR1.OUT
(binary) velocity transfer file = [.TRN_FILES.R1]NF2K_CRA1_R1_F001_PM.TRN
diagnostic/debug file = [.DBG_FILES.R1]vtran_CRA1_R1_F001_PM.DBG
(ascii) velocity output file = None
title                 = CRA 1 (all vectors and replicates)
format                = (448e16.8)
iscrn                 = 0
ncolmf                = 448
nrowmf                = 614
jshftx                = 172
ishfty                = 391
ncx                   = 150
ncy                   = 108
Using input format ( 1) = (448e16.8)
VTRAN >> Reading budget file
VTRAN >> Processing velocities
VTRAN >> Writing velocity transfer file
VTRAN >> Cleaning up
VTRAN >> Normal Completion
```

A.5 vtran2 Verification

The `vtran2` utility code was verified using two test cases. Case 1 demonstrates the conversion of volumetric flux to Darcy velocities, the sign change of the y-direction velocities and the inclusion of ghost nodes. Case 2 demonstrates that the indexing selects the correct subregion.

Both test cases use the mesh layout shown in Figure 8. The volume fluxes are specified on the 10×15 cell mesh. The 4×3 cell subregion outlined in red represents the transport domain. The dashed lines indicate the ghost nodes. We run `vtran2` such that it writes the output in both ASCII and binary format, so we can visually inspect the ASCII file to verify the results.

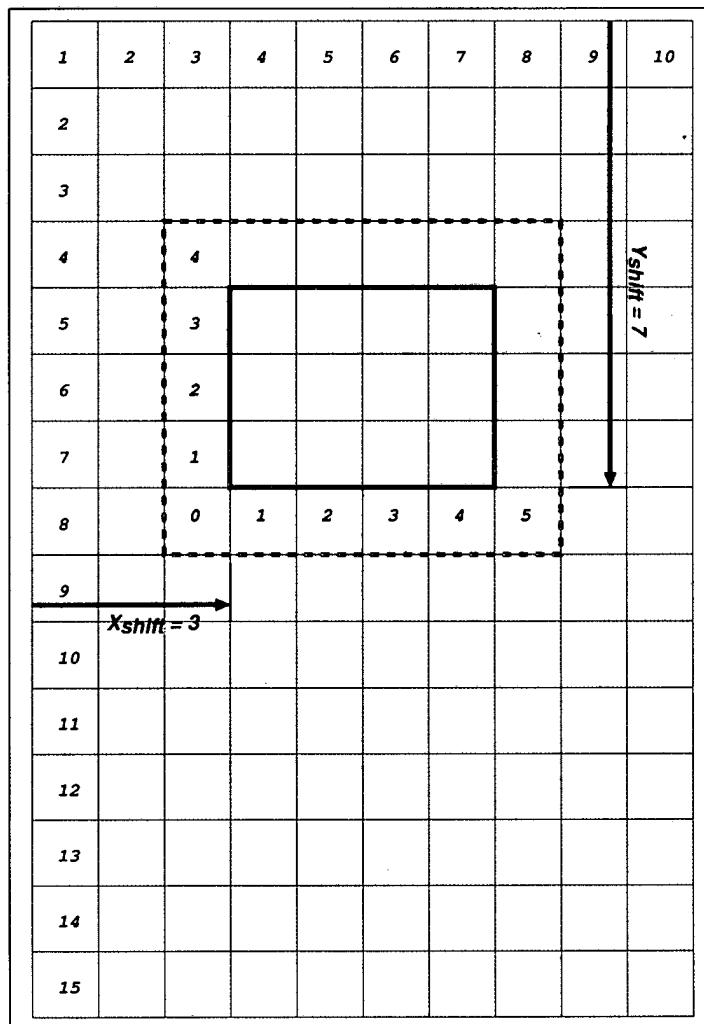


Figure 8: Mesh for `vtran2` Verification

A.5.1 vtran2 Verification Test Case 1

In this test we use a uniform volume flux ($Q_x = Q_y = 1$), and choose $dx = 1$, and $dy = dz = 2$, in the `vtran2` command file such that $A_x = 4$ and $A_y = 2$. Thus, for the transport mesh, we will have $u = 0.25$ and $v = 0.5$ for all cell faces except for the left and bottom boundaries. $u = 0$ at the left boundary and $v = 0$ at the bottom because the respective velocity at these faces is undefined in the `secotp2d` convention.

First we generate a uniform volume flux field ($Q_x = Q_y = 1$) on the 10×15 cell mesh with the Fortran code `vgen1.f`

vgen1.f

```
PROGRAM vgen1
  PARAMETER( ncol=10, nrow=15)
  DOUBLE PRECISION vx(ncol,nrow), vy(ncol,nrow)
  INTEGER iunout
  DO j=1,nrow
    DO i=1,ncol
      count = count+1
      vx(i,j) = 1.d0
      vy(i,j) = 1.d0
    END DO
  END DO
  iunout = 11
  irecln = 100*ncol
  OPEN(iunout, file='vtran2_test_1.bud',
+    status='unknown',form='formatted',
+    access='sequential',recl=irecln, iostat=ierr)
  IF ( ierr .ne. 0 ) THEN
    WRITE(*,*) 'ierr = ',ierr
    STOP
  ENDDIF
  DO j=1,nrow
    WRITE(iunout,150) (vx(i,j), i=1,ncol)
  END DO
  WRITE(iunout,*)
  DO j=1,nrow
    WRITE(iunout,150) (vy(i,j), i=1,ncol)
  END DO
150 FORMAT(500e16.8)
  CLOSE(iunout)
  STOP
END
```

which produces the output file `vtran2_test_1.bud`:

[illegible]

vtran_2_test_1.cmd

on this file using the `vtran2_test_1.com` script

vtran_2_test_1.com

```
$? Vtranz2 test_1
$
$ write sys$output " "
$ write sys$output "-----"
$ write sys$output "| Vtranz2.test_1          "
$ write sys$output "-----"
$ write sys$output " "
$
$
$
$ cmd_file = "vtranz2.test_1.cmd"
$ bud_file = "vtranz2.test_1.bud"
$ trn_file = "vtranz2.test_1.trn"
$ dbg_file = "vtranz2.test_1.dbg"
$ vel_file = "vtranz2.test_1.vel"
$
$
vtranz2_exe := "$spawork:[shared.jffkanne.codes.veltrn.test2]vtranz2.exe"
vtranz2_exe 'cmd_file' 'bud_file' 'trn_file' 'dbg_file' 'vel_file'
$
```

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vtran_2_test_1.vel

```
  4      3      0.0000000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00
0.0000000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00
0.0000000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00
0.0000000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00
0.0000000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00      0.2500000E+00
0.0000000E+00      0.0000000E+00      0.0000000E+00      0.0000000E+00      0.0000000E+00      0.0000000E+00
-0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00
-0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00
-0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00
-0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00
-0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00      -0.5000000E+00
```

vtran_2_test_1.dbg

```
command file          = VTRAN2_TEST_1.CMD
budget file           = VTRAN2_TEST_1.BUD
(binary) velocity transfer file = VTRAN2_TEST_1.TRN
diagnostic/debug file = VTRAN2_TEST_1.DBG
(ascii) velocity output file = VTRAN2_TEST_1.VEL
author   = Joseph F. Kanney
date     = 2003.09.24
title    = vtran2 test 1
format   = (448e16.8)
iscrn    = 0
ncolmf   = 10
nrowmf   = 15
jshftx   = 3
ishfty   = 7
ncx      = 4
ncy      = 3
dx       = 0.1000E+01
dy       = 0.2000E+01
dz       = 0.2000E+01
Using input format ( 1 ) = (448e16.8)
VTRAN >> Reading budget file
VTRAN >> Processing velocities
VTRAN >> Writing velocity transfer file
VTRAN >> Writing ascii velocity output file
VTRAN >> Cleaning up
VTRAN >> Normal Completion
```

We note that u and v are 0.25 and -0.5 as expected. We also note that the 4×3 transport domain has been appropriately padded with ghost cells to make a 6×5 array for each velocity component.

A.5.2 vtran2 Verification Test Case 2

In this test we generate a synthetic volume flux field on the 10×15 such that the modulus of the velocity component equals the row number and the fractional part equals the column number. Thus the cell number is embedded in the value of the flux component. We then specify $dx = dy = dz = 1$ in the `vtran2` command file. In this way, we can visually inspect the velocity file to verify that the correct row and column indices were extracted.

First we generate the volume flux field on the 10×15 cell mesh with the Fortran code `vgen2.f`

vgen2.f

```
PROGRAM vgen2
  PARAMETER( ncol=10, nrow=15)
  DOUBLE PRECISION vx(ncol,nrow), vy(ncol,nrow)
  *
  INTEGER iunout
  jcount = 0
  DO j=1,nrow
    jcount=jcount+1
    icount=0
    DO i=1,ncol
      icount = icount+1
      vx(i,j) = jcount + 0.01*icount
      vy(i,j) = jcount + 0.01*icount
    END DO
  END DO

  iunout = 11
  irecln = 100*ncol
  OPEN(iunout, file='vtran2_test_2.bud',
  +   status='unknown',form='formatted',
  +   access='sequential',recl=irecln, iostat=ierr)

  IF ( ierr .ne. 0 ) THEN
    WRITE(*,*) 'ierr = ',ierr
    STOP
  ENDIF

  DO j=1,nrow
    WRITE(iunout,150) (vx(i,j), i=1,ncol)
  END DO

  WRITE(iunout,*)

  DO j=1,nrow
    WRITE(iunout,150) (vy(i,j), i=1,ncol)
  END DO

  150 FORMAT(500e16.8)

  CLOSE(iunout)

  STOP
  END
```

which produces the file `vtran2_test_2.bud`,

vtran_2.test_2.bud

```
0.10100000E+01 0.10200000E+01 0.10300000E+01 0.10400000E+01 0.10500000E+01 0.10599999E+01 0.10700001E+01 0.10800000E+01 0.10900000E+01 0.11000000E+01
0.20100000E+01 0.20200000E+01 0.20300000E+01 0.20400000E+01 0.20500000E+01 0.20599999E+01 0.20699999E+01 0.20799999E+01 0.20899999E+01 0.20999999E+01
0.30100000E+01 0.30200000E+01 0.30300000E+01 0.30400000E+01 0.30500000E+01 0.30599999E+01 0.30699999E+01 0.30799999E+01 0.30899999E+01 0.30999999E+01
0.40100000E+01 0.40200000E+01 0.40300000E+01 0.40400000E+01 0.40500000E+01 0.40599999E+01 0.40699999E+01 0.40799999E+01 0.40899999E+01 0.40999999E+01
0.50100000E+01 0.50200000E+01 0.50300000E+01 0.50400000E+01 0.50500000E+01 0.50599999E+01 0.50699999E+01 0.50799999E+01 0.50899999E+01 0.50999999E+01
0.60100000E+01 0.60200000E+01 0.60300000E+01 0.60400000E+01 0.60500000E+01 0.60599999E+01 0.60699999E+01 0.60799999E+01 0.60899999E+01 0.60999999E+01
0.70100000E+01 0.70200000E+01 0.70300000E+01 0.70400000E+01 0.70500000E+01 0.70599999E+01 0.70699999E+01 0.70799999E+01 0.70899999E+01 0.70999999E+01
0.80100000E+01 0.80200000E+01 0.80299999E+01 0.80400000E+01 0.80500000E+01 0.80599999E+01 0.80699999E+01 0.80799999E+01 0.80899999E+01 0.81000000E+01
0.90100000E+01 0.90200000E+01 0.90299999E+01 0.90400000E+01 0.90500000E+01 0.90599999E+01 0.90699999E+01 0.90799999E+01 0.90899999E+01 0.91000000E+01
0.10010000E+02 0.10020000E+02 0.10030000E+02 0.10040000E+02 0.10050000E+02 0.10059999E+02 0.10069999E+02 0.10079999E+02 0.10089999E+02 0.10099999E+02
0.11010000E+02 0.11020000E+02 0.11030000E+02 0.11040000E+02 0.11050000E+02 0.11059999E+02 0.11069999E+02 0.11079999E+02 0.11089999E+02 0.11099999E+02
0.12010000E+02 0.12020000E+02 0.12030000E+02 0.12040000E+02 0.12050000E+02 0.12059999E+02 0.12069999E+02 0.12079999E+02 0.12089999E+02 0.12099999E+02
0.13010000E+02 0.13020000E+02 0.13030000E+02 0.13040000E+02 0.13050000E+02 0.13059999E+02 0.13069999E+02 0.13079999E+02 0.13089999E+02 0.13099999E+02
0.14010000E+02 0.14020000E+02 0.14030000E+02 0.14040000E+02 0.14050000E+02 0.14059999E+02 0.14069999E+02 0.14079999E+02 0.14089999E+02 0.14099999E+02
0.15010000E+02 0.15020000E+02 0.15030000E+02 0.15040000E+02 0.15050000E+02 0.15059999E+02 0.15069999E+02 0.15079999E+02 0.15089999E+02 0.15099999E+02
0.10100000E+01 0.10200000E+01 0.10300000E+01 0.10400000E+01 0.10500000E+01 0.10599999E+01 0.10700001E+01 0.10800000E+01 0.10900000E+01 0.11000000E+01
0.20100000E+01 0.20200000E+01 0.20300000E+01 0.20400000E+01 0.20500000E+01 0.20599999E+01 0.20699999E+01 0.20799999E+01 0.20899999E+01 0.20999999E+01
0.30100000E+01 0.30200000E+01 0.30300000E+01 0.30400000E+01 0.30500000E+01 0.30599999E+01 0.30699999E+01 0.30799999E+01 0.30899999E+01 0.30999999E+01
0.40100000E+01 0.40200000E+01 0.40300000E+01 0.40400000E+01 0.40500000E+01 0.40599999E+01 0.40699999E+01 0.40799999E+01 0.40899999E+01 0.40999999E+01
0.50100000E+01 0.50200000E+01 0.50300000E+01 0.50400000E+01 0.50500000E+01 0.50599999E+01 0.50699999E+01 0.50799999E+01 0.50899999E+01 0.50999999E+01
0.60100000E+01 0.60200000E+01 0.60300000E+01 0.60400000E+01 0.60500000E+01 0.60599999E+01 0.60699999E+01 0.60799999E+01 0.60899999E+01 0.60999999E+01
0.70100000E+01 0.70200000E+01 0.70300000E+01 0.70400000E+01 0.70500000E+01 0.70599999E+01 0.70699999E+01 0.70799999E+01 0.70899999E+01 0.70999999E+01
0.80100000E+01 0.80200000E+01 0.80299999E+01 0.80400000E+01 0.80500000E+01 0.80599999E+01 0.80699999E+01 0.80799999E+01 0.80899999E+01 0.81000000E+01
0.90100000E+01 0.90200000E+01 0.90299999E+01 0.90400000E+01 0.90500000E+01 0.90599999E+01 0.90699999E+01 0.90799999E+01 0.90899999E+01 0.91000000E+01
0.10010000E+02 0.10020000E+02 0.10030000E+02 0.10040000E+02 0.10050000E+02 0.10059999E+02 0.10069999E+02 0.10079999E+02 0.10089999E+02 0.10099999E+02
0.11010000E+02 0.11020000E+02 0.11030000E+02 0.11040000E+02 0.11050000E+02 0.11059999E+02 0.11069999E+02 0.11079999E+02 0.11089999E+02 0.11099999E+02
0.12010000E+02 0.12020000E+02 0.12030000E+02 0.12040000E+02 0.12050000E+02 0.12059999E+02 0.12069999E+02 0.12079999E+02 0.12089999E+02 0.12099999E+02
0.13010000E+02 0.13020000E+02 0.13030000E+02 0.13040000E+02 0.13050000E+02 0.13059999E+02 0.13069999E+02 0.13079999E+02 0.13089999E+02 0.13099999E+02
0.14010000E+02 0.14020000E+02 0.14030000E+02 0.14040000E+02 0.14050000E+02 0.14059999E+02 0.14069999E+02 0.14079999E+02 0.14089999E+02 0.14099999E+02
0.15010000E+02 0.15020000E+02 0.15030000E+02 0.15040000E+02 0.15050000E+02 0.15059999E+02 0.15069999E+02 0.15079999E+02 0.15089999E+02 0.15099999E+02
```

Now run vtran2 with the command file vtran2.test_2.cmd

vtran_2.test_2.cmd

```
* author
Joseph F. Kanney
* date
2003.09.24
* title
vtran2 test 2
* input format type
(448e16.8)
* iscrn > 0 will print to screen, otherwise to dbg file
0
* ncol nrow
10 15
* jshftz ishfty ncz ncy
3 7 4 3
* dx dy dz (3e10.3)
1.000E+00 1.000E+00 1.000E+00
```

on this file using the vtran2.test_2.com script

vtran_2.test_2.com

```
$! Vtran2 test_2
$
$ write sys$output " "
$ write sys$output "-----"
$ write sys$output "| Vtran2.test_2 "
$ write sys$output "-----"
$ write sys$output " "
$
$
$ cmd_file = "vtran2.test_2.cmd"
$ bud_file = "vtran2.test_2.bud"
$ trn_file = "vtran2.test_2.trn"
$ dbg_file = "vtran2.test_2.dbg"
$ vel_file = "vtran2.test_2.vel"
$
$ vtran2_exe := "$pawork:[shared.jfkanne.codes.veltrn.test2]vtran2.exe"
$ vtran2_exe 'cmd_file' 'bud_file' 'trn_file' 'dbg_file' 'vel_file'
$
```

which produces the following ASCII velocity and diagnostic files

vtran_2.test.2.vel

```
4      3      0.0000000E+00
0.0000000E+00 0.8029999E+01 0.8040000E+01 0.8050000E+01 0.8060000E+01 0.8069999E+01
0.0000000E+00 0.7030000E+01 0.7040000E+01 0.7050000E+01 0.7059999E+01 0.7070000E+01
0.0000000E+00 0.6030000E+01 0.6040000E+01 0.6050000E+01 0.6059999E+01 0.6070000E+01
0.0000000E+00 0.5030000E+01 0.5040000E+01 0.5050000E+01 0.5059999E+01 0.5070000E+01
0.0000000E+00 0.4030000E+01 0.4040000E+01 0.4050000E+01 0.4059999E+01 0.4070000E+01
0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00
-0.7030000E+01 -0.7040000E+01 -0.7050000E+01 -0.7059999E+01 -0.7070000E+01 -0.7079999E+01
-0.6030000E+01 -0.6040000E+01 -0.6050000E+01 -0.6059999E+01 -0.6070000E+01 -0.6079999E+01
-0.5030000E+01 -0.5040000E+01 -0.5050000E+01 -0.5059999E+01 -0.5070000E+01 -0.5079999E+01
-0.4030000E+01 -0.4040000E+01 -0.4050000E+01 -0.4059999E+01 -0.4070000E+01 -0.4079999E+01
```

vtran_2.test.2.dbg

```
command file      = VTRAN2_TEST_2.CMD
budget file      = VTRAN2_TEST_2.BUD
(binary) velocity transfer file = VTRAN2_TEST_2.TRN
diagnostic/debug file = VTRAN2_TEST_2.DBG
(ascii) velocity output file = VTRAN2_TEST_2.VEL
author   = Joseph F. Kanney
date    = 2003.09.24
title   = vtran2 test 2
format  = (448e16.8)
iscrn   = 0
ncolmf  = 10
nrowmf  = 15
jshftx  = 3
ishfty  = 7
ncx     = 4
ncy     = 3
dx      = 0.1000E+01
dy      = 0.1000E+01
dz      = 0.1000E+01
Using input format ( 1 ) = (448e16.8)
VTRAN >> Reading budget file
VTRAN >> Processing velocities
VTRAN >> Writing velocity transfer file
VTRAN >> Writing ascii velocity output file
VTRAN >> Cleaning up
VTRAN >> Normal Completion
```

We note from the velocity component values that the correct translation of indices between the two meshes has been effected.

Appendix B: Flow Field Extraction Input and Log Files

B.1 Replicate 1

vtran2_cra1_r1.cmd

```
* author
Joseph F. Kanney
* date
2003 09 24
* title
CRA1_R1 Vtran2 command file
* input format type
(448e16.8)
* iscrn > 0 will print to screen, otherwise to dbg file
0
* ncol nrow
448 614
* jshftz ishfty ncz ncy
172 391 150 108
* dx dy dz
50 50 4
```

vtran2_run_cra1_r1.inp

```
! Input file for the vtran_run script
! Associates mf2k output files with flow field
!
! Created by Joseph Kanney
! Sept 15, 2003
D01R02FR1 F001_FM
D01R02PR1 F001_FM
D01R04FR1 F002_FM
D01R04PR1 F002_FM
D01R07FR1 F003_FM
D01R07PR1 F003_FM
D01R10FR1 F004_FM
D01R10PR1 F004_FM
D02R02FR1 F005_FM
D02R02PR1 F005_FM
D03R01FR1 F006_FM
D03R01PR1 F006_FM
D03R03FR1 F007_FM
D03R03PR1 F007_FM
D03R06FR1 F008_FM
D03R06PR1 F008_FM
D03R07FR1 F009_FM
D03R07PR1 F009_FM
D03R08FR1 F010_FM
D03R08PR1 F010_FM
D03R09FR1 F011_FM
D03R09PR1 F011_FM
D04R01FR1 F012_FM
D04R01PR1 F012_FM
D04R02FR1 F013_FM
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D04R04FR1 F015_FM
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D04R05FR1 F016_FM
D04R05PR1 F016_FM
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vtran2_run_cra1_r1.log

Starting Time Stamp: 24-SEP-2003 15:13:12.16

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budget file dir  = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.BUD_FILES.R1]
trn file dir     = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.TRN_FILES.R1]
dbg file dir     = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.DBG_FILES.R1]
vtran2_run input file = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_RUN_CRA1_R1.IMP
vtran2_run log file   = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_RUN_CRA1_R1.LOG
vtran2_cmd_file      = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_CRA1_R1.CMD
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Opening vtran2_run input file

mf2k budget file mf2k velocity transfer file

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D01R07FR1.OUT	MF2K_CRA1_R1_F003_FM.TRN
D01R07PR1.OUT	MF2K_CRA1_R1_F003_PM.TRN
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Closing vtran2_run input file

Ending Time Stamp: 24-SEP-2003 15:18:44.86

B.2 Replicate 2

vtran2_cra1_r2.cmd

```
* author
Joseph F. Kanney
* date
2003 09 26
* title
CRA1_R2 Vtran2 command file
* input format type
(448e16.8)
* iscrn > 0 will print to screen, otherwise to dbg file
0
* ncol nrow
448 614
* jshftx ishfty ncx ncy
172 391 160 108
* dx dy dz
50 50 4
```

vtran2_run_cra1_r2.inp

```
! Input file for the vtran_run script
! Associates mf2k output files with flow field
! CRA1 R2
! Created by Joseph Kanney
! Sept 26, 2003
D01R02FR2 F001_FM
D01R02FR2 F001_FM
D01R04FR2 F002_FM
D01R04FR2 F002_FM
D01R07FR2 F003_FM
D01R07FR2 F003_FM
D01R10FR2 F004_FM
D01R10FR2 F004_FM
D02R02FR2 F005_FM
D02R02FR2 F005_FM
D03R01FR2 F006_FM
D03R01FR2 F006_FM
D03R03FR2 F007_FM
D03R03FR2 F007_FM
D03R06FR2 F008_FM
D03R06FR2 F008_FM
D03R07FR2 F009_FM
D03R07FR2 F009_FM
D03R08FR2 F010_FM
D03R08FR2 F010_FM
D03R09FR2 F011_FM
D03R09FR2 F011_FM
D04R01FR2 F012_FM
D04R01FR2 F012_FM
D04R02FR2 F013_FM
D04R02FR2 F013_FM
D04R03FR2 F014_FM
D04R03FR2 F014_FM
D04R04FR2 F015_FM
D04R04FR2 F015_FM
D04R05FR2 F016_FM
D04R05FR2 F016_FM
D04R06FR2 F017_FM
D04R06FR2 F017_FM
D04R07FR2 F018_FM
D04R07FR2 F018_FM
D04R08FR2 F019_FM
D04R08FR2 F019_FM
D04R10FR2 F020_FM
D04R10FR2 F020_FM
D05R03FR2 F021_FM
D05R03FR2 F021_FM
D05R07FR2 F022_FM
D05R07FR2 F022_FM
D06R02FR2 F023_FM
D06R02FR2 F023_FM
D06R03FR2 F024_FM
D06R03FR2 F024_FM
D06R04FR2 F025_FM
D06R04FR2 F025_FM
D06R05FR2 F026_FM
D06R05FR2 F026_FM
D06R06FR2 F027_FM
D06R06FR2 F027_FM
D06R07FR2 F028_FM
D06R07FR2 F028_FM
D06R10FR2 F029_FM
D06R10FR2 F029_FM
D07R01FR2 F030_FM
```

D07R01PR2 F030_PM
D07R02FR2 F031_FM
D07R02PR2 F031_PM
D07R05FR2 F032_FM
D07R05PR2 F032_PM
D07R06FR2 F033_FM
D07R06PR2 F033_PM
D07R07FR2 F034_FM
D07R07PR2 F034_PM
D07R08FR2 F035_FM
D07R08PR2 F035_PM
D07R09FR2 F036_FM
D07R09PR2 F036_PM
D07R10FR2 F037_FM
D07R10PR2 F037_PM
D08R01FR2 F038_FM
D08R01PR2 F038_PM
D08R02FR2 F039_FM
D08R02PR2 F039_PM
D08R03FR2 F040_FM
D08R03PR2 F040_PM
D08R04FR2 F041_FM
D08R04PR2 F041_PM
D08R05FR2 F042_FM
D08R05PR2 F042_PM
D08R06FR2 F043_FM
D08R06PR2 F043_PM
D08R07FR2 F044_FM
D08R07PR2 F044_PM
D09R02FR2 F045_FM
D09R02PR2 F045_PM
D09R03FR2 F046_FM
D09R03PR2 F046_PM
D09R04FR2 F047_FM
D09R04PR2 F047_PM
D09R05FR2 F048_FM
D09R05PR2 F048_PM
D09R06FR2 F049_FM
D09R06PR2 F049_PM
D09R07FR2 F050_FM
D09R07PR2 F050_PM
D09R08FR2 F051_FM
D09R08PR2 F051_PM
D09R09FR2 F052_FM
D09R09PR2 F052_PM
D09R10FR2 F053_FM
D09R10PR2 F053_PM
D10R02FR2 F054_FM
D10R02PR2 F054_PM
D10R03FR2 F055_FM
D10R03PR2 F055_PM
D10R04FR2 F056_FM
D10R04PR2 F056_PM
D10R06FR2 F057_FM
D10R06PR2 F057_PM
D10R07FR2 F058_FM
D10R07PR2 F058_PM
D10R08FR2 F059_FM
D10R08PR2 F059_PM
D10R09FR2 F060_FM
D10R09PR2 F060_PM
D10R10FR2 F061_FM
D10R10PR2 F061_PM
D11R01FR2 F062_FM
D11R01PR2 F062_PM
D11R02FR2 F063_FM
D11R02PR2 F063_PM
D11R06FR2 F064_FM
D11R06PR2 F064_PM
D11R07FR2 F065_FM
D11R07PR2 F065_PM
D11R08FR2 F066_FM
D11R08PR2 F066_PM
D11R09FR2 F067_FM
D11R09PR2 F067_PM
D11R10FR2 F068_FM
D11R10PR2 F068_PM
D12R01FR2 F069_FM
D12R01PR2 F069_PM
D12R02FR2 F070_FM
D12R02PR2 F070_PM
D12R03FR2 F071_FM
D12R03PR2 F071_PM
D12R05FR2 F072_FM
D12R05PR2 F072_PM
D12R06FR2 F073_FM
D12R06PR2 F073_PM
D12R07FR2 F074_FM
D12R07PR2 F074_PM
D12R08FR2 F075_FM
D12R08PR2 F075_PM

D12R09FR2 F076_FM
D12R09PR2 F076_PM
D13R01FR2 F077_FM
D13R01PR2 F077_PM
D13R02FR2 F078_FM
D13R02PR2 F078_PM
D13R03FR2 F079_FM
D13R03PR2 F079_PM
D13R05FR2 F080_FM
D13R05PR2 F080_PM
D13R06FR2 F081_FM
D13R06PR2 F081_PM
D13R07FR2 F082_FM
D13R07PR2 F082_PM
D13R08FR2 F083_FM
D13R08PR2 F083_PM
D13R09FR2 F084_FM
D13R09PR2 F084_PM
D21R01FR2 F085_FM
D21R01PR2 F085_PM
D21R02FR2 F086_FM
D21R02PR2 F086_PM
D21R03FR2 F087_FM
D21R03PR2 F087_PM
D21R04FR2 F088_FM
D21R04PR2 F088_PM
D21R05FR2 F089_FM
D21R05PR2 F089_PM
D21R06FR2 F090_FM
D21R06PR2 F090_PM
D21R07FR2 F091_FM
D21R07PR2 F091_PM
D21R10FR2 F092_FM
D21R10PR2 F092_PM
D22R02FR2 F093_FM
D22R02PR2 F093_PM
D22R03FR2 F094_FM
D22R03PR2 F094_PM
D22R04FR2 F095_FM
D22R04PR2 F095_PM
D22R05FR2 F096_FM
D22R05PR2 F096_PM
D22R07FR2 F097_FM
D22R07PR2 F097_PM
D22R08FR2 F098_FM
D22R08PR2 F098_PM
D22R09FR2 F099_FM
D22R09PR2 F099_PM
D22R10FR2 F100_FM
D22R10PR2 F100_PM

vtran2_run_cra1_r2.log

Starting Time Stamp: 26-SEP-2003 13:13:49.28

```
working dir      = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]
budget file dir  = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.BUD_FILES.R2]
trn file dir     = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.TRN_FILES.R2]
dbg file dir     = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.DBG_FILES.R2]
vtran2_run input file = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_RUN_CRA1_R2.INP
vtran2_run log file   = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_RUN_CRA1_R2.LOG
vtran2_cnd file      = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_CRA1_R2.CMD
```

Opening vtran2_run input file

mf2k budget file mf2k velocity transfer file

D01R02FR2.OUT	MF2K_CRA1_R2_F001_FM.TRN
D01R02PR2.OUT	MF2K_CRA1_R2_F001_PM.TRN
D01R04FR2.OUT	MF2K_CRA1_R2_F002_FM.TRN
D01R04PR2.OUT	MF2K_CRA1_R2_F002_PM.TRN
D01R07FR2.OUT	MF2K_CRA1_R2_F003_FM.TRN
D01R07PR2.OUT	MF2K_CRA1_R2_F003_PM.TRN
D01R10FR2.OUT	MF2K_CRA1_R2_F004_FM.TRN
D01R10PR2.OUT	MF2K_CRA1_R2_F004_PM.TRN
D02R02FR2.OUT	MF2K_CRA1_R2_F005_FM.TRN
D02R02PR2.OUT	MF2K_CRA1_R2_F005_PM.TRN
D03R01FR2.OUT	MF2K_CRA1_R2_F006_FM.TRN
D03R01PR2.OUT	MF2K_CRA1_R2_F006_PM.TRN
D03R03FR2.OUT	MF2K_CRA1_R2_F007_FM.TRN
D03R03PR2.OUT	MF2K_CRA1_R2_F007_PM.TRN
D03R06FR2.OUT	MF2K_CRA1_R2_F008_FM.TRN
D03R06PR2.OUT	MF2K_CRA1_R2_F008_PM.TRN
D03R07FR2.OUT	MF2K_CRA1_R2_F009_FM.TRN
D03R07PR2.OUT	MF2K_CRA1_R2_F009_PM.TRN
D03R08FR2.OUT	MF2K_CRA1_R2_F010_FM.TRN
D03R08PR2.OUT	MF2K_CRA1_R2_F010_PM.TRN
D03R09FR2.OUT	MF2K_CRA1_R2_F011_FM.TRN
D03R09PR2.OUT	MF2K_CRA1_R2_F011_PM.TRN
D04R01FR2.OUT	MF2K_CRA1_R2_F012_FM.TRN
D04R01PR2.OUT	MF2K_CRA1_R2_F012_PM.TRN
D04R02FR2.OUT	MF2K_CRA1_R2_F013_FM.TRN
D04R02PR2.OUT	MF2K_CRA1_R2_F013_PM.TRN
D04R03FR2.OUT	MF2K_CRA1_R2_F014_FM.TRN
D04R03PR2.OUT	MF2K_CRA1_R2_F014_PM.TRN
D04R04FR2.OUT	MF2K_CRA1_R2_F015_FM.TRN
D04R04PR2.OUT	MF2K_CRA1_R2_F015_PM.TRN
D04R05FR2.OUT	MF2K_CRA1_R2_F016_FM.TRN
D04R05PR2.OUT	MF2K_CRA1_R2_F016_PM.TRN
D04R06FR2.OUT	MF2K_CRA1_R2_F017_FM.TRN
D04R06PR2.OUT	MF2K_CRA1_R2_F017_PM.TRN
D04R07FR2.OUT	MF2K_CRA1_R2_F018_FM.TRN
D04R07PR2.OUT	MF2K_CRA1_R2_F018_PM.TRN
D04R08FR2.OUT	MF2K_CRA1_R2_F019_FM.TRN
D04R08PR2.OUT	MF2K_CRA1_R2_F019_PM.TRN
D04R10FR2.OUT	MF2K_CRA1_R2_F020_FM.TRN
D04R10PR2.OUT	MF2K_CRA1_R2_F020_PM.TRN
D05R03FR2.OUT	MF2K_CRA1_R2_F021_FM.TRN
D05R03PR2.OUT	MF2K_CRA1_R2_F021_PM.TRN
D05R07FR2.OUT	MF2K_CRA1_R2_F022_FM.TRN
D05R07PR2.OUT	MF2K_CRA1_R2_F022_PM.TRN
D06R02FR2.OUT	MF2K_CRA1_R2_F023_FM.TRN
D06R02PR2.OUT	MF2K_CRA1_R2_F023_PM.TRN
D06R03FR2.OUT	MF2K_CRA1_R2_F024_FM.TRN
D06R03PR2.OUT	MF2K_CRA1_R2_F024_PM.TRN
D06R04FR2.OUT	MF2K_CRA1_R2_F025_FM.TRN
D06R04PR2.OUT	MF2K_CRA1_R2_F025_PM.TRN
D06R05FR2.OUT	MF2K_CRA1_R2_F026_FM.TRN
D06R05PR2.OUT	MF2K_CRA1_R2_F026_PM.TRN
D06R06FR2.OUT	MF2K_CRA1_R2_F027_FM.TRN
D06R06PR2.OUT	MF2K_CRA1_R2_F027_PM.TRN
D06R07FR2.OUT	MF2K_CRA1_R2_F028_FM.TRN
D06R07PR2.OUT	MF2K_CRA1_R2_F028_PM.TRN
D06R10FR2.OUT	MF2K_CRA1_R2_F029_FM.TRN
D06R10PR2.OUT	MF2K_CRA1_R2_F029_PM.TRN
D07R01FR2.OUT	MF2K_CRA1_R2_F030_FM.TRN
D07R01PR2.OUT	MF2K_CRA1_R2_F030_PM.TRN
D07R02FR2.OUT	MF2K_CRA1_R2_F031_FM.TRN
D07R02PR2.OUT	MF2K_CRA1_R2_F031_PM.TRN
D07R05FR2.OUT	MF2K_CRA1_R2_F032_FM.TRN
D07R05PR2.OUT	MF2K_CRA1_R2_F032_PM.TRN
D07R06FR2.OUT	MF2K_CRA1_R2_F033_FM.TRN
D07R06PR2.OUT	MF2K_CRA1_R2_F033_PM.TRN
D07R07FR2.OUT	MF2K_CRA1_R2_F034_FM.TRN
D07R07PR2.OUT	MF2K_CRA1_R2_F034_PM.TRN
D07R08FR2.OUT	MF2K_CRA1_R2_F035_FM.TRN
D07R08PR2.OUT	MF2K_CRA1_R2_F035_PM.TRN
D07R09FR2.OUT	MF2K_CRA1_R2_F036_FM.TRN
D07R09PR2.OUT	MF2K_CRA1_R2_F036_PM.TRN
D07R10FR2.OUT	MF2K_CRA1_R2_F037_FM.TRN
D07R10PR2.OUT	MF2K_CRA1_R2_F037_PM.TRN

D08R01FR2.OUT	MF2K_CRA1_R2_F038_FM.TRN
D08R01PR2.OUT	MF2K_CRA1_R2_F038_PM.TRN
D08R02FR2.OUT	MF2K_CRA1_R2_F039_FM.TRN
D08R02PR2.OUT	MF2K_CRA1_R2_F039_PM.TRN
D08R03FR2.OUT	MF2K_CRA1_R2_F040_FM.TRN
D08R03PR2.OUT	MF2K_CRA1_R2_F040_PM.TRN
D08R04FR2.OUT	MF2K_CRA1_R2_F041_FM.TRN
D08R04PR2.OUT	MF2K_CRA1_R2_F041_PM.TRN
D08R05FR2.OUT	MF2K_CRA1_R2_F042_FM.TRN
D08R05PR2.OUT	MF2K_CRA1_R2_F042_PM.TRN
D08R06FR2.OUT	MF2K_CRA1_R2_F043_FM.TRN
D08R06PR2.OUT	MF2K_CRA1_R2_F043_PM.TRN
D08R07FR2.OUT	MF2K_CRA1_R2_F044_FM.TRN
D08R07PR2.OUT	MF2K_CRA1_R2_F044_PM.TRN
D08R02FR2.OUT	MF2K_CRA1_R2_F045_FM.TRN
D08R02PR2.OUT	MF2K_CRA1_R2_F045_PM.TRN
D08R03FR2.OUT	MF2K_CRA1_R2_F046_FM.TRN
D08R03PR2.OUT	MF2K_CRA1_R2_F046_PM.TRN
D08R04FR2.OUT	MF2K_CRA1_R2_F047_FM.TRN
D08R04PR2.OUT	MF2K_CRA1_R2_F047_PM.TRN
D08R05FR2.OUT	MF2K_CRA1_R2_F048_FM.TRN
D08R05PR2.OUT	MF2K_CRA1_R2_F048_PM.TRN
D08R06FR2.OUT	MF2K_CRA1_R2_F049_FM.TRN
D08R06PR2.OUT	MF2K_CRA1_R2_F049_PM.TRN
D08R07FR2.OUT	MF2K_CRA1_R2_F050_FM.TRN
D08R07PR2.OUT	MF2K_CRA1_R2_F050_PM.TRN
D08R08FR2.OUT	MF2K_CRA1_R2_F051_FM.TRN
D08R08PR2.OUT	MF2K_CRA1_R2_F051_PM.TRN
D08R09FR2.OUT	MF2K_CRA1_R2_F052_FM.TRN
D08R09PR2.OUT	MF2K_CRA1_R2_F052_PM.TRN
D08R10FR2.OUT	MF2K_CRA1_R2_F053_FM.TRN
D08R10PR2.OUT	MF2K_CRA1_R2_F053_PM.TRN
D10R02FR2.OUT	MF2K_CRA1_R2_F054_FM.TRN
D10R02PR2.OUT	MF2K_CRA1_R2_F054_PM.TRN
D10R03FR2.OUT	MF2K_CRA1_R2_F055_FM.TRN
D10R03PR2.OUT	MF2K_CRA1_R2_F055_PM.TRN
D10R04FR2.OUT	MF2K_CRA1_R2_F056_FM.TRN
D10R04PR2.OUT	MF2K_CRA1_R2_F056_PM.TRN
D10R06FR2.OUT	MF2K_CRA1_R2_F057_FM.TRN
D10R06PR2.OUT	MF2K_CRA1_R2_F057_PM.TRN
D10R07FR2.OUT	MF2K_CRA1_R2_F058_FM.TRN
D10R07PR2.OUT	MF2K_CRA1_R2_F058_PM.TRN
D10R08FR2.OUT	MF2K_CRA1_R2_F059_FM.TRN
D10R08PR2.OUT	MF2K_CRA1_R2_F059_PM.TRN
D10R09FR2.OUT	MF2K_CRA1_R2_F060_FM.TRN
D10R09PR2.OUT	MF2K_CRA1_R2_F060_PM.TRN
D10R10FR2.OUT	MF2K_CRA1_R2_F061_FM.TRN
D10R10PR2.OUT	MF2K_CRA1_R2_F061_PM.TRN
D11R01FR2.OUT	MF2K_CRA1_R2_F062_FM.TRN
D11R01PR2.OUT	MF2K_CRA1_R2_F062_PM.TRN
D11R02FR2.OUT	MF2K_CRA1_R2_F063_FM.TRN
D11R02PR2.OUT	MF2K_CRA1_R2_F063_PM.TRN
D11R06FR2.OUT	MF2K_CRA1_R2_F064_FM.TRN
D11R06PR2.OUT	MF2K_CRA1_R2_F064_PM.TRN
D11R07FR2.OUT	MF2K_CRA1_R2_F065_FM.TRN
D11R07PR2.OUT	MF2K_CRA1_R2_F065_PM.TRN
D11R08FR2.OUT	MF2K_CRA1_R2_F066_FM.TRN
D11R08PR2.OUT	MF2K_CRA1_R2_F066_PM.TRN
D11R09FR2.OUT	MF2K_CRA1_R2_F067_FM.TRN
D11R09PR2.OUT	MF2K_CRA1_R2_F067_PM.TRN
D11R10FR2.OUT	MF2K_CRA1_R2_F068_FM.TRN
D11R10PR2.OUT	MF2K_CRA1_R2_F068_PM.TRN
D12R01FR2.OUT	MF2K_CRA1_R2_F069_FM.TRN
D12R01PR2.OUT	MF2K_CRA1_R2_F069_PM.TRN
D12R02FR2.OUT	MF2K_CRA1_R2_F070_FM.TRN
D12R02PR2.OUT	MF2K_CRA1_R2_F070_PM.TRN
D12R03FR2.OUT	MF2K_CRA1_R2_F071_FM.TRN
D12R03PR2.OUT	MF2K_CRA1_R2_F071_PM.TRN
D12R05FR2.OUT	MF2K_CRA1_R2_F072_FM.TRN
D12R05PR2.OUT	MF2K_CRA1_R2_F072_PM.TRN
D12R06FR2.OUT	MF2K_CRA1_R2_F073_FM.TRN
D12R06PR2.OUT	MF2K_CRA1_R2_F073_PM.TRN
D12R07FR2.OUT	MF2K_CRA1_R2_F074_FM.TRN
D12R07PR2.OUT	MF2K_CRA1_R2_F074_PM.TRN
D12R08FR2.OUT	MF2K_CRA1_R2_F075_FM.TRN
D12R08PR2.OUT	MF2K_CRA1_R2_F075_PM.TRN
D12R09FR2.OUT	MF2K_CRA1_R2_F076_FM.TRN
D12R09PR2.OUT	MF2K_CRA1_R2_F076_PM.TRN
D13R01FR2.OUT	MF2K_CRA1_R2_F077_FM.TRN
D13R01PR2.OUT	MF2K_CRA1_R2_F077_PM.TRN
D13R02FR2.OUT	MF2K_CRA1_R2_F078_FM.TRN
D13R02PR2.OUT	MF2K_CRA1_R2_F078_PM.TRN
D13R03FR2.OUT	MF2K_CRA1_R2_F079_FM.TRN
D13R03PR2.OUT	MF2K_CRA1_R2_F079_PM.TRN
D13R05FR2.OUT	MF2K_CRA1_R2_F080_FM.TRN
D13R05PR2.OUT	MF2K_CRA1_R2_F080_PM.TRN
D13R06FR2.OUT	MF2K_CRA1_R2_F081_FM.TRN
D13R06PR2.OUT	MF2K_CRA1_R2_F081_PM.TRN
D13R07FR2.OUT	MF2K_CRA1_R2_F082_FM.TRN
D13R07PR2.OUT	MF2K_CRA1_R2_F082_PM.TRN
D13R08FR2.OUT	MF2K_CRA1_R2_F083_FM.TRN

D13R08PR2.OUT	MF2K_CRA1_R2_F083_PM.TRN
D13R09PR2.OUT	MF2K_CRA1_R2_F084_PM.TRN
D13R09PR2.OUT	MF2K_CRA1_R2_F084_PM.TRN
D21R01FR2.OUT	MF2K_CRA1_R2_F085_PM.TRN
D21R01PR2.OUT	MF2K_CRA1_R2_F085_PM.TRN
D21R02FR2.OUT	MF2K_CRA1_R2_F086_PM.TRN
D21R02PR2.OUT	MF2K_CRA1_R2_F086_PM.TRN
D21R03FR2.OUT	MF2K_CRA1_R2_F087_PM.TRN
D21R03PR2.OUT	MF2K_CRA1_R2_F087_PM.TRN
D21R04FR2.OUT	MF2K_CRA1_R2_F088_PM.TRN
D21R04PR2.OUT	MF2K_CRA1_R2_F088_PM.TRN
D21R05FR2.OUT	MF2K_CRA1_R2_F089_PM.TRN
D21R05PR2.OUT	MF2K_CRA1_R2_F089_PM.TRN
D21R06FR2.OUT	MF2K_CRA1_R2_F090_PM.TRN
D21R06PR2.OUT	MF2K_CRA1_R2_F090_PM.TRN
D21R07FR2.OUT	MF2K_CRA1_R2_F091_PM.TRN
D21R07PR2.OUT	MF2K_CRA1_R2_F091_PM.TRN
D21R10FR2.OUT	MF2K_CRA1_R2_F092_PM.TRN
D21R10PR2.OUT	MF2K_CRA1_R2_F092_PM.TRN
D22R02FR2.OUT	MF2K_CRA1_R2_F093_PM.TRN
D22R02PR2.OUT	MF2K_CRA1_R2_F093_PM.TRN
D22R03FR2.OUT	MF2K_CRA1_R2_F094_PM.TRN
D22R03PR2.OUT	MF2K_CRA1_R2_F094_PM.TRN
D22R04FR2.OUT	MF2K_CRA1_R2_F095_PM.TRN
D22R04PR2.OUT	MF2K_CRA1_R2_F095_PM.TRN
D22R06FR2.OUT	MF2K_CRA1_R2_F096_PM.TRN
D22R06PR2.OUT	MF2K_CRA1_R2_F096_PM.TRN
D22R07FR2.OUT	MF2K_CRA1_R2_F097_PM.TRN
D22R07PR2.OUT	MF2K_CRA1_R2_F097_PM.TRN
D22R08FR2.OUT	MF2K_CRA1_R2_F098_PM.TRN
D22R08PR2.OUT	MF2K_CRA1_R2_F098_PM.TRN
D22R09FR2.OUT	MF2K_CRA1_R2_F099_PM.TRN
D22R09PR2.OUT	MF2K_CRA1_R2_F099_PM.TRN
D22R10FR2.OUT	MF2K_CRA1_R2_F100_PM.TRN
D22R10PR2.OUT	MF2K_CRA1_R2_F100_PM.TRN

Closing vtran2_run input file

Ending Time Stamp: 26-SEP-2003 13:16:27.95

B.3 Replicate 3'

vtran2_cra1_r3.cmd

```
* author
Joseph F. Kanney
* date
2003 09 29
* title
CRA1_R3 Vtran2 command file
* input format type
(448e16.8)
* iscrn > 0 will print to screen, otherwise to dbg file
0
* ncol nrow
448 614
* jshftx ishfty ncx ncy
172 391 150 108
* dx dy dz
50 50 4
```

vtran2_run_cra1_r3.inp

```
! Input file for the vtran_run script
! Associates mf2k output files with flow field
! CRA1 R3
! Created by Joseph Kanney
! Sept 29, 2003
D01R02FR3 F001_FM
D01R02FR3 F001_FM
D01R04FR3 F002_FM
D01R04FR3 F002_FM
D01R07FR3 F003_FM
D01R07FR3 F003_FM
D01R10FR3 F004_FM
D01R10FR3 F004_FM
D02R02FR3 F005_FM
D02R02FR3 F005_FM
D03R01FR3 F006_FM
D03R01FR3 F006_FM
D03R03FR3 F007_FM
D03R03FR3 F007_FM
D03R06FR3 F008_FM
D03R06FR3 F008_FM
D03R07FR3 F009_FM
D03R07FR3 F009_FM
D03R08FR3 F010_FM
D03R08FR3 F010_FM
D03R09FR3 F011_FM
D03R09FR3 F011_FM
D04R01FR3 F012_FM
D04R01FR3 F012_FM
D04R02FR3 F013_FM
D04R02FR3 F013_FM
D04R03FR3 F014_FM
D04R03FR3 F014_FM
D04R04FR3 F015_FM
D04R04FR3 F015_FM
D04R05FR3 F016_FM
D04R05FR3 F016_FM
D04R06FR3 F017_FM
D04R06FR3 F017_FM
D04R07FR3 F018_FM
D04R07FR3 F018_FM
D04R08FR3 F019_FM
D04R10FR3 F020_FM
D04R10FR3 F020_FM
D05R03FR3 F021_FM
D05R03FR3 F021_FM
D05R07FR3 F022_FM
D05R07FR3 F022_FM
D06R02FR3 F023_FM
D06R02FR3 F023_FM
D06R03FR3 F024_FM
D06R03FR3 F024_FM
D06R04FR3 F025_FM
D06R04FR3 F025_FM
D06R05FR3 F026_FM
D06R05FR3 F026_FM
D06R06FR3 F027_FM
D06R06FR3 F027_FM
D06R07FR3 F028_FM
D06R10FR3 F029_FM
D06R10FR3 F029_FM
D07R01FR3 F030_FM
```

D07R01PR3 F030_PM
D07R02FR3 F031_FM
D07R02PR3 F031_PM
D07R05FR3 F032_FM
D07R05PR3 F032_PM
D07R06FR3 F033_FM
D07R06PR3 F033_PM
D07R07FR3 F034_FM
D07R07PR3 F034_PM
D07R08FR3 F035_FM
D07R08PR3 F035_PM
D07R09FR3 F036_FM
D07R09PR3 F036_PM
D07R10FR3 F037_FM
D07R10PR3 F037_PM
D08R01FR3 F038_FM
D08R01PR3 F038_PM
D08R02FR3 F039_FM
D08R02PR3 F039_PM
D08R03FR3 F040_FM
D08R03PR3 F040_PM
D08R04FR3 F041_FM
D08R04PR3 F041_PM
D08R05FR3 F042_FM
D08R05PR3 F042_PM
D08R06FR3 F043_FM
D08R06PR3 F043_PM
D08R07FR3 F044_FM
D08R07PR3 F044_PM
D09R02FR3 F045_FM
D09R02PR3 F045_PM
D09R03FR3 F046_FM
D09R03PR3 F046_PM
D09R04FR3 F047_FM
D09R04PR3 F047_PM
D09R05FR3 F048_FM
D09R05PR3 F048_PM
D09R06FR3 F049_FM
D09R06PR3 F049_PM
D09R07FR3 F050_FM
D09R07PR3 F050_PM
D09R08FR3 F051_FM
D09R08PR3 F051_PM
D09R09FR3 F052_FM
D09R09PR3 F052_PM
D09R10FR3 F053_FM
D09R10PR3 F053_PM
D10R02FR3 F054_FM
D10R02PR3 F054_PM
D10R03FR3 F055_FM
D10R03PR3 F055_PM
D10R04FR3 F056_FM
D10R04PR3 F056_PM
D10R06FR3 F057_FM
D10R06PR3 F057_PM
D10R07FR3 F058_FM
D10R07PR3 F058_PM
D10R08FR3 F059_FM
D10R08PR3 F059_PM
D10R09FR3 F060_FM
D10R09PR3 F060_PM
D10R10FR3 F061_FM
D10R10PR3 F061_PM
D11R01FR3 F062_FM
D11R01PR3 F062_PM
D11R02FR3 F063_FM
D11R02PR3 F063_PM
D11R06FR3 F064_FM
D11R06PR3 F064_PM
D11R07FR3 F065_FM
D11R07PR3 F065_PM
D11R08FR3 F066_FM
D11R08PR3 F066_PM
D11R09FR3 F067_FM
D11R09PR3 F067_PM
D11R10FR3 F068_FM
D11R10PR3 F068_PM
D12R01FR3 F069_FM
D12R01PR3 F069_PM
D12R02FR3 F070_FM
D12R02PR3 F070_PM
D12R03FR3 F071_FM
D12R03PR3 F071_PM
D12R05FR3 F072_FM
D12R05PR3 F072_PM
D12R06FR3 F073_FM
D12R06PR3 F073_PM
D12R07FR3 F074_FM
D12R07PR3 F074_PM
D12R08FR3 F075_FM
D12R08PR3 F075_PM

D12R09FR3 F076_FM
D12R09PR3 F076_PM
D13R01FR3 F077_FM
D13R01PR3 F077_PM
D13R02FR3 F078_FM
D13R02PR3 F078_PM
D13R03FR3 F079_FM
D13R03PR3 F079_PM
D13R05FR3 F080_FM
D13R05PR3 F080_PM
D13R06FR3 F081_FM
D13R06PR3 F081_PM
D13R07FR3 F082_FM
D13R07PR3 F082_PM
D13R08FR3 F083_FM
D13R08PR3 F083_PM
D13R09FR3 F084_FM
D13R09PR3 F084_PM
D21R01FR3 F085_FM
D21R01PR3 F085_PM
D21R02FR3 F086_FM
D21R02PR3 F086_PM
D21R03FR3 F087_FM
D21R03PR3 F087_PM
D21R04FR3 F088_FM
D21R04PR3 F088_PM
D21R05FR3 F089_FM
D21R05PR3 F089_PM
D21R06FR3 F090_FM
D21R06PR3 F090_PM
D21R07FR3 F091_FM
D21R07PR3 F091_PM
D21R10FR3 F092_FM
D21R10PR3 F092_PM
D22R02FR3 F093_FM
D22R02PR3 F093_PM
D22R03FR3 F094_FM
D22R03PR3 F094_PM
D22R04FR3 F095_FM
D22R04PR3 F095_PM
D22R05FR3 F096_FM
D22R05PR3 F096_PM
D22R07FR3 F097_FM
D22R07PR3 F097_PM
D22R08FR3 F098_FM
D22R08PR3 F098_PM
D22R09FR3 F099_FM
D22R09PR3 F099_PM
D22R10FR3 F100_FM
D22R10PR3 F100_PM

vtran2_run_cra1_r3.log

Starting Time Stamp: 29-SEP-2003 09:54:17.51

```
working dir      = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]
budget file dir  = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.BUD_FILES.R3]
trn file dir     = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.TRN_FILES.R3]
dbg file dir     = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS.DBG_FILES.R3]
vtran2_run input file = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_RUN_CRA1_R3.INP
vtran2_run log file   = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_RUN_CRA1_R3.LOG
vtran2_cmd_file      = PAWORK:[SHARED.JFKANNE.WRK.CRA1_CULEBRA_TRANSPORT.FLOW_FIELDS]VTRAN2_CRA1_R3.CMD
```

Opening vtran2_run input file

mf2k budget file mf2k velocity transfer file

D01R02FR3.OUT	MF2K_CRA1_R3_F001_FM.TRN
D01R02PR3.OUT	MF2K_CRA1_R3_F001_PM.TRN
D01R04FR3.OUT	MF2K_CRA1_R3_F002_FM.TRN
D01R04PR3.OUT	MF2K_CRA1_R3_F002_PM.TRN
D01R07FR3.OUT	MF2K_CRA1_R3_F003_FM.TRN
D01R07PR3.OUT	MF2K_CRA1_R3_F003_PM.TRN
D01R10FR3.OUT	MF2K_CRA1_R3_F004_FM.TRN
D01R10PR3.OUT	MF2K_CRA1_R3_F004_PM.TRN
D02R02FR3.OUT	MF2K_CRA1_R3_F005_FM.TRN
D02R02PR3.OUT	MF2K_CRA1_R3_F005_PM.TRN
D03R01FR3.OUT	MF2K_CRA1_R3_F006_FM.TRN
D03R01PR3.OUT	MF2K_CRA1_R3_F006_PM.TRN
D03R03FR3.OUT	MF2K_CRA1_R3_F007_FM.TRN
D03R03PR3.OUT	MF2K_CRA1_R3_F007_PM.TRN
D03R06FR3.OUT	MF2K_CRA1_R3_F008_FM.TRN
D03R06PR3.OUT	MF2K_CRA1_R3_F008_PM.TRN
D03R07FR3.OUT	MF2K_CRA1_R3_F009_FM.TRN
D03R07PR3.OUT	MF2K_CRA1_R3_F009_PM.TRN
D03R08FR3.OUT	MF2K_CRA1_R3_F010_FM.TRN
D03R08PR3.OUT	MF2K_CRA1_R3_F010_PM.TRN
D03R09FR3.OUT	MF2K_CRA1_R3_F011_FM.TRN
D03R09PR3.OUT	MF2K_CRA1_R3_F011_PM.TRN
D04R01FR3.OUT	MF2K_CRA1_R3_F012_FM.TRN
D04R01PR3.OUT	MF2K_CRA1_R3_F012_PM.TRN
D04R02FR3.OUT	MF2K_CRA1_R3_F013_FM.TRN
D04R02PR3.OUT	MF2K_CRA1_R3_F013_PM.TRN
D04R03FR3.OUT	MF2K_CRA1_R3_F014_FM.TRN
D04R03PR3.OUT	MF2K_CRA1_R3_F014_PM.TRN
D04R04FR3.OUT	MF2K_CRA1_R3_F015_FM.TRN
D04R04PR3.OUT	MF2K_CRA1_R3_F015_PM.TRN
D04R05FR3.OUT	MF2K_CRA1_R3_F016_FM.TRN
D04R05PR3.OUT	MF2K_CRA1_R3_F016_PM.TRN
D04R06FR3.OUT	MF2K_CRA1_R3_F017_FM.TRN
D04R06PR3.OUT	MF2K_CRA1_R3_F017_PM.TRN
D04R07FR3.OUT	MF2K_CRA1_R3_F018_FM.TRN
D04R07PR3.OUT	MF2K_CRA1_R3_F018_PM.TRN
D04R08FR3.OUT	MF2K_CRA1_R3_F019_FM.TRN
D04R08PR3.OUT	MF2K_CRA1_R3_F019_PM.TRN
D04R10FR3.OUT	MF2K_CRA1_R3_F020_FM.TRN
D04R10PR3.OUT	MF2K_CRA1_R3_F020_PM.TRN
D05R03FR3.OUT	MF2K_CRA1_R3_F021_FM.TRN
D05R03PR3.OUT	MF2K_CRA1_R3_F021_PM.TRN
D05R07FR3.OUT	MF2K_CRA1_R3_F022_FM.TRN
D05R07PR3.OUT	MF2K_CRA1_R3_F022_PM.TRN
D06R02FR3.OUT	MF2K_CRA1_R3_F023_FM.TRN
D06R02PR3.OUT	MF2K_CRA1_R3_F023_PM.TRN
D06R03FR3.OUT	MF2K_CRA1_R3_F024_FM.TRN
D06R03PR3.OUT	MF2K_CRA1_R3_F024_PM.TRN
D06R04FR3.OUT	MF2K_CRA1_R3_F025_FM.TRN
D06R04PR3.OUT	MF2K_CRA1_R3_F025_PM.TRN
D06R05FR3.OUT	MF2K_CRA1_R3_F026_FM.TRN
D06R05PR3.OUT	MF2K_CRA1_R3_F026_PM.TRN
D06R06FR3.OUT	MF2K_CRA1_R3_F027_FM.TRN
D06R06PR3.OUT	MF2K_CRA1_R3_F027_PM.TRN
D06R07FR3.OUT	MF2K_CRA1_R3_F028_FM.TRN
D06R07PR3.OUT	MF2K_CRA1_R3_F028_PM.TRN
D06R10FR3.OUT	MF2K_CRA1_R3_F029_FM.TRN
D06R10PR3.OUT	MF2K_CRA1_R3_F029_PM.TRN
D07R01FR3.OUT	MF2K_CRA1_R3_F030_FM.TRN
D07R01PR3.OUT	MF2K_CRA1_R3_F030_PM.TRN
D07R02FR3.OUT	MF2K_CRA1_R3_F031_FM.TRN
D07R02PR3.OUT	MF2K_CRA1_R3_F031_PM.TRN
D07R05FR3.OUT	MF2K_CRA1_R3_F032_FM.TRN
D07R05PR3.OUT	MF2K_CRA1_R3_F032_PM.TRN
D07R06FR3.OUT	MF2K_CRA1_R3_F033_FM.TRN
D07R06PR3.OUT	MF2K_CRA1_R3_F033_PM.TRN
D07R07FR3.OUT	MF2K_CRA1_R3_F034_FM.TRN
D07R07PR3.OUT	MF2K_CRA1_R3_F034_PM.TRN
D07R08FR3.OUT	MF2K_CRA1_R3_F035_FM.TRN
D07R08PR3.OUT	MF2K_CRA1_R3_F035_PM.TRN
D07R09FR3.OUT	MF2K_CRA1_R3_F036_FM.TRN
D07R09PR3.OUT	MF2K_CRA1_R3_F036_PM.TRN
D07R10FR3.OUT	MF2K_CRA1_R3_F037_FM.TRN

D07R10PR3.OUT	MF2K_CRA1_R3_F037_PM.TRN
D08R01FR3.OUT	MF2K_CRA1_R3_F038_FM.TRN
D08R01PR3.OUT	MF2K_CRA1_R3_F038_PM.TRN
D08R02FR3.OUT	MF2K_CRA1_R3_F039_FM.TRN
D08R02PR3.OUT	MF2K_CRA1_R3_F039_PM.TRN
D08R03FR3.OUT	MF2K_CRA1_R3_F040_FM.TRN
D08R03PR3.OUT	MF2K_CRA1_R3_F040_PM.TRN
D08R04FR3.OUT	MF2K_CRA1_R3_F041_FM.TRN
D08R04PR3.OUT	MF2K_CRA1_R3_F041_PM.TRN
D08R05FR3.OUT	MF2K_CRA1_R3_F042_FM.TRN
D08R05PR3.OUT	MF2K_CRA1_R3_F042_PM.TRN
D08R06FR3.OUT	MF2K_CRA1_R3_F043_FM.TRN
D08R06PR3.OUT	MF2K_CRA1_R3_F043_PM.TRN
D08R07FR3.OUT	MF2K_CRA1_R3_F044_FM.TRN
D08R07PR3.OUT	MF2K_CRA1_R3_F044_PM.TRN
D09R02FR3.OUT	MF2K_CRA1_R3_F045_FM.TRN
D09R02PR3.OUT	MF2K_CRA1_R3_F045_PM.TRN
D09R03FR3.OUT	MF2K_CRA1_R3_F046_FM.TRN
D09R03PR3.OUT	MF2K_CRA1_R3_F046_PM.TRN
D09R04FR3.OUT	MF2K_CRA1_R3_F047_FM.TRN
D09R04PR3.OUT	MF2K_CRA1_R3_F047_PM.TRN
D09R05FR3.OUT	MF2K_CRA1_R3_F048_FM.TRN
D09R05PR3.OUT	MF2K_CRA1_R3_F048_PM.TRN
D09R06FR3.OUT	MF2K_CRA1_R3_F049_FM.TRN
D09R06PR3.OUT	MF2K_CRA1_R3_F049_PM.TRN
D09R07FR3.OUT	MF2K_CRA1_R3_F050_FM.TRN
D09R07PR3.OUT	MF2K_CRA1_R3_F050_PM.TRN
D09R08FR3.OUT	MF2K_CRA1_R3_F051_FM.TRN
D09R08PR3.OUT	MF2K_CRA1_R3_F051_PM.TRN
D09R09FR3.OUT	MF2K_CRA1_R3_F052_FM.TRN
D09R09PR3.OUT	MF2K_CRA1_R3_F052_PM.TRN
D09R10FR3.OUT	MF2K_CRA1_R3_F053_FM.TRN
D09R10PR3.OUT	MF2K_CRA1_R3_F053_PM.TRN
D10R02FR3.OUT	MF2K_CRA1_R3_F054_FM.TRN
D10R02PR3.OUT	MF2K_CRA1_R3_F054_PM.TRN
D10R03FR3.OUT	MF2K_CRA1_R3_F055_FM.TRN
D10R03PR3.OUT	MF2K_CRA1_R3_F055_PM.TRN
D10R04FR3.OUT	MF2K_CRA1_R3_F056_FM.TRN
D10R04PR3.OUT	MF2K_CRA1_R3_F056_PM.TRN
D10R06FR3.OUT	MF2K_CRA1_R3_F057_FM.TRN
D10R06PR3.OUT	MF2K_CRA1_R3_F057_PM.TRN
D10R07FR3.OUT	MF2K_CRA1_R3_F058_FM.TRN
D10R07PR3.OUT	MF2K_CRA1_R3_F058_PM.TRN
D10R08FR3.OUT	MF2K_CRA1_R3_F059_FM.TRN
D10R08PR3.OUT	MF2K_CRA1_R3_F059_PM.TRN
D10R09FR3.OUT	MF2K_CRA1_R3_F060_FM.TRN
D10R09PR3.OUT	MF2K_CRA1_R3_F060_PM.TRN
D10R10FR3.OUT	MF2K_CRA1_R3_F061_FM.TRN
D10R10PR3.OUT	MF2K_CRA1_R3_F061_PM.TRN
D11R01FR3.OUT	MF2K_CRA1_R3_F062_FM.TRN
D11R01PR3.OUT	MF2K_CRA1_R3_F062_PM.TRN
D11R02FR3.OUT	MF2K_CRA1_R3_F063_FM.TRN
D11R02PR3.OUT	MF2K_CRA1_R3_F063_PM.TRN
D11R06FR3.OUT	MF2K_CRA1_R3_F064_FM.TRN
D11R06PR3.OUT	MF2K_CRA1_R3_F064_PM.TRN
D11R07FR3.OUT	MF2K_CRA1_R3_F065_FM.TRN
D11R07PR3.OUT	MF2K_CRA1_R3_F065_PM.TRN
D11R08FR3.OUT	MF2K_CRA1_R3_F066_FM.TRN
D11R08PR3.OUT	MF2K_CRA1_R3_F066_PM.TRN
D11R09FR3.OUT	MF2K_CRA1_R3_F067_FM.TRN
D11R09PR3.OUT	MF2K_CRA1_R3_F067_PM.TRN
D11R10FR3.OUT	MF2K_CRA1_R3_F068_FM.TRN
D11R10PR3.OUT	MF2K_CRA1_R3_F068_PM.TRN
D12R01FR3.OUT	MF2K_CRA1_R3_F069_FM.TRN
D12R01PR3.OUT	MF2K_CRA1_R3_F069_PM.TRN
D12R02FR3.OUT	MF2K_CRA1_R3_F070_FM.TRN
D12R02PR3.OUT	MF2K_CRA1_R3_F070_PM.TRN
D12R03FR3.OUT	MF2K_CRA1_R3_F071_FM.TRN
D12R03PR3.OUT	MF2K_CRA1_R3_F071_PM.TRN
D12R05FR3.OUT	MF2K_CRA1_R3_F072_FM.TRN
D12R05PR3.OUT	MF2K_CRA1_R3_F072_PM.TRN
D12R06FR3.OUT	MF2K_CRA1_R3_F073_FM.TRN
D12R06PR3.OUT	MF2K_CRA1_R3_F073_PM.TRN
D12R07FR3.OUT	MF2K_CRA1_R3_F074_FM.TRN
D12R07PR3.OUT	MF2K_CRA1_R3_F074_PM.TRN
D12R08FR3.OUT	MF2K_CRA1_R3_F075_FM.TRN
D12R08PR3.OUT	MF2K_CRA1_R3_F075_PM.TRN
D12R09FR3.OUT	MF2K_CRA1_R3_F076_FM.TRN
D12R09PR3.OUT	MF2K_CRA1_R3_F076_PM.TRN
D13R01FR3.OUT	MF2K_CRA1_R3_F077_FM.TRN
D13R01PR3.OUT	MF2K_CRA1_R3_F077_PM.TRN
D13R02FR3.OUT	MF2K_CRA1_R3_F078_FM.TRN
D13R02PR3.OUT	MF2K_CRA1_R3_F078_PM.TRN
D13R03FR3.OUT	MF2K_CRA1_R3_F079_FM.TRN
D13R03PR3.OUT	MF2K_CRA1_R3_F079_PM.TRN
D13R05FR3.OUT	MF2K_CRA1_R3_F080_FM.TRN
D13R05PR3.OUT	MF2K_CRA1_R3_F080_PM.TRN
D13R06FR3.OUT	MF2K_CRA1_R3_F081_FM.TRN
D13R06PR3.OUT	MF2K_CRA1_R3_F081_PM.TRN
D13R07FR3.OUT	MF2K_CRA1_R3_F082_FM.TRN
D13R07PR3.OUT	MF2K_CRA1_R3_F082_PM.TRN

D13R08FR3.OUT	MF2K_CRA1_R3_F083_FM.TRN
D13R08PR3.OUT	MF2K_CRA1_R3_F083_PM.TRN
D13R09FR3.OUT	MF2K_CRA1_R3_F084_FM.TRN
D13R09PR3.OUT	MF2K_CRA1_R3_F084_PM.TRN
D21R01FR3.OUT	MF2K_CRA1_R3_F085_FM.TRN
D21R01PR3.OUT	MF2K_CRA1_R3_F085_PM.TRN
D21R02FR3.OUT	MF2K_CRA1_R3_F086_FM.TRN
D21R02PR3.OUT	MF2K_CRA1_R3_F086_PM.TRN
D21R03FR3.OUT	MF2K_CRA1_R3_F087_FM.TRN
D21R03PR3.OUT	MF2K_CRA1_R3_F087_PM.TRN
D21R04FR3.OUT	MF2K_CRA1_R3_F088_FM.TRN
D21R04PR3.OUT	MF2K_CRA1_R3_F088_PM.TRN
D21R05FR3.OUT	MF2K_CRA1_R3_F089_FM.TRN
D21R05PR3.OUT	MF2K_CRA1_R3_F089_PM.TRN
D21R06FR3.OUT	MF2K_CRA1_R3_F090_FM.TRN
D21R06PR3.OUT	MF2K_CRA1_R3_F090_PM.TRN
D21R07FR3.OUT	MF2K_CRA1_R3_F091_FM.TRN
D21R07PR3.OUT	MF2K_CRA1_R3_F091_PM.TRN
D21R10FR3.OUT	MF2K_CRA1_R3_F092_FM.TRN
D21R10PR3.OUT	MF2K_CRA1_R3_F092_PM.TRN
D22R02FR3.OUT	MF2K_CRA1_R3_F093_FM.TRN
D22R02PR3.OUT	MF2K_CRA1_R3_F093_PM.TRN
D22R03FR3.OUT	MF2K_CRA1_R3_F094_FM.TRN
D22R03PR3.OUT	MF2K_CRA1_R3_F094_PM.TRN
D22R04FR3.OUT	MF2K_CRA1_R3_F095_FM.TRN
D22R04PR3.OUT	MF2K_CRA1_R3_F095_PM.TRN
D22R06FR3.OUT	MF2K_CRA1_R3_F096_FM.TRN
D22R06PR3.OUT	MF2K_CRA1_R3_F096_PM.TRN
D22R07FR3.OUT	MF2K_CRA1_R3_F097_FM.TRN
D22R07PR3.OUT	MF2K_CRA1_R3_F097_PM.TRN
D22R08FR3.OUT	MF2K_CRA1_R3_F098_FM.TRN
D22R08PR3.OUT	MF2K_CRA1_R3_F098_PM.TRN
D22R09FR3.OUT	MF2K_CRA1_R3_F099_FM.TRN
D22R09PR3.OUT	MF2K_CRA1_R3_F099_PM.TRN
D22R10FR3.OUT	MF2K_CRA1_R3_F100_FM.TRN
D22R10PR3.OUT	MF2K_CRA1_R3_F100_PM.TRN

Closing vtran2_run input file

Ending Time Stamp: 29-SEP-2003 09:57:38.43

Appendix C: Input Files Used in Culebra Transport Calculations

C.1: genmesh Input File

gm_st2d_cra1.inp

```
-----
: Grid for 2003 CRA calculations
: Created for SECOTP2D by Joshua Stein
: June 25, 2003
:-----
:
*SETUP
DIM=2
ORIG=0.0000E+00,0.0000E+00
IJOMAX=151, 109
:
*GRID,
DEL, COORD=X, DEL=50., INRANGE=1,151
:
DEL, COORD=Y, DEL=50., INRANGE=1,109
:
*REGions
REC=1, IRANGE=1,151, JRANGE=1,109
:
:
*ELEV
LOC, THICK=4.0, ELEVAT=0.0, IRANGE=1,151 JRANGE=1,109
*END
:-----
```

C.2: matset Input File

ms_st2d_cra1.inp

```
-----
! TITLE:      SECO INPUT 1996: The WIPP PA CCA Calculation
! ANALYSTS:   C. T. STOCKMAN, R. L. BLAINE
! CREATED:    JUNE 12, 1996
! MODIFIED:
! PURPOSE:    PREPARE DATABASE FOR PRESECO
!-----
!
! *HEADING
! RUN=0
! SCALE=SOURCE
! SCENARIO=00
! TITLE=SECO
!
! *PRINT_ASSIGNED_VALUES
!
! *UNITS=SI
!
! *CREATE_BLOCK
! BLOCKID=      2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13
! *RETRIEVE+NAME
! COORDINATE, DIM=2, NAMES=X, Y
! MATERIAL,    1=CULEBRA, 2=GLOBAL, 3=REFCON, &
!              4=AM241, 5=PU239, 6=TH230, 7=U234, &
!              8=AM+3, 9=PU+3, 10=PU+4, 11=TH+4, 12=U+4, 13=U+6
!
! PROPERTY, MATERIAL=CULEBRA, NAMES =APOROS,DPOROS,DISP_L,DISPT_L
! PROPERTY, MATERIAL=CULEBRA, NAMES =FTORT,DTORT
! PROPERTY, MATERIAL=CULEBRA, NAMES =JMBLKLT,SKIN_RES,DNSGRAIN
! PROPERTY, MATERIAL=GLOBAL,  NAMES =OXSTAT,CLINTIDX, TRANSIDX
! PROPERTY, MATERIAL=REFCON,  NAMES =YRSEC
! ISOTOPES
! PROPERTY MATERIAL=Am241,    NAMES =ATWEIGHT,HALFLIFE
! PROPERTY MATERIAL=Pu239,    NAMES =ATWEIGHT,HALFLIFE
! PROPERTY MATERIAL=Th230,    NAMES =ATWEIGHT,HALFLIFE
! PROPERTY MATERIAL=U234,     NAMES =ATWEIGHT,HALFLIFE
!
! PROPERTY MATERIAL=AM+3,     NAMES =MKD_AM, MDO
! PROPERTY MATERIAL=PU+3,     NAMES =MKD_PU, MDO
! PROPERTY MATERIAL=PU+4,     NAMES =MKD_PU, MDO
! PROPERTY MATERIAL=TH+4,     NAMES =MKD_TH, MDO
! PROPERTY MATERIAL=U+4,     NAMES =MKD_U, MDO
! PROPERTY MATERIAL=U+6,     NAMES =MKD_U, MDO
!
! *END
!-----
```

C.3: prelhs Input File, Replicate 1

lhs1_st2d_cra1_a1.inp

```
! TITLE: BRAGFLO 2003 CRA1 (LHS1)
! SCENARIO: S1, S2, S3, S4, S5, and S6
! ANALYSTS: Joshua Stein and Bill Zelinski
! CREATED: April 2003
! MODIFIED: April 7
!
! LMSCALC = CRA1 REALIZATION 1
!-----
! DESCRIPTION:
! WIPP 2003 Compliance Recertification Analyses (CRA)
!
! This input file to PRELHS is used to generate, as an output file, an LHS
! input file containing all distribution information and execution options
! required to create a sample for Replicate R1 for the WIPP 2003 CRA
!
! Modified for CRA analyses: LHSBLANK dummy changed to LHSBLANK and
! REFCON MATERIAL (LHSBLANK) changed to REFCON
! #59 dummy replaced with VOLSPALL
!----- No Comments Allowed between *ECHO and *ENDECHO -----
!
! *ECHOLHS
! TITLE 2002 TEM PA Calculation, Replicate R1 Input File for the LHS Code
! NOBS 100
! RANDOM SEED 921196800
! CORRELATION MATRIX
! 3
! 18 19 -0.99
! 20 21 -0.99
! 28 29 -0.76
! OUTPUT CORR HIST DATA
! *ENDECHO
!
! == PROPERTIES TO BE RETRIEVED FROM WIPP 1997 PA CALCULATION DATABASE ==
!
! *RETRIEVE
!1 MATERIALS, STEEL
! PROPERTIES, CORRMCO2
!2 MATERIALS, WAS_AREA
! PROPERTIES, PROBDEG
!3 MATERIALS, WAS_AREA
! PROPERTIES, GRATHICI
!4 MATERIALS, WAS_AREA
! PROPERTIES, GRATHICH
!5 MATERIALS, CELLULS
! PROPERTIES, FBETA
!6 MATERIALS, WAS_AREA
! PROPERTIES, SAT_RGAS
!7 MATERIALS, WAS_AREA
! PROPERTIES, SAT_RBRN
!8 MATERIALS, WAS_AREA
! PROPERTIES, SAT_WICK
!9 MATERIALS, DRZ_PCS
! PROPERTIES, PRMX_LOG
!10 MATERIALS, CONC_PCS
! PROPERTIES, PRMX_LOG
!11 MATERIALS, SOLU4
! PROPERTIES, SOLCIM
!12 MATERIALS, SOLTH4
! PROPERTIES, SOLCIM
!13 dummy placeholder
! MATERIALS, REFCON
! PROPERTIES, LHSBLANK
!14 MATERIALS, CONC_PCS
! PROPERTIES, SAT_RGAS
!15 MATERIALS, CONC_PCS
! PROPERTIES, SAT_RBRN
!16 MATERIALS, CONC_PCS
```

PROPERTIES, PORE_DIS
 117 MATERIALS, S_HALITE
 PROPERTIES, POROSITY
 118 MATERIALS, S_HALITE
 PROPERTIES, PRMX_LOG
 119 MATERIALS, S_HALITE
 PROPERTIES, COMP_RCK
 120 MATERIALS, S_MB139
 PROPERTIES, PRMX_LOG
 121 MATERIALS, S_MB139
 PROPERTIES, COMP_RCK
 122 MATERIALS, S_MB139
 PROPERTIES, RELP_MOD
 123 MATERIALS, S_MB139
 PROPERTIES, SAT_RBRN
 124 MATERIALS, S_MB139
 PROPERTIES, SAT_RGAS
 125 MATERIALS, S_MB139
 PROPERTIES, PORE_DIS
 126 MATERIALS, S_HALITE
 PROPERTIES, PRESSURE
 127 MATERIALS, CASTILER
 PROPERTIES, PRESSURE
 128 MATERIALS, CASTILER
 PROPERTIES, PRMX_LOG
 129 MATERIALS, CASTILER
 PROPERTIES, COMP_RCK
 130 MATERIALS, BK_SAND
 PROPERTIES, PRMX_LOG
 131 MATERIALS, DRZ_1
 PROPERTIES, PRMX_LOG
 132 MATERIALS, CONC_PLG
 PROPERTIES, PRMX_LOG
 133 dummy placeholder
 MATERIALS, REFCOM
 PROPERTIES, LMSBLANK
 134 MATERIALS, SOLAM3
 PROPERTIES, SOLSIM
 135 MATERIALS, SOLAM3
 PROPERTIES, SOLCIM
 136 MATERIALS, SOLPU3
 PROPERTIES, SOLSIM
 137 MATERIALS, SOLPU3
 PROPERTIES, SOLCIM
 138 MATERIALS, SOLPU4
 PROPERTIES, SOLSIM
 139 MATERIALS, SOLPU4
 PROPERTIES, SOLCIM
 140 MATERIALS, SOLU4
 PROPERTIES, SOLSIM
 141 MATERIALS, SOLU6
 PROPERTIES, SOLSIM
 142 MATERIALS, SOLU6
 PROPERTIES, SOLCIM
 143 MATERIALS, SOLTH4
 PROPERTIES, SOLSIM
 144 MATERIALS, PHUMOX3
 PROPERTIES, PHUMCIN
 145 MATERIALS, GLOBAL
 PROPERTIES, OXSTAT
 146 MATERIALS, CULEBRA
 PROPERTIES, MINP_FAC

C.4: prelhs Input File, Replicate 2

lhs1.st2d.cra1.a2.inp

```
! TITLE: BRAGLO 2003 CRA1 (LHS1)
! SCENARIO: S1, S2, S3, S4, S5, and S6
! ANALYSTS: Joshua Stein and Bill Zelinski
! CREATED: April 2003
! MODIFIED: April 7

! LNSCALC = CRA1 REALIZATION 1
-----
! DESCRIPTION:
! WIPP 2003 Compliance Recertification Analyses (CRA)
! This input file to PRELHS is used to generate, as an output file, an LHS
! input file containing all distribution information and execution options
! required to create a sample for Replicate R1 for the WIPP 2003 CRA
! Modified for CRA analyses: LHSBLANK dummy changed to LHSBLANK and
! REFCON MATERIAL (LHSBLANK) changed to REFCON
! #59 dummy replaced with VOLSPALL
!----- No Comments Allowed between *ECHO and *ENDECHO -----
*ECHOLHS
TITLE 2002 TEN PA Calculation, Replicate R1 Input File for the LHS Code
NOBS 100
RANDOM SEED 921196800
CORRELATION MATRIX
3
18 19 -0.99
20 21 -0.99
28 29 -0.78
OUTPUT CORR HIST DATA
*ENDECHO
!
!-- PROPERTIES TO BE RETRIEVED FROM WIPP 1997 PA CALCULATION DATABASE --
!
*RETRIEVE
!1
MATERIALS, STEEL
PROPERTIES, CORRMCO2
!2
MATERIALS, WAS_AREA
PROPERTIES, PROBDEG
!3
MATERIALS, WAS_AREA
PROPERTIES, GRATHICI
!4
MATERIALS, WAS_AREA
PROPERTIES, GRATHICH
!5
MATERIALS, CELLULS
PROPERTIES, FBETA
!6
MATERIALS, WAS_AREA
PROPERTIES, SAT_RGAS
!7
MATERIALS, WAS_AREA
PROPERTIES, SAT_RBRN
!8
MATERIALS, WAS_AREA
PROPERTIES, SAT_WICK
!9
MATERIALS, DRZ_PCS
PROPERTIES, PRMX_LOG
!10
MATERIALS, CONC_PCS
PROPERTIES, PRMX_LOG
!11
MATERIALS, SOLU4
PROPERTIES, SOLCIM
!12
MATERIALS, SOLTH4
PROPERTIES, SOLCIM
!13 dummy placeholder
MATERIALS, REFCON
PROPERTIES, LHSBLANK
!14
MATERIALS, CONC_PCS
PROPERTIES, SAT_RGAS
!15
MATERIALS, CONC_PCS
PROPERTIES, SAT_RBRN
!16
MATERIALS, CONC_PCS
```

PROPERTIES, PORE_DIS
 !17 MATERIALS, S_HALITE
 PROPERTIES, POROSITY
 !18 MATERIALS, S_HALITE
 PROPERTIES, PRMX_LOG
 !19 MATERIALS, S_HALITE
 PROPERTIES, COMP_RCK
 !20 MATERIALS, S_MB139
 PROPERTIES, PRMX_LOG
 !21 MATERIALS, S_MB139
 PROPERTIES, COMP_RCK
 !22 MATERIALS, S_MB139
 PROPERTIES, RELP_MOD
 !23 MATERIALS, S_MB139
 PROPERTIES, SAT_RBRN
 !24 MATERIALS, S_MB139
 PROPERTIES, SAT_RGAS
 !25 MATERIALS, S_MB139
 PROPERTIES, PORE_DIS
 !26 MATERIALS, S_HALITE
 PROPERTIES, PRESSURE
 !27 MATERIALS, CASTILER
 PROPERTIES, PRESSURE
 !28 MATERIALS, CASTILER
 PROPERTIES, PRMX_LOG
 !29 MATERIALS, CASTILER
 PROPERTIES, COMP_RCK
 !30 MATERIALS, BH_SAND
 PROPERTIES, PRMX_LOG
 !31 MATERIALS, DRZ_1
 PROPERTIES, PRMX_LOG
 !32 MATERIALS, CONC_PLG
 PROPERTIES, PRMX_LOG
 !33 dummy placeholder
 MATERIALS, REFCON
 PROPERTIES, LHSBLANK
 !34 MATERIALS, SOLAM3
 PROPERTIES, SOLSIM
 !35 MATERIALS, SOLAM3
 PROPERTIES, SOLCIM
 !36 MATERIALS, SOLPU3
 PROPERTIES, SOLSIM
 !37 MATERIALS, SOLPU3
 PROPERTIES, SOLCIM
 !38 MATERIALS, SOLPU4
 PROPERTIES, SOLSIM
 !39 MATERIALS, SOLPU4
 PROPERTIES, SOLCIM
 !40 MATERIALS, SOLU4
 PROPERTIES, SOLSIM
 !41 MATERIALS, SOLU6
 PROPERTIES, SOLSIM
 !42 MATERIALS, SOLU6
 PROPERTIES, SOLCIM
 !43 MATERIALS, SOLTH4
 PROPERTIES, SOLSIM
 !44 MATERIALS, PHUMX3
 PROPERTIES, PHUNCIM
 !45 MATERIALS, GLOBAL
 PROPERTIES, OXSTAT
 !46 MATERIALS, CULEBRA
 PROPERTIES, MINP_FAC


```

1
147 MATERIALS, GLOBAL
   PROPERTIES, TRANSIDX
148 MATERIALS, GLOBAL
   PROPERTIES, CLINTIDX
149 MATERIALS, CULEBRA
   PROPERTIES, HMBLXLIT
150 MATERIALS, CULEBRA
   PROPERTIES, APOROS
151 MATERIALS, CULEBRA
   PROPERTIES, DPOROS
152 MATERIALS, U+6
   PROPERTIES, MKD_U
153 MATERIALS, U+4
   PROPERTIES, MKD_U
154 MATERIALS, PU+3
   PROPERTIES, MKD_PU
155 MATERIALS, PU+4
   PROPERTIES, MKD_PU
156 MATERIALS, TH+4
   PROPERTIES, MKD_TH
157 MATERIALS, AM+3
   PROPERTIES, MKD_AM
158 MATERIALS, BOREHOLE
   PROPERTIES, TAUFALL
159 dummy placeholder for VOLSPALL
   MATERIALS, WAS_AREA
   PROPERTIES, VOLSPALL
160 MATERIALS, GLOBAL
   PROPERTIES, FBRINE
161 MATERIALS, BOREHOLE
   PROPERTIES, DOMECA
162 MATERIALS, SHFTU
   PROPERTIES, SAT_RBRN
163 MATERIALS, SHFTU
   PROPERTIES, SAT_RGAS
164 MATERIALS, SHFTU
   PROPERTIES, PRMX_LOG
165 MATERIALS, SHFTL_T1
   PROPERTIES, PRMX_LOG
166 MATERIALS, SHFTL_T2
   PROPERTIES, PRMX_LOG
167 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
168 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
169 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
170 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
171 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
172 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
173 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
174 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
175 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
!
!-----
!
!
*END

```

C.5: prelhs Input File, Replicate 3

lhs1_st2d_cra1_a3.inp

```
! TITLE: BRAGFLO 2003 CRA1 (LHS1)
! SCENARIO: S1, S2, S3, S4, S5, and S6
! ANALYSTS: Joshua Stein and Bill Zelinski
! CREATED: April 2003
! MODIFIED: April 7
!
! LHSCALC = CRA1 REALIZATION 1
!-----
! DESCRIPTION:
! WIPP 2003 Compliance Recertification Analyses (CRA)
! This input file to PRELHS is used to generate, as an output file, an LHS
! input file containing all distribution information and execution options
! required to create a sample for Replicate R1 for the WIPP 2003 CRA
! Modified for CRA analyses: LHSBLANK dummy changed to LHSBLANK and
! REFCON MATERIAL (LHSBLANK) changed to REFCON
! #59 dummy replaced with VOLSPALL
!----- No Comments Allowed between *ECHO and *ENDECHO -----
!
! *ECHOLHS
! TITLE 2002 TBM PA Calculation, Replicate R1 Input File for the LHS Code
! NOBS 100
! RANDOM SEED 921196800
! CORRELATION MATRIX
! 3
! 18 19 -0.99
! 20 21 -0.99
! 28 29 -0.75
! OUTPUT CORR HIST DATA
! *ENDECHO
!
! == PROPERTIES TO BE RETRIEVED FROM WIPP 1997 PA CALCULATION DATABASE ==
!
! *RETRIEVE
!1
! MATERIALS, STEEL
! PROPERTIES, CORRMCO2
!2
! MATERIALS, WAS_AREA
! PROPERTIES, PROBDEG
!3
! MATERIALS, WAS_AREA
! PROPERTIES, CRATMICI
!4
! MATERIALS, WAS_AREA
! PROPERTIES, CRATHICH
!5
! MATERIALS, CELLULS
! PROPERTIES, FBETA
!6
! MATERIALS, WAS_AREA
! PROPERTIES, SAT_RGAS
!7
! MATERIALS, WAS_AREA
! PROPERTIES, SAT_RBRN
!8
! MATERIALS, WAS_AREA
! PROPERTIES, SAT_WICK
!9
! MATERIALS, DRZ_PCS
! PROPERTIES, PRMX_LOG
!10
! MATERIALS, CONC_PCS
! PROPERTIES, PRMX_LOG
!11
! MATERIALS, SOLU4
! PROPERTIES, SOLCIN
!12
! MATERIALS, SOLTH4
! PROPERTIES, SOLCIN
!13 dummy placeholder
! MATERIALS, REFCON
! PROPERTIES, LHSBLANK
!14
! MATERIALS, CONC_PCS
! PROPERTIES, SAT_RGAS
!15
! MATERIALS, CONC_PCS
! PROPERTIES, SAT_RBRN
!16
! MATERIALS, CONC_PCS
```

PROPERTIES, PORE_DIS
 117 MATERIALS, S_HALITE
 PROPERTIES, POROSITY
 118 MATERIALS, S_HALITE
 PROPERTIES, PRMX_LOG
 119 MATERIALS, S_HALITE
 PROPERTIES, COMP_RCK
 120 MATERIALS, S_MB139
 PROPERTIES, PRMX_LOG
 121 MATERIALS, S_MB139
 PROPERTIES, COMP_RCK
 122 MATERIALS, S_MB139
 PROPERTIES, RELP_MOD
 123 MATERIALS, S_MB139
 PROPERTIES, SAT_RERN
 124 MATERIALS, S_MB139
 PROPERTIES, SAT_RGAS
 125 MATERIALS, S_MB139
 PROPERTIES, PORE_DIS
 126 MATERIALS, S_HALITE
 PROPERTIES, PRESSURE
 127 MATERIALS, CASTILER
 PROPERTIES, PRESSURE
 128 MATERIALS, CASTILER
 PROPERTIES, PRMX_LOG
 129 MATERIALS, CASTILER
 PROPERTIES, COMP_RCK
 130 MATERIALS, BH_SAND
 PROPERTIES, PRMX_LOG
 131 MATERIALS, DRZ_1
 PROPERTIES, PRMX_LOG
 132 MATERIALS, CONC_PLG
 PROPERTIES, PRMX_LOG
 133 dummy placeholder
 MATERIALS, REFCOM
 PROPERTIES, LHSBLANK
 134 MATERIALS, SOLAM3
 PROPERTIES, SOLSIM
 135 MATERIALS, SOLAM3
 PROPERTIES, SOLCIM
 136 MATERIALS, SOLPU3
 PROPERTIES, SOLSIM
 137 MATERIALS, SOLPU3
 PROPERTIES, SOLCIM
 138 MATERIALS, SOLPU4
 PROPERTIES, SOLSIM
 139 MATERIALS, SOLPU4
 PROPERTIES, SOLCIM
 140 MATERIALS, SOLU4
 PROPERTIES, SOLSIM
 141 MATERIALS, SOLU6
 PROPERTIES, SOLSIM
 142 MATERIALS, SOLU6
 PROPERTIES, SOLCIM
 143 MATERIALS, SOLTH4
 PROPERTIES, SOLSIM
 144 MATERIALS, PHUMOX3
 PROPERTIES, PHUMCIM
 145 MATERIALS, GLOBAL
 PROPERTIES, OXSTAT
 146 MATERIALS, CULEBRA
 PROPERTIES, MINP_FAC

```

147 MATERIALS, GLOBAL
   PROPERTIES, TRANSIDX
148 MATERIALS, GLOBAL
   PROPERTIES, CLINTIDX
149 MATERIALS, CULEBRA
   PROPERTIES, HMBLKLIT
150 MATERIALS, CULEBRA
   PROPERTIES, APOROS
151 MATERIALS, CULEBRA
   PROPERTIES, DPOROS
152 MATERIALS, U+6
   PROPERTIES, MKD_U
153 MATERIALS, U+4
   PROPERTIES, MKD_U
154 MATERIALS, PU+3
   PROPERTIES, MKD_PU
155 MATERIALS, PU+4
   PROPERTIES, MKD_PU
156 MATERIALS, TH+4
   PROPERTIES, MKD_TH
157 MATERIALS, AM+3
   PROPERTIES, MKD_AM
158 MATERIALS, BOREHOLE
   PROPERTIES, TAUFALL
159 dummy placeholder for VOLSPALL
   MATERIALS, WAS_AREA
   PROPERTIES, VOLSPALL
160 MATERIALS, GLOBAL
   PROPERTIES, PERINE
161 MATERIALS, BOREHOLE
   PROPERTIES, DOMEGA
162 MATERIALS, SFTU
   PROPERTIES, SAT_RBRN
163 MATERIALS, SFTU
   PROPERTIES, SAT_RGAS
164 MATERIALS, SFTU
   PROPERTIES, PMX_LOG
165 MATERIALS, SFTL_T1
   PROPERTIES, PMX_LOG
166 MATERIALS, SFTL_T2
   PROPERTIES, PMX_LOG
167 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
168 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
169 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
170 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
171 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
172 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
173 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
174 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
175 MATERIALS, REFCON
   PROPERTIES, LHSBLANK
!
!-----
!
•END

```

C.6: postlhs Input File

lhs3_st2d_cra1.inp

```
=====
! Dummy file required for postlhs to be run
=====
```

*end

C.7: algebracdb Input File

alg_st2d_cra1.inp

```
-----
!TITLE: PREPARE CDB FOR PRESECO
!ANALYSTS: C.T. STOCKMAN, R.L. BLAINE
!CREATED: JUNE 13, 1996
!MODIFIED:
!MODIFIED:
-----
!OX IS NEG AND 0 FOR LOW OX STATE AND POSITIVE FOR HIGH OX STATE
OX=OXSTAT[B:2]-0.5
ACTCONST=1.128E+13
! Convert the transmissivity index to an integer
! between 1 and 100 to correspond to a given t-field
TRANSIDX = AINT(TRANSIDX*100) + 1
!
!USE CULEBRA BLOCK=1
LIMIT BLOCK 1
!
!AM241=4, AM+3=8
DC_AM241=MAKEPROP(LOG(2)/HALFLIFE[B:4])
SA_AM241=MAKEPROP(ACTCONST/ATWEIGHT[B:4]/HALFLIFE[B:4])
MKD_AM=MAKEPROP(MKD_AM[B:8])
MDO_AM=MAKEPROP(MDO[B:8])
MRTRD_AM=1.0 + DNSGRAIN*(1-DPOROS)*MKD_AM/DPOROS
ZRTRD_AM=MAKEPROP(1.0)
!
!PU239=5, PU+3=9, PU+4=10
DC_PU239=MAKEPROP(LOG(2)/HALFLIFE[B:5])
SA_PU239=MAKEPROP(ACTCONST/ATWEIGHT[B:5]/HALFLIFE[B:5])
MKD_PU=MAKEPROP(IFGTO(OX,MKD_PU[B:10],MKD_PU[B:9]))
MDO_PU=MAKEPROP(IFGTO(OX,MDO[B:10],MDO[B:9]))
MRTRD_PU=1.0 + DNSGRAIN*(1-DPOROS)*MKD_PU/DPOROS
ZRTRD_PU=MAKEPROP(1.0)
!
!TH230=6, TH+4=11
DC_TH230=MAKEPROP(LOG(2)/HALFLIFE[B:6])
SA_TH230=MAKEPROP(ACTCONST/ATWEIGHT[B:6]/HALFLIFE[B:6])
MKD_TH=MAKEPROP(MKD_TH[B:11])
MDO_TH=MAKEPROP(MDO[B:11])
MRTRD_TH=1.0 + DNSGRAIN*(1-DPOROS)*MKD_TH/DPOROS
ZRTRD_TH=MAKEPROP(1.0)
!
!U234=7, U+4=12, U+6=13
DC_U234=MAKEPROP(LOG(2)/HALFLIFE[B:7])
SA_U234=MAKEPROP(ACTCONST/ATWEIGHT[B:7]/HALFLIFE[B:7])
MKD_U=MAKEPROP(IFGTO(OX,MKD_U[B:13],MKD_U[B:12]))
MDO_U=MAKEPROP(IFGTO(OX,MDO[B:13],MDO[B:12]))
MRTRD_U=1.0 + DNSGRAIN*(1-DPOROS)*MKD_U/DPOROS
ZRTRD_U=MAKEPROP(1.0)
!
LIMIT BLOCK 1
DISP_TRN=MAKEATTR(DISP_L*DISPT_L)
DISP_LNG=MAKEATTR(DISP_L)
FPOROS=MAKEATTR(APOROS)
MPOROS=MAKEATTR(DPOROS)
MTORT=MAKEATTR(DTORT)
F_TORT=MAKEATTR(FTORT)
END
```

C.8: relate Input File

rel_st2d.cra1.inp

```
-----
! Input file to run RELATE for PRESECOTP preparation
! Need to remove all elements blocks except for CULEBRA
! Created by Rebecca Blaine
! June 15, 1996
-----
```

```
*LOCATION,
  XOBJ=0.0, YOBJ=0.0, ANGLE=0.0, UNITS=1.0
```

*ATTRIBUTE

```
DISP_TRN = NEAREST CULEBRA DISP_TRN
DISP_LNG = NEAREST CULEBRA DISP_LNG
FPOROS   = NEAREST CULEBRA FPOROS
MPOROS   = NEAREST CULEBRA MPOROS
F_TORT   = NEAREST CULEBRA F_TORT
MTORT    = NEAREST CULEBRA MTORT
```

*PROPERTY

```
HMBLKL7  = XFERED CULEBRA HMBLKL7
SKIN_RES = XFERED CULEBRA SKIN_RES
DC_AM241 = XFERED CULEBRA DC_AM241
DC_PU239 = XFERED CULEBRA DC_PU239
DC_TH230 = XFERED CULEBRA DC_TH230
DC_U234  = XFERED CULEBRA DC_U234
SA_AM241 = XFERED CULEBRA SA_AM241
SA_PU239 = XFERED CULEBRA SA_PU239
SA_TH230 = XFERED CULEBRA SA_TH230
SA_U234  = XFERED CULEBRA SA_U234
MDO_AM   = XFERED CULEBRA MDO_AM
MDO_PU   = XFERED CULEBRA MDO_PU
MDO_TH   = XFERED CULEBRA MDO_TH
MDO_U    = XFERED CULEBRA MDO_U
MRTRD_AM = XFERED CULEBRA MRTRD_AM
MRTRD_PU = XFERED CULEBRA MRTRD_PU
MRTRD_TH = XFERED CULEBRA MRTRD_TH
MRTRD_U  = XFERED CULEBRA MRTRD_U
ZRTRD_AM = XFERED CULEBRA ZRTRD_AM
ZRTRD_PU = XFERED CULEBRA ZRTRD_PU
ZRTRD_TH = XFERED CULEBRA ZRTRD_TH
ZRTRD_U  = XFERED CULEBRA ZRTRD_U
CLIMTDX  = XFERED GLOBAL CLIMTDX
```

C.9: presecotp2d Input File

```

! Input file used to run PRESECOTP2D for the CRAI calculations.
!
! This input file:
! 1) Applies source coefficient only in y direction.
! 2) Uses fixed time steps
!
! Created by Joseph Kanney
! Oct. 8, 2003
! Input file version 05
!-----
*CONTROL
MEDIUM=DUAL
TIME_SCHEME=EULER
LIMITER=MUSCL
CLIMATE=CLINTIDX
SOURCE_COEFF, AX=0.0, AY=1.0
!-----
*VELOCITY
STEADY=YES
STEP=1
!-----
*OUTPUT
STEP=2000
SCREEN_IO=OFF
DISCHARGE_STEP=20
!-----
*TIME
TIME_GEN=AUTO
START_TIME=0.0
STOP_TIME =3.15569E+11
NUM_STEP=20000
!-----
*SPECIES
NUCLIDE SYMBOL=PU239, INDEX=1, LAMBDA=DC_PU239, FREE_H2O_DIFF=H2O_PU &
NUCLIDE SYMBOL=U234, INDEX=2, LAMBDA=DC_U234, FREE_H2O_DIFF=H2O_U &
CURIE=SA_U234
NUCLIDE SYMBOL=TH230, INDEX=3, LAMBDA=DC_TH230, FREE_H2O_DIFF=H2O_TH &
CURIE=SA_TH230
NUCLIDE SYMBOL=AM241, INDEX=4, LAMBDA=DC_AM241, FREE_H2O_DIFF=H2O_AM &
CURIE=SA_AM241
NUCLIDE SYMBOL=TH23A, INDEX=5, LAMBDA=DC_TH230, FREE_H2O_DIFF=H2O_TH &
CURIE=SA_TH230
CHAIN CHAIN_NUM=1 NUM_SPECIES=1 NUC_INDICES=1
CHAIN CHAIN_NUM=2 NUM_SPECIES=2 NUC_INDICES=2,3
CHAIN CHAIN_NUM=3 NUM_SPECIES=1 NUC_INDICES=4
CHAIN CHAIN_NUM=4 NUM_SPECIES=1 NUC_INDICES=5
!-----
*PROPERTY
DIFF TORT=MTORT, POROSITY=MPOROS, RETARD=MRTRD
DUAL BLOCK_LEN=HMBLKLIT SKIN_RESIST=SKIN_RES
ADVEC DISP_LNG=DISP_LNG, DISP_TRN=DISP_TRN, TORT= F_TORT, &
POROSITY=FPOROS, RETARD=ZRTRD
!-----
*SOURCE
TERM_DEF SYMBOL=PU239, NUM_POINTS= 2, &
TIMES= 0.0, 1.577845E+9, &
VALUES= 0.0, 1.0, &
IRANGE=67,67 JRANGE=76,76
TERM_DEF SYMBOL=U234, NUM_POINTS= 2, &
TIMES= 0.0, 1.577845E+9, &
VALUES= 0.0, 1.0, &
IRANGE=67,67 JRANGE=76,76
TERM_DEF SYMBOL=TH23A, NUM_POINTS= 2, &
TIMES= 0.0, 1.577845E+9, &
VALUES= 0.0, 1.0, &
IRANGE=67,67 JRANGE=76,76
TERM_DEF SYMBOL=AM241, NUM_POINTS= 2, &
TIMES= 0.0, 1.577845E+9, &
VALUES= 0.0, 1.0, &
IRANGE=67,67 JRANGE=76,76
!-----
*DP_MESH
AUTO INIT_DIST=.001, NUM_NODES=21
!-----
*DISCHARGE_BOUND
NUM_BNDS=2
! Waste Panel Area
BOUND_DEF TOP_LEFT=60,82, BOTTOM_RIGHT=75,70
! LWB
BOUND_DEF TOP_LEFT=7,100, BOTTOM_RIGHT=136,22
!-----
*END

```