# Integration OfDeterministic And Stochastic Models In A 1,4-Dioxane Contaminated Glacial Aquifer System, Washtenaw County, Michigan 

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# INTEGRATION OF DETERMINISTIC AND STOCHASTIC 

 MODELS IN A 1,4-DIOXANE CONTAMINATED GLACIAL AQUIFER SYSTEM, WASHTENAW COUNTY, MICHIGANby

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## THESIS

Submitted to the Graduate School of Wayne State University,

Detroit, Michigan
in partial fulfillment of the requirements

for the degree of<br>MASTER OF SCIENCE<br>2016<br>MAJOR: GEOLOGY

Approved By:

Date

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## Chapter 1 - Introduction

### 1.1. Introduction

Management of contaminated groundwater can be a pervasive and costly problem facing communities that depend on aquifers for their water supply. Accurate conceptualization of the extent and impact of groundwater pollution influences management strategies and ultimately the risk and financial cost to the affected population. Since the advent of numerical groundwater flow and contaminant transport models in the 1960s and 70s, computer simulation has been used to help solve groundwater pollution problems of increasing complexity (Lahkim and Garcia, 1999). Two general and potentially complimentary approaches for conceptualizing aquifer systems within numerical models have been followed: deterministic interpretation by a geologist or engineer (e.g.,Frahm, 2011) and stochastic modeling using geostatistical tools (e.g.,Lahkim and Garcia, 1999 Cypher, 2009, Gao 2011).

It is recognized that, in complicated sedimentary environments, groundwater flow (and therefore movement of dissolved contaminants) preferentially follows pathways of high sediment permeability. Therefore, the incorporation of hydraulic conductivity distributions is an essential part of the groundwater flow and contaminant transport modeling process. Deterministic interpretive methods can oversimplify complex geologic environments, particularly when they rely on effective hydraulic parameters. Additionally, geologic interpretation can be limited by inadequate data density which restricts the effectiveness of numerical modeling in aquifer remediation applications. To address these limitations, this study attempts to integrate both deterministic and stochastic methods. The goal of this hybrid approach is to identify multiple possible outcomes from which more robust conclusions can be drawn to improve the effectiveness of proposed groundwater remediation strategies.

### 1.2 Site Overview

The site for this study is located in Washtenaw County, Michigan. Groundwater within an area of approximately 10 square miles ( $25.9 \mathrm{~km}^{2}$ ) has been affected by 1,4-dioxane within Scio Township, the
northern sections of Lodi and Pittsfield Townships, and the western sections of Ann Arbor Township. The identified source area of the 1,4-dioxane is located at the former Gelman Sciences, Inc. facility located at 600 South Wagner Road in Ann Arbor, which consists of office buildings, manufacturing buildings, water treatment ponds, and undeveloped land (Figure 1-1). The source area is situated within the Huron River watershed and atop the Fort Wayne moraine (Figure 1-2), which is a part of the Thumb Uplands, a regional topographical high stretching from central southern Michigan up to the Saginaw Bay area (Leverett and Taylor, 1915). Additionally, the Fort Wayne moraine is composed of complex Pleistocene glacial sediments (Leverett and Taylor, 1915). Due to the site location on a prominent topographic ridge and the complexity of underlying sediments, impacted groundwater migrated away from the source area in multiple directions (Figure 1-1).

Observed 1,4-dioxane movement in different directions at different depths has led to the designation and description of separate 'plumes' at the site, although the independence of these plumes has been questioned (Lemke, 2004). Currently, different zones of impacted groundwater are described as the Little Lake Area plume (greater than 1ppb surrounding Little Lake), the Core Area and Evergreen plume (greater than 85 ppb surrounding the source area), and the Unit E or Deep Aquifer plume (greater than 85 ppb extending eastward from the source area). Figure 1-1 also depicts the area containing greater than 1 ppb dioxane, delineating the total extent of the impact as estimated by Washtenaw County Public Health (City of Ann Arbor, 2016).

Additionally, because 1,4-dioxane has migrated in separate directions, it is also described in terms of its primary direction, i.e. the western plume, located west of the source area within Scio Township, and the eastern plume located east of the source area within the northern sections of Lodi and Pittsfield Townships, the western sections of Ann Arbor Township and the City of Ann Arbor. 1,4-Dioxane concentrations range from the detection limit of 1 ppb up to several hundred thousand ppb (MDEQ, 2016), which exceed current MDEQ Residential Drinking Water Criteria of 85 ppb. Data were obtained
from a large publically available data set for the Gelman Sciences, Inc. Contamination Site (MDEQ, 2016).

### 1.3 Site History

Gelman Sciences, Inc. began using 1,4-dioxane in medical filter manufacturing operations in 1966 (City of Ann Arbor, 2016). Process wastewater containing 1,4-dioxane was disposed of onsite using several methods including disposal into unlined seepage ponds, spray irrigation onto facility property, and deep well injection. Gelman Sciences continued to use 1,4-dioxane until 1986. Total loading of 1,4dioxane into the subsurface over the 20-year time period is unknown; however, in 1980 PLS reported using 60,000 pounds annually. Discovery of the impact occurred in 1985 when 1,4-dioxane was detected in Third Sister Lake, located approximately 500 feet ( $1,640 \mathrm{~m}$ ) west of the source area (City of Ann Arbor, 2016).

Following discovery in 1986, Gelman discontinued use of 1,4-dioxane and entered into a consent judgement requiring the company to delineate the extent of groundwater contamination and remediate groundwater to MDEQ criteria using pump and treat facilities. After its acquisition of Gelman Sciences in 1997, Pall Life Sciences expanded groundwater monitoring and cleanup operations including the installation of a horizontal well for groundwater extraction and transmission and a series of improved 1,4-dioxane treatment systems (MDEQ, 2004). In 2005, a court ordered institutional control was implemented in the form of a prohibition zone within which groundwater is not permitted to be used for potable water (Figure 1-1). The prohibition zone was later expanded northward effective March 8, 2011 (Washtenaw County Circuit Court, 2005).


Figure 1-1. Site overview and groundwater monitoring well location map, former Gelman Sciences site, Washtenaw County, MI


Figure 1-2. Hydrogeologic setting of former Gelman Sciences site, Washtenaw County, MI

Today, the groundwater monitoring program continues, including quarterly sampling of site-wide groundwater monitoring wells to determine current plume location and pump and treat systems to remove 1,4-dioxane. Over 200 stratigraphic boreholes, monitoring wells, and groundwater extraction or purge wells have been drilled and installed since remediation began onsite. Approximately 7.5 billion gallons of water have been treated and 91,900 pounds of 1,4-dioxane have been removed since the expansion of the pump and treat system by PLS in 1997 (Fotouhi, 2016). Further management of the plume migrating east-northeast underneath the City of Ann Arbor has prompted additional investigation into the timing, position, and concentration of 1,4-dioxane arriving at the Huron River.

### 1.4 1,4-Dioxane

1,4-Dioxane is used as a solvent in manufacturing, and according to the United States Environmental Protection Agency (EPA) air toxics database, is classified as a probable human carcinogen (USEPA, 2000). Chronic exposure from drinking water caused an increase in tumor rates and damage to liver and kidneys in rats (USEPA, 2000). The chemical formula for 1,4-dioxane is $\mathrm{C}_{4} \mathrm{H}_{8} \mathrm{O}_{2}$. It is a hydrocarbon ether arranged in an aromatic ring with oxygen atoms substituted for carbons 1 and 4 . The opposing positioning of the oxygen atoms creates a partial dipole moment across the molecule which, when in solution, allows it to be miscible in water, and therefore has a low $\mathrm{K}_{\mathrm{ow}}$ (USEPA, 2014). Additionally, 1,4dioxane's $K_{o c}$ is 1.23 , which indicates it is weakly retarded by sorption to soil particles, and will readily move from soil to groundwater (USEPA, 2014). The Henry's Law Constant at standard temperature and pressure is $4.80 \times 10^{-6} \mathrm{~atm}^{*} \mathrm{~m}^{3} / \mathrm{mol}$, which indicates it has low volatility. The aromatic structure also deters natural degradation through chemical or biological means (USEPA, 2014). This combination of properties, including 1,4-dioxane's high miscibility coupled with it low degradation, adsorption, and volatility rates allows the molecule to act essentially as a groundwater tracer. For this reason, the documented historical presence and movement of 1,4-dioxane through the subsurface in Washtenaw

County, Michigan, make it useful for studying alternative models representing the distribution of hydraulic conductivity $(K)$ in the complex glacial aquifer system located there.

### 1.5 Hydrostratigraphic Correlation.

Within sedimentary bodies, deposited materials can be classified into two basic categories with respect to groundwater storage and transmissivity: aquifer and aquitard. Aquifer materials have a high capacity for groundwater storage, and are typically associated with coarse-grained materials, such as sand and gravel. These materials have the capacity for larger, well connected pore spaces that allow for a relatively larger, more mobile groundwater mass. In contrast, aquitard materials have a low capacity to transmit groundwater, and are typically associated with poorly sorted or fine-grained sediment, such as clay or silt. Groundwater is likely to exist in smaller volume in these types of sediments, and if it does exist, the interconnectivity of the pore spaces is low, preventing accessibility of any groundwater existing in this area.

Measurements taken on sediment cores collected from boreholes installed throughout the site can be classified as aquifer or aquitard material. When these classifications are assigned to a geographical location, deterministic interpretation can be used to delineate the extent of the two sediment types. Traditionally, stratigraphic interpretation is based on the principle that sedimentary units are laid down in a series of depositional events arranged in a time-progressive pattern, with younger beds atop older beds. Erosional processes form the surficial topography of the sedimentary units. Classical correlation methods, used to interpolate between control points (i.e., subsurface monitoring wells and stratigraphic borings), rely on lithostratigraphic approaches (Prothero and Schwab, 2013) which attempt to correlate aquifer and aquitard materials as bodies of sediment with their own two- or three-dimensional extents. Alternatively, allostratigraphic methods (Prothero and Schwab, 2013) focus on the correlation of bounding surfaces, such as erosional or depositional surfaces. In a previous study, Frahm (2011) used the allostratigraphic approach to complete a deterministic interpretation of the site reconciling
hydrologic data, including hydraulic head and concentration data, with a correlation of natural gamma radiation response to particle size.

### 1.6 Prior Modeling.

Initial groundwater models constructed for the site were grid-based, with hydrologic units assigned uniform thickness and properties. Due to their simplicity, the models were primarily used to determine the efficiency of the groundwater monitoring well network, as it existed at the time the models were constructed. Models did not at that time incorporate the complexity to determine contaminant flow pathways (Cypher, 2009).

Subsequent models, such as that constructed by Brode (2002), incorporated hydrostratigraphic units and surficial water bodies. Brode's model was built within MODFLOW as a three-dimensional finite difference grid consisting of four model layers representing regional aquifer and aquitard units. The layers were assigned hydraulic conductivities that represented two high quality confined aquifers bounded by confining layers with lower permeability. Brode used forward particle tracking through advective transport to examine travel times and concentrations in the Western Plume area as a result of surface water and groundwater interactions.
(Cypher and Lemke, 2009) used MODFLOW to evaluate three alternative three-dimensional conceptualizations of the site based on an increasingly complex discretization of the subsurface. Model complexity ranged from a regional effective aquifer (Model A), through a layered confined aquifer (Model B) similar to the Brode (2002) model in which a uniform $K$ was applied to each layer, to a discretely heterogeneous aquifer (Model $C$ ) in which aquifer $K$ properties were assigned based on zones within aquifer structures. Models were subjected to steady-state and transient flow simulations and calibrated to 1995 head observations at 33 control points which were taken prior to active pumping operations in the western portion of the site. Model outcomes indicated an increasing confidence in
particle pathway predictions with increasing complexity of the hydrogeological environment (Cypher and Lemke, 2009).

### 1.7 Project Outline and Hypotheses

The focus of this study was to compare and contrast differences in predicted groundwater flow pathways simulated using a hybrid approach that integrates two traditional methodologies: deterministic and stochastic modeling. The earlier allohydrostratigraphic model developed by Frahm (2011) provided a deterministic framework to identify aquifer and aquitard units within the subsurface monitoring well data set as well as within a numerical groundwater flow and transport model. The distribution of hydraulic conductivity ( $K$ ) within the aquifer and aquitard units was simulated stochastically using two different geostatistical methods: Sequential Gaussian Simulation (SGS) and Sequential Indicator Simulation (SIS) (Deutsch and Jounel, 1998). The K fields constructed using these methods were inserted into a modified version of a pre-existing groundwater flow and contaminant transport model of the site (Cypher and Lemke, 2009) in a way that incorporated both the deterministic framework along with stochastic variability. Advective transport was simulated to evaluate the rates and pathways by which 1,4-dioxane could be expected to migrate from the source area at the site toward the Huron River several miles to the east. It was expected that the ensemble behavior of SGS and SIS models evaluated using Monte Carlo analysis would differ. Specifically, it was hypothesized that:

1. As transport proceeds downgradient of the source area, the simulated spatial distribution of groundwater contamination would initially disperse, but eventually reorganize into channelized preferential flow pathways, reflecting changes in the relative influence of deterministic versus stochastic model components;
2. Monte Carlo analysis of 1,4-dioxane transport using Sequential Gaussian and Sequential Indicator Simulation outcomes would predict preferential particle discharge locations along the Huron River as a result of channelized flow pathways; and
3. SIS outcomes would exhibit greater spatial variability of preferential flow pathways and discharge locations than SGS outcomes.

Details of the data set and modeling methods used to test these hypotheses are provided in Chapter 2 of this thesis. Results are documented in Chapter 3 and discussed along with a presentation of conclusions in Chapter 4.

## Chapter 2 - Methods

Testing of the hypotheses described in the previous chapter was accomplished using a combination of steps to construct two ensembles of stochastically-generated hydraulic conductivity fields which were subsequently embedded within a numerical groundwater flow model and used to simulate transport of 1,4-dioxane through the glacial aquifer system. The process involved analysis of natural gamma radiation logs from 77 monitoring wells, measurement of hydraulic conductivity in glacial sediment core samples, geostatistical simulation of hydraulic conductivity fields in aquifer and aquitard units, modification of a pre-existing regional MODFLOW model to incorporate a hybrid combination of deterministic and stochastic hydraulic conductivity distributions, and simulation of advective solute transport to evaluate differences in flow and transport model predictions. Each of these steps is described in detail in the sections that follow in this chapter.

### 2.1 Borehole, Well Log, and Core Data

More than 200 monitoring wells, stratigraphic boreholes, and groundwater extraction or purge wells have been drilled since investigations began in 1985. Borehole logs were completed for each of the wells drilled as part of site investigation and remediation activities. Borehole logs included the following information: well identification, date of installation, ground and top of casing (TOC) elevations, total depth, screened interval, static water level (feet bgs), drilling method, and sampling method. Additionally, a geologist's description of sediments, sample depths, and well construction detail was included in each borehole log.

Groundwater monitoring wells were installed in glacial sediments at shallow, intermediate, and deep levels to help delineate the spatial extent of 1,4-dioxane contamination throughout the aquifer system. These descriptors are relative and do not refer to specific depths or elevations. Monitoring wells were drilled using a hollow stem auger, with the exception of MW-96, which was completed with a
rotosonic drill rig. Sediments extracted from MW-96 rotosonic core were collected in polyethylene bags, placed in 5-foot core boxes, and stored within the core storage facility at Wayne State University.

Natural gamma radiation response was logged within 102 wells from their total depth up to ground surface using a Keck analog gamma ray logging unit with a time constant of 5 seconds and a logging speed of 10 feet per minute. Most of these gamma logs were run through hollow stem augers in the drill hole prior to installation of the final well casing. In addition to analog gamma logging through rotosonic override casing, MW-96 was also logged with a Mount Sopris MGXII digital logging unit. Both the analog and digital logging methods utilized a Thallium-activated sodium iodide crystal as a scintillator. A total of 26 well gamma log datasets were identified as unusable for analysis due to incomplete or corrupt data; therefore, 77 wells were utilized for gamma radiation analysis as described below in Section 2.3 and shown in Figure 2-1.

### 2.2 MODFLOW Model

Cypher and Lemke (2009) constructed a numerical groundwater model of the source area using Visual MODFLOW Pro Version 4.2 (Waterloo Hydrogeologic Inc., 2004). Visual MODFLOW (VMODFLOW) uses a finite difference scheme to solve the following groundwater flow equation (Harbaugh et al., 2000):

$$
\begin{equation*}
\delta\left(K_{x x} \delta h / \delta x\right) / \delta x+\delta\left(K_{y y} \delta h / \delta y\right) / \delta y+\delta\left(K_{z z} \delta h / \delta z\right) / \delta z+W=S_{s} \delta h / \delta t \tag{2.1}
\end{equation*}
$$

where $K_{x x}, K_{y y}$, and $K_{z z}$ are hydraulic conductivity vectors in the $x, y$, and $z$ directions respectively; $h$ is the potentiometric head; $W$ is a source or sink term expressed as a volumetric flux per unit volume; $\mathrm{S}_{\mathrm{s}}$ is the specific storage of the porous material; and t is time.

The model was constructed to investigate the Western plume. Using the Michigan State Plane, South Zone coordinate system (1983 Datum), northing and easting extents of the model ranged from 272,000 to 308,500 feet and $13,250,000$ to $13,300,000$ feet, respectively. Telescopically-refined variable grid spacing in the $x-y$ plane created 83 rows ( $x$ ) and 80 columns (y) in the original Cypher (2009) model.

Rows ranged from 312 to 2,250 feet wide and columns ranged from 230 to 400 feet wide. The model extends for 36 layers in the $z$ direction, ranging from 600 to 1,100 feet above mean sea level (amsl). All layers are 10 feet thick, with the exception of the upper most layer, which is 150 feet thick.

The site is located within the Huron River watershed, which exerts a strong influence on surface and groundwater movement within the study area. Surface water bodies in the vicinity of the study area including the Huron River, Mill Creek, Honey Creek, and several significant lakes and ponds were assigned river boundary conditions in the model. River boundaries require specification of three parameters: river bottom elevation, river stage elevation, and conductance. River stage elevation was obtained from the 1983 USGS 7.5 Minute Ann Arbor West Topographic Quadrangle. River bottom elevation was estimated at 5-10 feet below river stage elevation. Conductance is dependent upon several physical properties, including river reach, width, bottom thickness and vertical hydraulic conductivity of the river sediments (Kz) which are not available for all relevant surface water bodies. Therefore, conductance was treated as a fitting parameter and adjusted as a part of the calibration process. Parameter values for river boundaries within the model are provided in Table 2-1.

In addition to river boundary conditions, no flow boundary conditions were utilized in several areas, including cells north of the Huron River drainage divide, south of the surface water drainage divide, and the underlying Coldwater Shale bedrock surface. (See Pruehs (2016) for an analysis of model behavior when the latter assumption of no flow across the bedrock surface is relaxed. Cells located in the upper model layers were designated as inactive.)

Recharge was assigned to the upper-most active cells within the model. To determine recharge values, historical precipitation data were acquired for the University of Michigan collection station in Ann Arbor for the period from 1980 to 2007, which showed average precipitation to be approximately 37 inches per year. Average recharge for soil types which exist in the vicinity of the source area is


Figure 2-1. Location of groundwater wells with natural gamma radiation response measurements, former Gelman Sciences site, Washtenaw County, MI

| Table 2-1. MODFLOW Model River Boundary Condition Parameters |  |  |  |
| :---: | :---: | :---: | :---: |
| River | Stage (feet amsl) | River Bottom (feet amsl) | Conductance (ft²${ }^{\mathbf{} / \text { day })}$ |
| Huron River | $750-830$ | $745-825$ | 2,500 |
| Mill Creek | $830-853$ | $825-848$ | 1,250 |
| Honey Creek | $800-880$ | $795-875$ | 1,250 |
| Honey Creek Tributary | $847-910$ | $845-908$ | 625 |
| $1^{\text {st }}$ Sister Lake | 902 | 890 | 625 |
| $2^{\text {nd }}$ Sister Lake | 905 | 880 | 2,500 |
| $3^{\text {rd }}$ Sister Lake | 905 | 880 | 312.5 |
| Dolph Pond | 902 | 895 | 625 |

approximately 20 percent; however, calibration required an adjustment to recharge rates (Table 2-2) which ranged from $11 \%$ to $15 \%$. Downward adjustment of recharge rates was justified by additional developments constructed in the vicinity of the site, as described by Cypher (2009). Storage parameters, such as effective porosity, specific yield, and specific storage, were also assigned uniform values in the model as shown in Table 2-2. Additional changes made to hydraulic conductivity values within the hybrid model area are discussed in Section 2.2.2.

| Table 2-2. MODFLOW Model Storage Parameters |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| Recharge Zone 2 (in/yr) | Recharge Zone 3 (in/yr) | Effective Porosity | Specific Yield | Specific Storage |
| 5.5 | 4.0 | 0.15 | 0.20 | $3.05 \mathrm{E}-6$ |

### 2.2.1 Grid Refinement

For this study, the original (Cypher and Lemke, 2009) VMODFLOW model grid was refined to facilitate integration of subsequent stochastic and deterministic modeling, which was conducted at a finer resolution. External boundaries of the VMODFLOW model remained the same ( $\mathrm{x}: 13,250,000$ to $13,300,000$ feet, $\mathrm{y}: 272,000$ to 308,500 feet, and z : 600 to 1,100 feet); however, the central portion of the model ranging from $13,268,200$ to $13,292,800$ feet in the $x$ direction and 281,100 to 290,700 feet in the y direction was modified. Grid refinement within this area was resolved to 100 feet ( x ) by 100 feet (y) by 10 feet (z) ( 30 m by 30 m by 3 m ) cells within the central model. The area of the refined VMODFLOW grid corresponds to the extent of the deterministic model discussed in Section 2.2, and is
herein referred to as the "hybrid model area." Grid spacing from the hybrid model area out to external model boundaries was telescoped from 100 to 2,500 feet in the $x$ direction and 100 to 900 feet in the $y$ direction (Figure 2-2).


Figure 2-2. Grid refinement and hybrid model area displayed over active (white) and inactive (blue) cells in VMODFLOW model image, layer 21

### 2.2.2 Boundary Conditions

Grid refinement moved some existing river boundaries away from stream locations; therefore, assigned river boundaries were adjusted to better reflect accurate stream locations. Historically, Allen Creek drained approximately 3,500 acres in the west-central portion of the current City of Ann Arbor prior to the City's development. As the City grew, much of Allen Creek was confined to a series of underground culverts constructed between the early 1920s and 1950, transforming it into a currentlyactive drain. The Allen Creek drain discharges into the Huron River through a single outfall located south of Argo Pond. To accurately model subsurface hydrologic conditions, drain boundary conditions were
added to MODFLOW model cells corresponding to the location and elevation at which subsurface drains are buried, extending from 910 feet to 760 feet amsl at the drain outfall at the Huron River (Figure 2-3).


Figure 2-3. Location of Allen Creek drainshed and drain boundary conditions in VMODFLOW model, layer 18.

### 2.2.3 Model Calibration

The 2009 model created by Cypher was originally calibrated using data from 33 well locations, and adjusted to honor recharge rates, groundwater flux into the Huron River, and equipotential orientation (Cypher and Lemke, 2009). The revised model was recalibrated using 140 head observation control points in steady state simulations. Adjustments were made using a deterministic model, and then checked after each individual stochastic model run. Correlation coefficients ranged from 0.927 and 0.946 for SIS-based simulations and 0.930 to 0.934 for SGS-based simulations. Additional calibration (i.e., model parameter adjustment) was not performed for individual stochastic ensemble realizations.

### 2.3 Deterministic Modeling

Frahm (2011) created a deterministic 3D model of the hydrostratigraphic architecture of the glacial aquifer system that forms the framework used to define the distribution of aquifer and aquitard units across the central portion of the area modeled in the study area of this thesis. Frahm constructed his
deterministic model using a series of steps including detailed sediment physical and chemical analysis, natural gamma response correlation to sediment characteristics, allostratigraphic interpretation of hydrogeologic units on a network of hydrostratigraphic cross sections, and mapping of identified allostratographic surfaces to construct a 3D model of the hydrostratigraphic architecture (Frahm, 2011). Frahm collected sediment samples from the MW-96 rotosonic core and identified sediment texture and mineralogy using sieve analysis, gamma well spectrometry on representative size fractions, optical point counting of grain mounted thin sections for the establishment of mineralogical fractions, and X-ray diffraction analysis for geochemistry of clay-sized minerals. He then compared the sediment dataset generated to natural gamma responses to identify a correlation between sediment characteristics and gamma response.

Frahm (2011) concurrently constructed eight hydrostratigraphic cross-sections which extended the length of the eastern and western plumes using geologists' logs, including gamma logs for lithological control and available groundwater monitoring datasets for hydrological control. Importantly, he constructed his model within an allostratographic framework that emphasized correlation of depositional and erosional surfaces that bounded aquifer and aquitard units. Frahm also used available hydrogeologic data including hydraulic head and contaminant concentration data from the monitoring wells to interpret hydraulic connectivity of aquifer units. Cross sections were interconnected and aligned in N-S and E-W directions, reaching from 13,269,500 to 13,272,000 and 282,500 to 289,500 feet, respectively, which corresponds to the extents of the VMODFLOW hybrid model area that was refined to facilitate integration of subsequent stochastic and deterministic modeling, as mentioned above. Frahm entered the elevation of hydrostratigraphic subunits for each control point into a Rockworks database to interpret his 3D deterministic model. He then interpreted these elevations to create nine bounding surfaces used to separate intervals categorized as predominantly aquifer or aquitard material
and these surfaces were exported as Surfer grids that were used in this study to incorporate Frahm's deterministic hydrostratigraphic model into MODFLOW (Figure 2-4).


Figure 2-4. Visualization of deterministic model aquifer (yellow) and aquitard (green) layers (After Frahm, 2011).

### 2.4 Normalization of Gamma Values

Natural gamma radiation logs were digitized and subsequently converted from depth below top of casing (BTOC) to elevation in feet amsl (Figure 2-5). In bedrock penetrations, gamma responses associated with the underlying Mississippian Coldwater Shale were identified based on their high natural radioactivity. These values were removed from the dataset to restrict gamma analysis to Pleistocene glacial sediments. MW-61 was identified as an outlier and removed from the population because it contained consistently higher than average gamma readings. To account for variation in drilling equipment and casing material, gamma counts were normalized to the highest and lowest gamma response values within the glacial drift section of each well.


Figure 2-5 Natural gamma radiation response measurements in counts per second (cps) from 77 groundwater monitoring wells located across the site

### 2.5 Classification of Aquifer and Aquitard Gamma Populations

Natural gamma radiation response data were compiled into a single dataset and separated into two populations, aquifer and aquitard based on their deterministic classifications as identified by Frahm (Frahm). Additional information regarding the classification of Pleistocene glacial sediments into hydrostratigraphic units within the study area is provided in Section 2.2. For wells drilled after the completion of Frahm's thesis, or those not included in his cross sections and maps, aquifer and aquitard intervals were identified based on the depths of the nine interpolated surface maps generated by Frahm. Population statistics were then calculated independently for the aquifer and aquitard gamma measurement datasets, and a two-tailed t-test was applied to confirm the existence of two separate populations.

### 2.6 Laboratory K Determination

The total natural gamma response logged in MW-96 using the Mount Sopris MGXII digital logging tool was analyzed, and general statistics were calculated (Table 2-3).

| Table 2-3. MW-96 Gamma Log Statistics (cps) |  |
| :--- | ---: |
| Average | 794 |
| Maximum | 1,474 |
| Minimum | 451 |
| Standard Deviation | 179 |
| Mean - 1 Standard Deviation | 615 |
| Mean + 1 Standard Deviation | 973 |

Gamma responses were classified to identify values which varied by one or more standard deviation from the mean. Depths at which these conditions were met for 10 or more successive gamma response measurements were identified for sediment sampling. Sediment samples collected from intervals with higher gamma counts tended to correspond to finer grained glacial sediment (i.e., aquitard) and intervals with lower gamma counts generally corresponded to coarser sediment (i.e., aquifer). Core depths for each interval were identified at the time of sampling to account for shifting of unconsolidated sediment in the rotosonic core bags and boxes. Sediment samples collected from each identified interval were packed into columns and analyzed using falling head parameters to determine their K value. For each sample, three runs were performed and the average was used as the $K$ value.

### 2.7 Gamma to K Correlation

The measured K value of each sediment sample was plotted against the gamma value associated with the corresponding sample depth. An average gamma response value was used when sample depths corresponded to two or more successive gamma readings. K values were then plotted as a function of gamma response. A potential outlier on this plot was identified at sample depth 165'. Upon secondary visual inspection of core sediments, discrepancies between logging description and sediment material were identified. Sample $165^{\prime}$ was therefore removed from the dataset. The K and gamma response datasets were divided into separate aquifer and aquitard populations and fitted with empirical correlations.

### 2.8 Variography

Variography is the process of quantifying the variance of measured values as a function of the distance separating measurement points in time or space (Isaaks and Srivastava, 1989). For spatial relationships, pairs of measurements separated by known distances or lags falling within specified tolerances are used to create experimental semi-variogram plots using the following equation:

$$
\begin{equation*}
\gamma(h)=\frac{1}{2}(N(h)) \sum_{i=1}^{N(h)}\left(x_{i}-y_{i}\right)^{2} \tag{2.4}
\end{equation*}
$$

where $\gamma(h)$ is the calculated semi-variogram value, $N(h)=$ number of data pairs separated by the lag vector $h, x_{i}$ is the property value at the start of the separation vector, and $y_{i}$ is the property value at the end of the separation vector. $\quad X_{i}$ and $y_{i}$ pair values are identified based on defined lag parameters and their tolerances, such as separation distance, azimuth angle and


Figure 2-6. Exponential semiviogram model example. bandwidth. To quantity spatial variability in three dimensions, dip, dip tolerance and vertical bandwidth were also defined.

Normalized gamma data were used as irregularly-spaced data for the calculation of isotropic 3D experimental variograms using the Geostatistical Software Library (GSLIB) GAMV program (Deutsch and Jounel, 1998). Variograms were calculated separately for aquifer and aquitard gamma populations with vertical and horizontal orientations, resulting in four experimental variograms (vertical and horizontal aquifer and vertical and horizontal aquitard). Vertical variograms incorporated small lag distances (1 ft or 30 cm ) to account for high data density in the vertical direction. Vertical variograms were oriented at a 90 degree dip with a 2.5 foot horizontal radius to calculate vertical variation within each well independently. Average horizontal distance between control points (wells) was determined using a
custom-built Fortran program. As a consequence of the low well density within the large study area for this investigation, horizontal variograms used the average distance between wells (1,600 ft or 490 m ) as the lag distance. Horizontal variograms were constrained by a 3 foot vertical window oriented in horizontal slices across the site. GAMV parameter files for vertical and horizontal semi-variograms are included in Appendix A. Experimental variograms (Figure 2-6) were fit with exponential variogram models conforming to the following equation:

$$
\begin{equation*}
\gamma(h)=n+c *\left(1-e^{(-3 h / a)}\right) \tag{2.5}
\end{equation*}
$$

where $\gamma(\mathrm{h})$ is the semi-variogram value, n is the nugget contribution attributable to measurement uncertainty, c is the positive variance contribution value or sill, h is the separation or lag distance, and a is the effective range where $95 \%$ of the maximum semi-variance is reached. Variogram models provide the basis for the subsequent stochastic simulation described below.

### 2.9 Stochastic Simulation

SGS and SIS are stochastic simulation methods that sequentially add estimated values to a conditioning data set (measured or specified values) from which the estimated values are calculated (Deutsch and Journel, 1998). Both methods visit unsampled locations in a randomly determined order, derive an estimate at that location based on a weighted linear combination of information from nearby conditioning or previously estimated points, and continue to the next randomly selected location until all unsampled locations are estimated. Both simulation methods use the variogram model as described above to determine values at locations not directly measured, allowing for population estimation with incomplete sampling and ensuring that the spatial structure of the simulated population represents the variogram model.

More specifically, SGS uses ordinary kriging to calculate a local conditional cumulative distribution function (LCCDF) at unestimated locations whereas SIS uses indicator kriging to calculate the LCCDF. A random generator is then used to select an estimated value from the LCCDF. That value is assigned to
the point and the process is repeated at the next randomly selected location with all previously simulated values treated as conditioning data to calculate the new local conditional probability distribution.

SGS assumes populations are normally distributed, whereas SIS allows for nonparametric distributions. This represents a major advantage for SIS in that indicator classes can be defined based on threshold values that allow high, intermediate, and low classes of values to be simulated differently. As a result, realizations created using SGS tend to maximize the entropy of values throughout the simulated domain, whereas SIS can create distributions that maintain modeled continuity among high, intermediate, and low values within different modeled regions. This added flexibility comes at the cost of needing to model variograms for each of the indicator classes specified during SIS. Both SGS and SIS are capable of creating an infinite number of equally probable realizations of stochastic simulation results for a given set of conditioning data and variogram models.

In this study, normalized aquifer and aquitard gamma values were used as conditioning data in GSLIB SGSIM and SISSIM programs (Deutsch and Jounel, 1998). Gamma values were assigned $\mathrm{x}, \mathrm{y}$, and z coordinate to allow for three-dimensional simulation within the hybrid model area as described in Section 2.2.1. A single gamma value was simulated for each cell and assigned the cell's center-point coordinates. Ensembles of 100 SGS-based and 100 SIS-based realizations were created for aquifer and aquitard gamma populations separately, creating a total of 400 simulations. Parameter files used for SGS and SIS simulation are included in Appendix A.

### 2.10 Combined Deterministic-Stochastic Models

Two FORTRAN programs (DETERMINE.for and GSL2VMF16.for) were written and used to combine the deterministic and stochastic models in the hybrid model area of the VMODFLOW model. Copies of DETERMINE.for and GSL2VMF.for are included in Appendix B.

First, DETERMINE.for compared the central $x-y-z$ coordinates of each MODFLOW model cell with the elevations of Frahm's (2011) hydrostratigraphic surfaces to determine whether the cell should be classified as aquifer, aquitard, or bedrock. Minor discrepancies identified between the bottom of the Frahm (2011) hydrostratigraphic surfaces and the top of the bedrock layer in the pre-existing VMODFLOW model were randomly assigned as aquifer or aquitard in the same proportions found in the remainder of the hybrid model area.

Second, GSL2VMF16.for integrated SGS or SIS simulation results with DETERMINE.for results to create formatted MODFLOW property (.vmp) files for use within the modified VMODFLOW model. Stochastic gamma values from the SGS or SIS aquifer and aquitard simulations were assigned to the corresponding cell in the hybrid model grid area based on their classification in the DETERMINE.for output file. Aquifer and aquitard gamma values were then converted to hydraulic conductivity values using independent correlations. The model was given an $x$ :y anisotropy at a factor of 2:1. Vertical K values were divided by 10 to impose a $10: 1$ horizontal to vertical anisotropy in $K$ values. $K$ values generated through these processes were then coded with one of 40 different pre-assigned property values and used to define K indices in the .vmp property file. Property values are shown in Table 2-4.

K values for cells outside the hybrid model area were assigned a uniform value, property value \#1 as described above in Table 2-1, based on the geometric average $K$ values within the hybrid model area. The property values anisotropy in the $K_{x}-K_{y}$ vs $K_{z}$ dimensions were consistent (10:1 ratio) with the values assigned within the hybrid model area. Bedrock cells were inactivated so that the underlying bedrock surface was treated as a no-flow boundary. This process was repeated for each realization of the SGS and SIS ensembles, resulting in a total of 200 .vmp files.

| Table 2-4. MODFLOW K Class Values |  |  |  |
| :---: | :---: | :---: | :---: |
| Property Value \# | $\mathbf{K}_{\mathbf{x}}(\mathrm{ft} /$ day $)$ | $\mathbf{K}_{\mathbf{y}}(\mathrm{ft} /$ day $)$ | $\mathbf{K}_{\mathbf{z}}(\mathrm{ft} /$ day $)$ |
| 1 | $0.11100 \mathrm{E}+02$ | $0.11100 \mathrm{E}+02$ | $0.11100 \mathrm{E}+01$ |
| 2 | $0.50000 \mathrm{E}-02$ | $0.50000 \mathrm{E}-02$ | $0.50000 \mathrm{E}-03$ |
| 3 | $0.30000 \mathrm{E}-01$ | $0.30000 \mathrm{E}-01$ | $0.30000 \mathrm{E}-02$ |
| 4 | $0.75000 \mathrm{E}-01$ | $0.75000 \mathrm{E}-01$ | $0.75000 \mathrm{E}-02$ |
| 5 | $0.15000 \mathrm{E}+00$ | $0.15000 \mathrm{E}+00$ | $0.15000 \mathrm{E}-01$ |
| 6 | $0.25000 \mathrm{E}+00$ | $0.25000 \mathrm{E}+00$ | $0.25000 \mathrm{E}-01$ |
| 7 | $0.35000 \mathrm{E}+00$ | $0.35000 \mathrm{E}+00$ | $0.35000 \mathrm{E}-01$ |
| 8 | $0.45000 \mathrm{E}+00$ | $0.45000 \mathrm{E}+00$ | $0.45000 \mathrm{E}-01$ |
| 9 | $0.55000 \mathrm{E}+00$ | $0.55000 \mathrm{E}+00$ | $0.55000 \mathrm{E}-01$ |
| 10 | $0.65000 \mathrm{E}+00$ | $0.65000 \mathrm{E}+00$ | $0.65000 \mathrm{E}-01$ |
| 11 | $0.80000 \mathrm{E}+00$ | $0.80000 \mathrm{E}+00$ | $0.80000 \mathrm{E}-01$ |
| 12 | $0.95000 \mathrm{E}+00$ | $0.95000 \mathrm{E}+00$ | $0.95000 \mathrm{E}-01$ |
| 13 | $0.12500 \mathrm{E}+01$ | $0.12500 \mathrm{E}+01$ | $0.12500 \mathrm{E}+00$ |
| 14 | $0.20000 \mathrm{E}+01$ | $0.20000 \mathrm{E}+01$ | $0.20000 \mathrm{E}+00$ |
| 15 | $0.37500 \mathrm{E}+01$ | $0.37500 \mathrm{E}+01$ | $0.37500 \mathrm{E}+00$ |
| 16 | $0.75000 \mathrm{E}+01$ | $0.75000 \mathrm{E}+01$ | $0.75000 \mathrm{E}+00$ |
| 17 | $0.15000 \mathrm{E}+02$ | $0.15000 \mathrm{E}+02$ | $0.15000 \mathrm{E}+01$ |
| 18 | $0.25000 \mathrm{E}+02$ | $0.25000 \mathrm{E}+02$ | $0.25000 \mathrm{E}+01$ |
| 19 | $0.40000 \mathrm{E}+02$ | $0.40000 \mathrm{E}+02$ | $0.40000 \mathrm{E}+01$ |
| 20 | $0.60000 \mathrm{E}+02$ | $0.60000 \mathrm{E}+02$ | $0.60000 \mathrm{E}+01$ |
| 21 | $0.85000 \mathrm{E}+02$ | $0.85000 \mathrm{E}+02$ | $0.85000 \mathrm{E}+01$ |
| 22 | $0.11500 \mathrm{E}+03$ | $0.11500 \mathrm{E}+03$ | $0.11500 \mathrm{E}+02$ |
| 23 | $0.14500 \mathrm{E}+03$ | $0.14500 \mathrm{E}+03$ | $0.14500 \mathrm{E}+02$ |
| 24 | $0.17500 \mathrm{E}+03$ | $0.17500 \mathrm{E}+03$ | $0.17500 \mathrm{E}+02$ |
| 25 | $0.20500 \mathrm{E}+03$ | $0.20500 \mathrm{E}+03$ | $0.20500 \mathrm{E}+02$ |
| 26 | $0.23500 \mathrm{E}+03$ | $0.23500 \mathrm{E}+03$ | $0.23500 \mathrm{E}+02$ |
| 27 | $0.27500 \mathrm{E}+03$ | $0.27500 \mathrm{E}+03$ | $0.27500 \mathrm{E}+02$ |
| 28 | $0.35000 \mathrm{E}+03$ | $0.35000 \mathrm{E}+03$ | $0.35000 \mathrm{E}+02$ |
| 29 | $0.45000 \mathrm{E}+03$ | $0.45000 \mathrm{E}+03$ | $0.45000 \mathrm{E}+02$ |
| 30 | $0.55000 \mathrm{E}+03$ | $0.55000 \mathrm{E}+03$ | $0.55000 \mathrm{E}+02$ |
| 31 | $0.70000 \mathrm{E}+03$ | $0.70000 \mathrm{E}+03$ | $0.70000 \mathrm{E}+02$ |
| 32 | $0.90000 \mathrm{E}+03$ | $0.90000 \mathrm{E}+03$ | $0.90000 \mathrm{E}+02$ |
| 33 | $0.12500 \mathrm{E}+04$ | $0.12500 \mathrm{E}+04$ | $0.12500 \mathrm{E}+03$ |
| 34 | $0.17500 \mathrm{E}+04$ | $0.17500 \mathrm{E}+04$ | $0.17500 \mathrm{E}+03$ |
| 35 | $0.25000 \mathrm{E}+04$ | $0.25000 \mathrm{E}+04$ | $0.25000 \mathrm{E}+03$ |
| 36 | $0.35000 \mathrm{E}+04$ | $0.35000 \mathrm{E}+04$ | $0.35000 \mathrm{E}+03$ |
| 37 | $0.45000 \mathrm{E}+04$ | $0.45000 \mathrm{E}+04$ | $0.45000 \mathrm{E}+03$ |
| 38 | $0.55000 \mathrm{E}+04$ | $0.55000 \mathrm{E}+04$ | $0.55000 \mathrm{E}+03$ |
| 39 | $0.67500 \mathrm{E}+04$ | $0.67500 \mathrm{E}+04$ | $0.67500 \mathrm{E}+03$ |
| 40 | $0.87500 \mathrm{E}+04$ | $0.87500 \mathrm{E}+04$ | $0.87500 \mathrm{E}+03$ |

### 2.11 Hybrid Groundwater Flow and Transport Modeling

Because of the size of the modeled area relative to the number of well control points, simulation outcomes were expected to vary greatly from realization to realization. Therefore, Monte Carlo analysis was used to assess model prediction uncertainty for the SGS and SIS hybrid model ensembles. Completed .vmp files generated by GSL2VMF16.for were manually copied into the modified VMODFLOW model project file and individually run and assessed for each realization (Figure 2-7). Each


Figure-2-7. Map view of VMODFLOW model layer 20 showing integrated aquifer and aquitard simulated $K$ values within the hybrid model area. Lighter color values indicate aquifer material, whereas darker color values indicate aquitard material
model was run in steady state and mass balance errors were checked to ensure they were less than $0.5 \%$ and that volumetric flux of water out of the model through the Allen Creek Drain conformed to historical average flow rates. The head calibration for each run was checked using plots of predicted versus observed head values for 77 head observation well control points.

Advective 1,4-dioxane transport was simulated using MODPATH (Pollock, 1994) forward particle tracking. Forward particle tracking uses the steady state head gradient and hydraulic conductivity field to calculate a velocity and subsequent travel path through the finite difference model grid for individual particles during each time step of the numerical simulation. Consequently, it provides a representation of advective particle transport pathways, but does not account for dispersion of solute contaminants in
response to small-scale mechanical mixing or chemical gradients. For this study, a total of 100 particles were placed as line sources near Wagner Road in row 112 of the modified VModflow model (Figure 2-8). Particles were placed in aquifer material in layers 11, 18, 22, 26, and 29 at depths corresponding to 1,4dioxane detection in monitoring wells documented in Frahm's (2011) cross section B-B'. Particles were positioned so that the cell to particle ratio was 1:1.


Figure 2-8. South-north cross section from VMODFLOW model column 112 showing particle placement locations. Cells located between the black lines are active, with deterministic classifications of aquifer and aquitard.

Following completion of each run, information including the calibration curve, a pathline map image, particle tracking pathline data (.mpF file), and Allen Creek Drain flux were collected. Pathline data included in each .mpF file indicated the position within the grid for each particle as it moved through individual model cells from the line source to its eventual point of discharge.

### 2.12 Post Processing of Transport Simulation Results

Two additional computer programs (WALL.for and POLYPATH.for) were written and used to collect and compare advective transport results for the SGS and SIS ensembles. Both programs interrogated individual particle pathline information from the set of 100 .mpF files in each ensemble. In total, 100
particles in each of 100 realizations yielded information on the predicted pathways of 100,000 particles in each ensemble.

WALL.for calculated the position of particles passing through nine down-gradient cross-sectional areas positioned between the source area and the Huron River. Each cross section or 'wall' that the particles passed through was oriented in a north-south direction, parallel to MODFLOW model columns and approximately perpendicular to the primary east-west direction of transport (Figure 2-9). Sections were spaced $500 \mathrm{~m}(1,600 \mathrm{ft})$ apart, beginning 500 m downgradient from the particle line source location at Wagner Road, with the exception of the last section which was positioned at the Huron River, approximately 467 m east of the eighth section. For each section, the model cell in which each particle first passed into the section was recorded. If particles passed along the section, or, in the rare event that particles passed through the section and then reentered it from the east, those cells were not included in the count for each section. Output from WALL.for was used to generate statistics for hypothesis evaluation and to create ensemble averaged $y-z$ particle density profiles illustrating areas of high particle counts, or preferential flow pathways through each of the seven sections. WALL.for was also used to identify and compile statistics for particles intercepted by the Allen Creek Drain before exiting the model at the Huron River. A copy of WALL.for is included in Appendix B.

Similarly, POLYPATH.for also used information from the .mpF files to track the $x-y$ coordinates of particles as they moved through the MODFLOW model. Output from POLYPATH.for was used to generate statistics for hypothesis evaluation and to create ensemble averaged $x-y$ particle density maps illustrating differences in probable pathways for the SGS and SIS ensembles. Ensemble results collated using WALL.for and POLYPATH.for used to evaluate the study hypotheses are reported in Chapter 3. Comparative statistics include cell counts, mean, standard deviation, and variance analysis of particle coordinate distributions relative to the principle model axes. A copy of POLYPATH.for is included in Appendix B.


Figure 2-9. WALL cross section locations where downgradient particle pathway locations were compared

## Chapter 3 - Results

Results from the glacial sediment gamma radiation and hydraulic conductivity analysis, MODFLOW model modification, and advective transport modelling activities described in the prior chapter are reported here.

### 3.1 Gamma and Hydraulic Conductivity Analysis

Gamma values were segregated into aquifer and aquitard populations based on the Frahm (2011)


Figure 3-1. Distributions of normalized gamma response data separated into two populations based on deterministic
aquifer/aquitard classifications. Population means are shown.
deterministic hydrostratigraphic surfaces described in Section 2.3. Probability distribution functions created from normalized natural gamma response data showed overlap in the two datasets (Figure 3-1). Additionally, the means for aquifer and aquitard data were 0.387 cps and 0.309 cps respectively; therefore, data were subjected to statistical testing to validate separation
into different populations.
Data were subjected to a Chi-Squared test where the null hypothesis was the data were normally distributed and the alternative hypothesis was the data were not normally distributed. The null hypothesis failed to be rejected at a confidence level of 0.05 . Because the data populations were identified as normally distributed, they were subjected to the parametric two-tailed F -Test with the null hypothesis set that the variances of aquifer and aquitard population datasets are equal and the alternative hypothesis set that the variances of the aquifer and aquitard population are not equal to each other. The test rejected the null hypothesis at a confidence level of 0.05 ; therefore, the alternative hypothesis was accepted.

Because the two applied tests indicated the two populations were both normally distributed with different variances, a two-tailed Paring-Design t-test was applied with a null hypothesis that the means of the aquifer and aquitard datasets are equal to one another and the alternative hypothesis that the means of the two populations are different. The test rejected the null hypothesis at a confidence level of 0.05 . Because statistical testing indicates the two separated datasets are normally distributed with different variances and means, the populations were treated as separate. A summary of statistical tests applied and their outcome is described in Table 3-1.

| Table 3-1. Aquifer and Aquitard Natural Gamma Radiation Response Datasets Probability <br> Distribution Function and Statistical Tests |  |  |
| :---: | :---: | :---: |
| Test | Result | Confidence Level |
| Chi-Squared | Fail to reject $H_{o}$ | 0.05 |
| F-Test (two-tailed) | Reject $H_{o}$ | 0.05 |
| Pairing Design t-Test (two-tailed) | Reject $H_{o}$ | 0.05 |

### 3.2 Gamma to K Associations

K values for samples collected from aquifer segments of the MW-96 core ranged from $4.08 \times 10^{-7}$ $\mathrm{cm} / \mathrm{s}$ to $3.59 \times 10^{-4} \mathrm{~cm} / \mathrm{s}$. K values for aquitard segments samples ranged from $1.58 \times 10^{-6} \mathrm{~cm} / \mathrm{s}$ to $2.91 \times 10^{-}$ ${ }^{4} \mathrm{~cm} / \mathrm{s}$. Aquifer and aquitard-based empirical K values were plotted against a corresponding gamma value (Figures 3.2 and 3.3 ) and fitted with the following regressions:

$$
\begin{align*}
& K_{a q}=0.003 e^{-0.005 \gamma}  \tag{3.1}\\
& K_{a t}=3 \times 10^{-7}+0.0004 \gamma \tag{3.2}
\end{align*}
$$

where $K_{a q}$ is equal to the hydraulic conductivity for aquifer material, $\mathrm{K}_{\mathrm{at}}$ is the hydraulic conductivity for aquitard material, and $\gamma$ is equal to the measured natural gamma response in counts per minute. $R^{2}$ values are 0.63 and 0.70 for aquifer and aquitard datasets, respectively. Summaries of aquifer and aquitard-based correlations are provided in Figure 3.2 and 3.3.


Figure 3-2. Gamma response to K empirical correlation for aquifer dataset


Figure 3-3. Gamma response to $K$ empirical correlation for aquitard dataset.

### 3.3 Variography

Two sets of variogram models were constructed to support stochastic simulation using 1) SGS, and 2) SIS. In the first case, vertical variogram exponential models calculated for normalized aquifer and aquitard datasets with all gamma responses measured in the shale bedrock removed. Both SGS and SIS variograms used a nugget of 0.0085 (Figure 3-4). Variogram values showed a periodicity, alternating between high and low semivariogram values approximately every 5 feet. Maximum variation in the vertical direction was reached at 120 feet and 80 feet for aquifer and aquitard data, respectively (Figure 3-4). Horizontal exponential variogram models used the nugget identified through vertically oriented variogram modeling, 0.0085 (Figure 3-5). Maximum variation in the horizontal direction was reached at 750 feet for aquifer data and 600 feet for aquitard data (Figure 3-5).

SIS requires a non-parametric model of the conditional cumulative distribution function (ccdf), which avoids assumptions about the distribution shape (e.g., Gaussian) and allows for correlation of extreme values (Goovaerts, 1997). Indicator variograms were therefore constructed for nine thresholds corresponding to deciles of the normalized gamma cumulative distribution function (cdf). Vertical and horizontal variograms were modeled independently using standardized sills. A geometric model of anisotropy was used to account for differing ranges in the N-S and E-W directions. The tails of each distribution were extrapolated using linear interpolation. Variogram model parameters for each indicator class are given in Table 3-2.


Figure 3-4. Vertical experimental variograms for aquifer and aquitard gamma data populations and corresponding variogram model parameters.


Figure 3-5. Horizontal experimental variograms for aquifer and aquitard gamma data populations and corresponding variogram model parameters

|  |  | Table 3-2. Indicator Variogram Model Parameters |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Indicator Class |  |  |  |  |  |  |  |  |
|  | Parameter | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| Aquitard Vertical | n | 0.61 | 0.61 | 0.53 | 0.46 | 0.47 | 0.51 | 0.62 | 0.65 | 0.58 |
|  | c | 0.17 | 0.30 | 0.35 | 0.35 | 0.33 | 0.23 | 0.12 | 0.10 | 0.08 |
|  | a (ft) | 18 | 30 | 38 | 35 | 35 | 18 | 12 | 15 | 15 |
| Aquifer Vertical | n | 0.6 | 0.58 | 0.45 | 0.43 | 0.46 | 0.52 | 0.58 | 0.55 | 0.48 |
|  | c | 0.17 | 0.30 | 0.30 | 0.30 | 0.25 | 0.18 | 0.12 | 0.10 | 0.08 |
|  | a (ft) | 6 | 40 | 35 | 40 | 35 | 35 | 35 | 15 | 15 |
| Aquitard Horizontal | n | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 |
|  | c | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 |
|  | $\mathrm{N}-\mathrm{S}$ a (ft) | 900 | 900 | 1,000 | 600 | 600 | 800 | 900 | 800 | 900 |
|  | E-W a (ft) | 1,200 | 800 | 700 | 800 | 800 | 800 | 1,200 | 800 | 1,300 |
|  | Vertical a (ft) | 18 | 30 | 38 | 35 | 35 | 18 | 12 | 15 | 15 |
| Aquifer Horizontal | n | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 |
|  | c | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 | 0.90 |
|  | N-S a (ft) | 700 | 800 | 900 | 1,000 | 1,100 | 1,000 | 900 | 800 | 700 |
|  | E-W a (ft) | 1,200 | 1,300 | 1,000 | 800 | 900 | 1,100 | 1,300 | 1,500 | 1,700 |
|  | Vertical a (ft) | 6 | 40 | 35 | 40 | 35 | 35 | 35 | 15 | 15 |

### 3.4 Stochastic Simulation

Stochastic simulation through SGSIM and SISIM produced a total of 400 simulations of gamma data, broken into four separate ensembles: 100 SGS-based aquifer simulations, 100-SGS-based aquitard simulations, 100 SIS-based aquifer simulations, and 100 SIS-based aquitard simulations. Simulations were created within the hybrid model area, with one simulated gamma value per $100 \times 100 \times 10$ foot cell.

### 3.5 Combined Deterministic-Stochastic Models

DETERMINE.for generated a 3D grid of aquifer and aquitard indicator values based on the 2D deterministic aquifer and aquitard surfaces described in Section 2.3. The DETERMINE.for output grid
was utilized in GSL2VMF16.for to integrate sets of SGS or SIS-based aquifer and aquitard simulated gamma values and produce an amalgamation of aquifer and aquitard-based simulated gamma values. The final integrated cube corresponding to the hybrid model area was converted to $K$ values based on empirically-derived relationships (Equations 3.2 and 3.3). This created 200 K value realizations, 100 based on SGS simulations and 100 based on SIS simulation for Monte Carlo analysis. Output files were formatted as MODFLOW .vmp property files for integration into VMODFLOW and subsequent flow and transport simulation.

### 3.6 Hybrid Groundwater Flow and Transport Modeling

Particle pathline images, calibration curves, and VMODFLOW .mpF files were collected from each simulation outcome as described in Section 2.6. During each simulation, model calibration of hydraulic head values was tracked; however, the MODFLOW model was calibrated prior to this study, and subsequent modification of boundary conditions and model parameters did not significantly alter the calibration beyond acceptable limits. Correlation coefficients between simulated and real hydraulic head data for SGS and SIS-based model runs were an average of 0.932 and 0.938 , respectively. A summary of calibration statistics for each model type is provided below in Table 3-3.

|  | Table 3-3. Head Calibration Summary for SIS and SGS-Based Model Runs |  |
| :---: | :---: | :---: |
|  | SGS-Based Model Averages | SIS-Based Model Averages |
| Residual Mean (ft) | 0.6306 | 0.1924 |
| Abs. Residual Mean (ft) | 4.971 | 4.572 |
| Standard Error (ft) | 0.6628 | 0.6319 |
| RMS (ft) | 7.839 | 7.597 |
| Normalized RMS (\%) | 5.707 | 5.578 |
| Correlation Coefficient (ft) | 0.9319 | 0.9375 |

Particle path line images recorded indicated groundwater flow and contaminant migration direction to primarily be to the east from the source area towards the Huron River. For the deterministic model, the majority of the particles travel within the hybrid model area (Figure 3-6). Particles which exited the hybrid model area entered a region of uniform K values and thereafter


Figure 3-6. $X-Y$ particle pathline image for deterministic model outcome. Particle pathlines are depicted as blue when moving towards the viewer (up), and brown when moving away (down).


Figure 3-7. X-Y particle pathline image for SGS-based outcome 001. Particle pathlines are depicted as blue when moving towards the viewer (up), and brown when moving away (down).


Figure 3-8. X-Y particle pathline image for SIS-based outcome 001. Particle pathlines are depicted as blue when moving towards the viewer (up) and brown when moving away (down).


Figure 3-9a. Y-Z Cross sectional views of the particle pathway ensembles for SGS and SIS-based hybrid model outcomes. View looking east (downgradient).


Figure 3-9b. Y-Z Cross sectional views of the particle pathway ensembles for SGS and SIS-based hybrid model outcomes. View looking east (downgradient).
migrate towards the regional sink, the Huron River. Representative realizations for the SGS and SIS model outcomes as shown in Figures 3-7 and 3-8, respectively.

### 3.7 Downgradient Cross-Sectional Analysis

Figures 3-9a and 3-9b depicts ensemble average particle distributions for the 100 SGS and SIS realizations at a series of downgradient profiles oriented perpendicular to the general eastward direction of advective transport (Figure 2-9). These cross sections ("walls") show patterns of similarity and differences for the two hybrid model types. Similarities between the SGS and SIS ensembles include similar gross patterns of particle distribution, reflecting the distribution of aquifer and aquitard units inherent in the deterministic model (i.e., particles concentrate in the aquifer units). Visually, the degree of particle concentration and spreading also appears similar, with the greatest concentration of particles apparent in the second profile located 3200 feet down gradient. Differences in the degree of spread and in the apparent center of mass for each ensemble are also apparent in Figure 3-10. Differences in particle counts and spreading as a function of migration distance downgradient of the source location at Wagner Road are explored quantitatively below.

### 3.7.1 Advective Particle Count Results

In both the SGS and SIS models, approximately 400 to 950 cells of the total 4,212 cells comprising each cross section had at least a single particle detection. Cells without particles were not included in subsequent analyses. Particle counts were statistically summarized, including the number of cells with at least a single particle detected (Count), sum total of all tracked particles for model ensembles (Sum), arithmetic average number of particles per cell (Mean), standard deviation of the particle counts (St Dev), and the maximum particle count detected (Max) (Tables 3-4 and 3-5). Similar statistics were calculated on the outcome of the deterministic model (Table 3-6); however, because the deterministic model represents a single realization, the Sum, Mean, and Max particle counts were scaled by 100 to make them comparable to the hybrid model ensemble outcomes.

For the hybrid model outcome ensembles, the number of cells with at least one particle detection (Count) increased as the distance from the source increased. This trend changed at approximately 11,200 to 12,800 feet downgradient and the number of cells with at least one detection began to decrease. This trend was not observed in the deterministic model outcome, which showed that the number of cells with at least one detection decreased prior to reaching the first downgradient cross section. This value stayed below the initial count number for the entire distance to the Huron River, with the lowest number ( 62 cells) observed at approximately 12,800 feet downgradient. All particles were counted in all downgradient cross-sections in the deterministic outcome.

Average number of particles per cell constantly decreased in both SGS and SIS-based hybrid models from the source area to the Huron River, from 100 particles per cell to 13.02 particles per cell and 7.69 particles per cell, respectively (Figure 3-10). However, the particle per cell averages for the deterministic outcome increased above the initial concentration of 100 particles per cell at the first cross section 1,600 feet downgradient to 119 particles per cell. The highest value (161 particles per cell) was detected at the second to last cross-section, approximately 12,800 feet downgradient.

The standard deviation of particle counts in the SGS and SIS based hybrid models both initially increased from 0 at the source area to their maximum values of 40.34 and 37.53 , respectively, at approximately 3,200 feet downgradient before again beginning to decrease until the last cross-section (Table 3-4). Additionally, the maximum detected concentration also followed this pattern, with the highest number of particles detected at the same distance, 3,200 feet downgradient, for both the SGSbased model (221 particles) and the SIS-based model (240 particles) (Figure 3-11).

| Table 3-4. Particle Pathway Statistics for SGS, SIS, and Deterministic Models Cross Section Data |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Down- <br> Gradient | 0 | 1,600 | 3,200 | 4,800 | 6,400 | 8,000 | 9,600 | 11,200 | 12,800 | 14,200 |
| SGS |  |  |  |  |  |  |  |  |  |  |
| Count | 100 | 421 | 460 | 460 | 620 | 858 | 991 | 926 | 681 | 594 |
| Sum | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 9,953 | 9,834 | 8,724 | 7,734 |
| Mean | 100 | 23.75 | 21.74 | 21.74 | 16.13 | 11.66 | 10.04 | 10.62 | 12.81 | 13.02 |
| St Dev | 0 | 23.54 | 40.34 | 25.08 | 19.93 | 14.35 | 11.36 | 10.41 | 12.93 | 11.99 |
| Max | 100 | 113 | 221 | 100 | 136 | 64 | 82 | 72 | 89 | 77 |
| SIS |  |  |  |  |  |  |  |  |  |  |
| Count | 100 | 461 | 520 | 523 | 719 | 856 | 870 | 899 | 707 | 585 |
| Sum | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 9,955 | 8,872 | 6,232 | 4,498 |
| Mean | 100 | 21.69 | 19.23 | 19.12 | 13.91 | 11.68 | 11.44 | 9.87 | 8.81 | 7.69 |
| St. Dev | 0 | 27.64 | 37.53 | 26.68 | 18.02 | 13.84 | 13.66 | 13.39 | 14.84 | 9.63 |
| Max | 100 | 173 | 240 | 211 | 92 | 85 | 69 | 83 | 96 | 49 |
| Deterministic |  |  |  |  |  |  |  |  |  |  |
| Count | 100 | 84 | 76 | 78 | 85 | 80 | 82 | 73 | 62 | 70 |
| Sum | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 | 10,000 |
| Mean | 100 | 119 | 132 | 128 | 118 | 125 | 122 | 137 | 161 | 143 |
| St. Dev | 0 | 0.424 | 0.677 | 0.556 | 0.413 | 0.516 | 0.522 | 0.755 | 0.947 | 0.714 |
| Max | 100 | 300 | 500 | 300 | 300 | 300 | 400 | 500 | 500 | 400 |



Figure 3-10. Graph of particle count averages by distance from source (feet downgradient) from SGS, SIS, and deterministic model cross section data.


Figure 3-11. Particle count maximums by distance from source in feet downgradient from SGS, SIS, and deterministic model cross section data.

### 3.7.2 Advective Particle Spread Results

Spread was observed in the distribution of particles through analysis of the standard deviation of the $Y$ and $Z$ coordinates of each particle passing through the downgradient profiles (Figures 3-12 and 313). Because both hybrid model types and the deterministic model utilized the same particle source locations, the standard deviations calculated from the initial spread at Wagner Road were the same in both the $Y$ ( 794.1 feet) and $Z$ ( 60.7 feet) directions for all models.
$Y$ coordinate analysis showed an increase in standard deviation as the distance from the source area increased for both hybrid model types; however, standard deviation of the Y coordinate in the deterministic model showed increasing and decreasing standard deviation values (Figure 3-12). Spread initially increased from the source area, decreasing between 3,200 and 4,800 feet downgradient. Spread again began to increase after 4,800 feet downgradient, and continued to increase until approximately 11,800 feet downgradient, when the standard deviation again began to decrease. Additionally, standard deviation of the hybrid model types showed less initial dispersion than the deterministic model outcome, until between 3,600 feet and 4,800 feet downgradient, when the standard deviation of the hybrid models began to exceed that of the deterministic model. The standard
deviation values of hybrid model types then exceeded the spread of the deterministic model for the rest of the distance downgradient. In general, standard deviation of $Y$ coordinate values in the SGS ensemble exceeded those of the SIS ensemble.

A similar pattern was observed in the $Z$ coordinate analysis, where the deterministic spread (standard deviation of $Z$ coordinate values) initially exceeded that of the hybrid model types until approximately 4,800 to 6,400 feet downgradient where they switched and the hybrid model standard deviation values then exceeded that of the deterministic model (Figure 3-13). However, the vertical spread of all three models initially decreased, until between 3,600 and 4,800 feet downgradient, where the hybrid models began to increase in spread. The deterministic model, however, continued to decrease in vertical standard deviation until 8,000 feet, when spread again began to increase overall. Unlike the pattern of spread in the Y-coordinate direction, no clear relationship between the SGS and SIS ensembles is evident in the Z-coordinate spreading as a function of downgradient transport distance.


Figure 3-12. $Y$ coordinate standard deviation for SGS, SIS, and deterministic model types as a function of distance from source.


Figure 3-13. Z coordinate standard deviation for SGS, SIS, and deterministic model types as a function of distance from source.

### 3.8 Map View Results

Map view analysis of particle dispersion was performed using POLYPATH.for output, which compiled particle $X-Y$ location data for the hybrid model ensembles. Images of the cumulative particle location data are shown in Figures 3-14 and 3-15 for the SGS and SIS-based models, respectively. Additionally, an image of the deterministic model particle location data is provided in Figure 3-16.

In the hybrid models, approximately 11,000 to 12,000 cells of the total 38,920 cells comprising map view had at least a single detection. Due to the large number of cells without a single particle detected, zero count cells were not included in the subsequent analysis. Analysis of map view ensembles were completed in a similar way to cross section ensembles, with Count, Mean, St Dev, and Max calculated. Similar statistics were also calculated on the outcome of the deterministic model; however, because the deterministic model was run once, the mean, and max values were multiplied by 100 to make them
comparable to the hybrid models outcome ensembles. Count values and standard deviation were not scaled. Results of this summarization are provided in Table 3-5.

| Table 3-5. Map-View Pathway Count Summary |  |  |  |
| :--- | :---: | :---: | :---: |
|  | SGS-Based Model | SIS-Based Model | Deterministic |
| Count | 11,115 | 12,146 | 5,527 |
| Mean | 187.50 | 153.45 | 368.41 |
| Max | 1,250 | 1,444 | 1,500 |
| St. Dev | 229.74 | 195.77 | 2.62 |

Spread of the particles was analyzed by comparing the average and standard deviation of the Y coordinates for each model type. Polypath Images show the majority of the particles in SIS and deterministic outcomes migrate primarily east, whereas particles within the SGS outcomes migrate to the east-northeast. As shown in Table 3-8, SGS pathlines travel toward the north more than the other model types with a Y coordinate average of 287,825 feet. Additionally, SGS-based model outcomes show the most spread with a standard deviation of 1,995 feet. SIS-based outcomes display less spread with a standard deviation of 1,372 feet and a more southerly trajectory with a Y coordinate average of 286,580 feet. The deterministic model has an average $Y$ coordinate of 287,144 feet with a standard deviation of 1,460 feet.

Spread of the $Y$ coordinate for the three model types was also compared within the last crosssection, located 14,200 feet downgradient, adjacent to the Huron River. Y coordinate averages +/- one standard deviation were calculated and depicted as blue rectangles on the cross-section on Figures 3-14,

3-15, and 3-16 as shown below.

Table 3-6. North-South Spread Statistics

|  | SGS-Based Model |  | SIS-Based Model |  | Deterministic |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Overall | $14,200^{\prime}$ <br> Downgradient | Overall | $14,200^{\prime}$ <br> Downgradient | Overall | $14,200^{\prime}$ <br> Downgradient |
|  | 287,825 | 289,856 | 286,580 | 288,158 | 287,144 | 288,585 |
| St.Dev (Y) ft | 1,995 | 1,510 | 1,372 | 1,320 | 1,460 | 1,204 |



Figure 3-14. POLYPATH outcome ensemble from SGS-based hybrid model with the last cross section depicted adjacent to the Huron River. Depicted in blue is the average location of the pathlines +/- one standard deviation along a N/S profile located 14,200 feet downgradient of the particle line source.


Figure 3-15. POLYPATH outcome ensemble from SIS-based hybrid model simulations with the last cross section depicted adjacent to the Huron River. Depicted in blue is the average location of the pathlines $+/-$ one standard deviation along a N/S profile located 14,200 feet downgradient of the particle line source.


Figure 3-16. POLYPATH outcome from deterministic model simulation with the last cross section depicted adjacent to the Huron River. Depicted in blue is the average location of the pathlines +/- one standard deviation along a N/S profile located 14,200 feet downgradient of the particle line source.

### 3.9 Allen Creek Drain Analysis

As described in Section 2.2.2, the Allen Creek drain is a buried stream system which underlies the southeastern portion of the City of Ann Arbor. According to model outcomes and field observations, migration of 1,4-dioxane is in the direction of the Allen Creek drain system. Therefore, drain boundaries were added into the MODFLOW models and particles were tallied when they entered the drain system. Drain collection data were summarized for both hybrid model types (Table 3-7). Because the deterministic model represents a single outcome, there is no range of values to report; however, the five particles terminate in the drain for this model.

| Table 3-7. Allen Creek Drain Particle Collection Summary |  |  |
| :--- | :---: | :---: |
|  | SGS-Based Model | SIS-Based Model |
| Minimum | 4 | 22 |
| Maximum | 17 | 88 |
| Average | 10 | 56 |

SGS-hybrid model outcomes assembled in POLYPATH show that the advective transport (particle movement) is to the east-northeast from the source area towards the Huron River. Many of the particles were observed to pass north of the Allen Creek Drain in the SGS ensemble (Figure 3-17). Drain particle collection counts reflect this observation, with the data ranging from 4 to 17 particles collected per run, for an average of 10 particles per run terminating in the drain (Table 3-7).

SIS hybrid model outcomes show that the particle flow direction is primarily to the east directly towards the Huron River (Figure 3-17). Consequently, a large number of the particles intercepted the Allen Creek drain, ranging from 22 to 88 particles per run, for an average of 56 particles per run (Table 37).


Figure 3-17. Allen Creek drain particle collection data for both SGS and SIS-hybrid models.


Figure 3-18. POLYPATH output for SGS-based ensemble intersecting the Allen Creek drainshed.


Figure 3-19. POLYPATH output for SIS-based ensemble intersecting the Allen Creek drainshed.

## Chapter 4 - Discussion

The incorporation of different groundwater flow conceptual models ultimately can affect the accuracy and efficiency of treatment and prevention strategies utilized. This study focused on integrating two traditional approaches to compare and contrast predicted groundwater flow pathways. A deterministic framework was obtained from an earlier allohydrostratigraphic model developed by Frahm (2011) that included the explicit identification of aquifer and aquitard subunits. Within these subunits, hydraulic conductivity fields were simulated stochastically using SGS and SIS. The two separate models were then integrated within a modified flow and contaminant transport model of the site (Cypher 2009). Termed hybrid models, these two simulation approaches were evaluated through Monte Carlo analysis.

Based on expected SGS and SIS ensemble model behavior, I hypothesized that: 1) the predicted contamination spatial distribution would initially disperse followed by increasing channelization as advective transport proceeded downgradient; 2) the channelized flow would generate preferential particle discharge locations along the Huron River; and 3) SIS outcomes would exhibit greater spatial variability than SGS outcomes. Evaluation of the hypotheses based on the methods and results described earlier in Chapters 2 and 3 is provided below.

### 4.1 Dispersion Patterns (Hypothesis 1 )

The predicted pattern of successive dispersive-then-channelized plume pathways was not supported. Monte Carlo analysis shows that dispersive patterning of the plume pathways is dependent on orientation, with pathways in the $Y$ direction dispersing from source to termination and pathways in the $Z$ direction following a channelization then dispersion pattern.

In the $Y$ direction, examination of the standard deviation indicates that hybrid model types have an initial stage of slow dispersion, reflected by the small positive slope of plotted standard deviation values (Figure 3-12). The dispersion rate of hybrid model pathways increases as the slope value approaches 1
from 4,800 feet to 9,600 feet downgradient. After this distance, the slope decreases as the pathways continue to termination. This observation is mirrored in the cell pathway averages (Figure 3-10), which indicate that the number of pathways per cell decrease approximately $80 \%$ between the source and the first cross section at 1,600 feet downgradient (Table 3-4). Averages then continue to decline with a small negative slope until termination.

In the $Z$ direction, dispersion follows a different pattern as revealed by analysis of the $Z$ coordinate standard deviation (Figure 3-13). Hybrid and deterministic model outcomes indicate that pathways initially channelize as indicated by the negative slope of the standard deviations, until approximately 3,200 feet and 8,000 feet downgradient, respectively, and then begin to disperse again as indicated by the positive slope in standard deviations. Examination of the cell pathway maximums (Figure 3-11) reveal the channelization observed in the $Z$ direction, with highest maximum values reached at the same distance, 3,200 feet downgradient, for hybrid and deterministic model types.

Ensemble hybrid model results did not conform to the hypothesized expectation; however, Y direction dispersion-channelization was observed in results for the deterministic model. Standard deviation for deterministic modeling in the $Y$ direction indicate that pathlines initially dispersed downgradient from the source (Figure 3-12). Pathlines then channelized between 3,200 and 4,800 feet downgradient as indicated by the negative slope of plotted standard deviation values. Pathlines then dispersed again until 11,200 feet downgradient, where they again began to channelize.

Results for deterministic and hybrid models are consistent with the interpreted lateral continuity of the glacial sediments (Frahm, 2011) where spread occurred primarily in the $Y$ direction as opposed to the $Z$ direction. Standard deviations indicate maximum spread in the $Y$ direction reached 2,129.2 feet (SGS model), whereas standard deviation analysis indicate spread in the $Z$ direction reached 61.2 feet (SGS model). Additionally, the degree of channelization as indicated by the negative slope of standard
deviations in both hybrid and deterministic modeling was greater in the $Z$ direction than that of $Y$ direction.

A factor influencing the observed spread patterns may be linked to the overall percentage of aquifer material present at each cross section location. As delineated in the deterministic model, the percentage of aquifer to aquitard material varies at different cross-sections downgradient (Figure 4-1)


Figure 4.1. Net to gross distribution of aquifer material as a function of distance from source. .
This may influence the pathline outcome possibilities as the distribution of preferred flow pathways is directly related to the amount of aquifer material present. Figure 4-1 indicates the lowest measured percentage of aquifer material occurs approximately 4,600 feet downgradient. This distance corresponds to the locations of the hybrid models' maximum particle pathline counts and the lowest spread values in the $Z$ direction. This suggests that model regions with lower percentages of aquifer material may create a bottle-neck dynamic in the preferred flow pathways that causes advective transport pathlines to converge (i.e. channelize).

### 4.2 Huron River Discharge (Hypothesis 2)

As hypothesized, different, yet overlapping, ranges of preferential outfall locations are predicted along the Huron River by SGS and SIS-based hybrid modeling (Figures 3-14 and 3-15). SGS-based model
outcomes predict the northern-most outfall locations with the largest outfall range, whereas the SISbased model outcomes predict the southern-most discharge locations (Table 3-4). The deterministic model outfall location was located between the SGS and SIS locations and, not surprisingly, had the smallest range. This corroborates the idea that preferential flow pathways and discharge locations are predicted by each model at the Huron River, and that these locations vary by model type. Additionally, this further supports the idea that the stochastic model component increases the potential for pathway spatial variability as the distance from the source area increased for hybrid model ensembles.

### 4.3 Comparison of Stochastic Ensembles (Hypothesis 3)

The hypothesis suggesting that a greater degree of spatial variability in SIS outcomes versus SGS outcomes was not supported. Pathway count data indicated that SIS had a higher degree of downgradient pathway density than did SGS outcomes (Table 3-4). Additionally, Y coordinates analyzed in downgradient cross sections showed that the spread of SGS outcomes exceeded that of SIS outcomes at all distances (Figure 3-12). Overall spread, measured in an XY analysis of the particle pathway ensembles, also mirrored the same relationship (Table 3-6), where the standard deviation of SGS outcomes exceeded that of the SIS outcomes. Cross sectional spread in the $Z$ direction showed that standard deviations of the SGS and SIS outcome ensembles switched relative positions, where one would exceed the other alternatingly as the distance from the source increased.

One factor that may contribute to this result is a more realistic representation of aquifer characteristics (i.e., hydraulic conductivity), allowed by indicator statistics. Additionally, SGS pathways migrated primarily to the east-northeast compared to the eastern direction of the SIS pathways. As the pathways moved north, they reached the northern boundary of the hybrid model area. Once outside this hybrid area, particles migrated under uniform model parameters (effective hydraulic conductivity and anisotropy). Particles then moved in a spreading pattern in response to curvilinear equipotentials,
as opposed to the behavior within the hybrid model area where pathlines were directed by variable hydraulic conductivity within deterministic aquifer and aquitard subunits.

## 5 Conclusions

This study indicates that preferential flow pathways influencing groundwater contamination migration can be modeled using a combination of deterministic and stochastic methods. Moreover, it demonstrates that predictions of downgradient contaminant location and concentration depend not only on head differentials and distance from the source area, but also on subsurface conditions including percentage of aquifer material present in the sediments (deterministic model component) and the finer scale distribution of hydraulic conductivity (stochastic model component).

Comparison of spread between the hybrid model ensembles and the deterministic model employed in this study indicates that although the deterministic model predicts greater initial spread, stochastic models have a greater overall rate of spread, and are the primary drivers of dispersive patterns observed further downgradient. The study suggests that SGS modeling maximizes the predicted spread of overall particle dispersion and increases the range of predicted outfall locations at the Huron River.

In addition to their direct relevance to ongoing remediation efforts at the Pall-Gelman Site in Ann Arbor, results from this study are likely to apply conceptually to other glacial aquifer systems impacted by emerging contaminants of concern, such as dioxane, ethanol and triclosan. These contaminants would likely follow a similar dispersion pattern, regulated by the percentage of aquifer located within the system. Additional investigation, specifically into the quantified relative contribution of deterministic and stochastic model components, could reveal relative importance and influence of each component on the overall hybrid model behavior.

## ACKNOWLEDGEMENTS

I would like to thank primarily Larry Lemke, whose knowledge, support, and patience has enabled this accomplishment. I would like to acknowledge the contributions made by other students, including the undergraduate students who diligently conducted laboratory work, and also graduate students, Joe Cypher, Andrew Frahm, and Amanda Pruehs. Their accomplishments enabled the comprehensive nature of this study.

I would also like to thank the MDEQ, Washtenaw County, the City of Ann Arbor, Pall Life Sciences, and the Scio Residents for Safe Water for providing ample data and intellectual support. This study was made possible through support from the National Science Foundation, under award no. EAR0746540. The interpretations and conclusions are solely those of the author and have not been subject to agency review.

Finally I would like to thank my family, whose backing throughout this endeavor has made completion possible and also my children, James and Michael, who have provided the inspiration.

## APPENDIX A - PARAMETER FILES

## SGS Modeling

```
Parameters for GAMV - Horizontal Aquifer
***************************************
START OF PARAMETERS:
./GAMV_Input/AquiferLayers.dat
1 24
1 6
-1.0 1.0e21
H_GCD_NormExSD_Elev_AF.out
5 0
100
50
1
0.0180.0 5000.0 0.0 2.5 1.5
0
1
1 1 1
```

Parameters for GAMV - Vertical Aquifer
**************************************
START OF PARAMETERS:
./GAMV_Input/AquiferLayers.dat
124
16
-1.0 1.0e21
V_GCD_NormExSD_Elev_AF.out
150
1.0
0.5
1
0.0180 .05 .090 .02 .51 .0
0
1
111
$\backslash$ file with data
\columns for $\mathrm{X}, \mathrm{Y}, \mathrm{Z}$ coordinates
\number of varables,column numbers
\trimming limits
$\backslash$ file for variogram output
\number of lags
\ag separation distance
\lag tolerance
\number of directions
\azm,atol,bandh,dip,dtol,bandv
\standardize sills? (0=no, 1=yes)
\number of variograms
\tail var., head var., variogram type
\file with data
\columns for $\mathrm{X}, \mathrm{Y}, \mathrm{Z}$ coordinates
\number of varables,column numbers
$\backslash$ trimming limits
\file for variogram output
\number of lags
\lag separation distance
\ag tolerance
\number of directions
\azm,atol,bandh,dip,dtol,bandv
\standardize sills? ( $0=$ no, $1=y e s$ )
\number of variograms
\tail var., head var., variogram type

## Parameters for GAMV - Horizontal Aquitard

***************************************

## START OF PARAMETERS:

./GAMV_Input/AquitardLayers.dat
124
16
-1.0 1.0e21
H_GCD_NormExSD_Elev_AT.out
50
150
75
1
$0.0180 .05000 .0 \quad 0.02 .51 .5$
0
1
111

## Parameters for GAMV - Vertical Aquitard

$* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *$

## START OF PARAMETERS:

./GAMV_Input/AquitardLayers.dat
124
16
-1.0 1.0e21
V_GCD_NormExSD_Elev_AT.out
150
1.0
0.5

1
0.0180 .05 .090 .02 .51 .0

0
1
111
\file with data
\columns for $\mathrm{X}, \mathrm{Y}, \mathrm{Z}$ coordinates
\number of varables,column numbers
\trimming limits
\file for variogram output
\number of lags
\lag separation distance
\lag tolerance
\number of directions
\azm,atol,bandh,dip,dtol,bandv
\standardize sills? ( $0=n o, 1=y e s$ )
\number of variograms
\tail var., head var., variogram type
\file with data
\columns for $\mathrm{X}, \mathrm{Y}, \mathrm{Z}$ coordinates
\number of varables,column numbers
\trimming limits
\file for variogram output
\number of lags
\lag separation distance
\lag tolerance
\number of directions
\azm,atol,bandh,dip,dtol,bandv
\standardize sills? ( $0=n o, 1=y e s$ )
\number of variograms
\tail var., head var., variogram type

## SIS Modeling

GAMV.PAR_Horiz_SIS.txt
Parameters for GAMV
*******************
START OF PARAMETERS:
../DATA/SIS/AT_All.txt
123
14
-1.0e21 1.0e21
gamvSIS_AT_HORZ_EW_SS.out
12
250
125
1
90.045 .01000 .00 .05 .020 .0

1
9
1190.1
1190.2
1190.3
1190.4
1190.5
1190.6
1190.7
1190.8
1190.9
90.045 .01000 .00 .05 .020 .0
0.045 .01000 .00 .05 .020 .0
90.045 .01000 .090 .045 .0100 .0
\file with data
\columns for $X, Y$, Z coordinates (1 2 4)
\number of varables,column numbers (16)
\trimming limits
\file for variogram output
\number of lags 12
\lag separation distance 250
\lag tolerance 125
\number of directions
\azm,atol,bandh,dip,dtol,bandv E-W
\standardize sills? ( $0=n o, 1=y e s$ )
\number of variograms
\tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \azm,atol,bandh,dip,dtol,bandv E-W \azm,atol,bandh,dip,dtol,bandv N-S
\azm,atol,bandh,dip,dtol,bandv vertical

## GAMV.PAR_Vert_SIS.txt Parameters for GAMV <br> *******************

START OF PARAMETERS:
../DATA/SIS/AT_All.txt
123
14
-1.0e21 1.0e21
gamvSIS_AT_VERT_SS.out
10
5
2.5

1
90.045 .01000 .090 .045 .0100 .0

1
9
\file with data
\columns for X, Y, Z coordinates (1 2 4)
\number of varables,column numbers (16)
\trimming limits
\file for variogram output
\number of lags 10
\lag separation distance 5
\lag tolerance 2.5
\number of directions
\azm,atol,bandh,dip,dtol,bandv vertical \standardize sills? (0=no, 1=yes)
\number of variograms
1190.1
1190.2
1190.3
1190.4
1190.5
1190.6
1190.7
1190.8
1190.9
90.045 .01000 .00 .05 .020 .0
0.045 .01000 .00 .05 .020 .0
90.045 .01000 .090 .045 .0100 .0
\tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut \tail var., head var., variogram type, ivcut
\tail var., head var., variogram type, ivcut
\tail var., head var., variogram type, ivcut
\tail var., head var., variogram type, ivcut
\azm,atol,bandh,dip,dtol,bandv E-W
\azm,atol,bandh,dip,dtol,bandv N-S
\azm,atol,bandh,dip,dtol,bandv vertical

## Parameters for SGSIM - Aquifer <br> $* * * * * * * * * * * * * * * * * * * * * * * * * * * * *$

## START OF PARAMETERS:

..\DATA\AquiferLayers.txt
124600
-1.0 1.0e21
1
sgsim.trn
0
histsmth.out
12
0.01 .0
10.0
115.0

1
AFsgsim.dbg
OUTPUT\ATsgsim_96-101.out
5
$225 \quad 13269500.0 \quad 100.0$
$70 \quad 282500.0 \quad 100.0$
$36 \quad 600.0 \quad 10$.
48101
016
12
1
13
0
10.010 .010 .0
$0.0 \quad 0.0 \quad 0.0$
$10.60 \quad 1.0$
../data/ydata.dat
4
10.33
$2 \quad 0.67 \quad 0.0 \quad 0.0 \quad 0.0$
750.0750 .0120 .0
\file with data
\columns for $X, Y, Z, v r, w t$, sec.var.
\trimming limits
\transform the data ( $0=$ no, $1=y e s$ )
\file for output trans table
\consider ref. dist (0=no, 1=yes)
$\backslash$ file with ref. dist distribution
\columns for vr and wt
\zmin,zmax(tail extrapolation)
\lower tail option, parameter
\upper tail option, parameter
\debugging level: 0,1,2,3
\file for debugging output
\file for simulation output
\number of realizations to generate
\nx,xmn,xsiz
\ny,ymn,ysiz
\nz,zmn,zsiz
\random number seed
$\backslash m i n$ and max original data for sim
\number of simulated nodes to use
\assign data to nodes ( $0=$ no, $1=y e s$ )
\multiple grid search ( $0=$ no, $1=y e s$ ), num
\maximum data per octant ( $0=$ not used)
\maximum search radii (hmax,hmin,vert)
\angles for search ellipsoid
\ktype: 0=SK,1=OK,2=LVM,3=EXDR,4=COLC
\file with LVM, EXDR, or COLC variable
\column for secondary variable
\nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert

## Parameters for SGSIM - Aquitard <br> ******************************

## START OF PARAMETERS:

..\DATA\AquitardLayers.txt
124600
-1.0 1.0e21
1
sgsim.trn
0
histsmth.out
12
0.01 .0
10.0
$1 \quad 15.0$
1
AFsgsim.dbg
OUTPUT\ATsgsim_96-101.out
5
$225 \quad 13269500.0 \quad 100.0$
$70 \quad 282500.0 \quad 100.0$
$36 \quad 600.010$.
48101
016
12
1
3
0
10.010 .010 .0
$0.0 \quad 0.0 \quad 0.0$
10.601 .0
../data/ydata.dat
4
10.24
20.760 .00 .00 .0
600.0600 .080 .0
\file with data
\columns for $\mathrm{X}, \mathrm{Y}, \mathrm{Z}, \mathrm{vr}, \mathrm{wt}$,sec.var.
\trimming limits
\transform the data ( $0=$ no, $1=$ yes)
\file for output trans table
\consider ref. dist (0=no, 1=yes)
\file with ref. dist distribution
\columns for vr and wt
\zmin,zmax(tail extrapolation)
\lower tail option, parameter
\upper tail option, parameter
\debugging level: 0,1,2,3
\file for debugging output
$\backslash$ file for simulation output
\number of realizations to generate
\nx,xmn,xsiz
\ny,ymn,ysiz
\nz,zmn,zsiz
\random number seed
\min and max original data for sim
\number of simulated nodes to use
\assign data to nodes ( $0=$ no, $1=$ yes)
\multiple grid search ( $0=$ no, $1=$ yes), num
\maximum data per octant (0=not used)
\maximum search radii (hmax,hmin,vert)
\angles for search ellipsoid
\ktype: 0=SK,1=OK,2=LVM,3=EXDR,4=COLC
\file with LVM, EXDR, or COLC variable
\column for secondary variable
\nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert

## Parameters for SISIM - Aquifer

$* * * * * * * * * * * * * * * * * * * * * * * * * * * *$

START OF PARAMETERS:
1
9 9
$\begin{array}{lllllllll}0.1 & 0.2 & 0.3 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.9\end{array}$
. 08 . 299 . 560 . 745 . 858 . 925 . 963 . 985 . 994
../data/SIS/AF_All3.txt
1246
direct.ik
12034567
0
0.610 .540 .560 .530 .29
-1.0e21 1.0e21
0.01 .0
10.0
11.0
130.0
cluster.dat
30
0
sisim.dbg
OUTPUT\AQUIFERoutput\AFsisim_11-15.out 5
22513269500.0100 .0
$70 \quad 282500.0 \quad 100.0$
$36 \quad 600.0 \quad 10.0$
48105
12
12
1
1
03
0
2000.02000 .050 .0
$0.0 \quad 0.0 \quad 0.0$
02.5

1
10.10
$2 \quad 0.7090 .0 \quad 0.0 \quad 0.0$ 12007006.0
10.10
$\begin{array}{llll}2 & 0.87 & 90.0 & 0.0\end{array} \quad 0.0$
130080040.0
10.10
$\begin{array}{lllll}2 & 0.80 & 90.0 & 0.0 & 0.0\end{array}$ 100090035.0
\1=continuous(cdf), 0=categorical(pdf)
\number thresholds/categories
\thresholds / categories
\global cdf / pdf
\file with data
\columns for $X, Y, Z$, and variable
$\backslash$ file with soft indicator input
\columns for $\mathrm{X}, \mathrm{Y}, \mathrm{Z}$, and indicators
$\backslash$ Markov-Bayes simulation ( $0=$ no, $1=y e s$ )
\calibration B(z) values
\trimming limits
\minimum and maximum data value
\lower tail option and parameter
\middle option and parameter
\upper tail option and parameter
\file with tabulated values
\columns for variable, weight
\debugging level: 0,1,2,3
\file for debugging output
\file for simulation output
\number of realizations
\nx,xmn,xsiz
\ny,ymn,ysiz
\nz,zmn,zsiz
\random number seed
\maximum original data for each kriging
\maximum previous nodes for each kriging
\maximum soft indicator nodes for kriging
\assign data to nodes? ( $0=$ no, $1=y e s$ )
\multiple grid search? ( $0=$ no,1=yes),num
\maximum per octant ( $0=$ not used)
\maximum search radii
\angles for search ellipsoid
$\backslash 0=$ full IK, 1=median approx. (cutoff)
$\backslash 0=S K, 1=O K$
\One nst, nugget effect AQUIFER VARIOGRAMS
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Two nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Three nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
10.10
$2 \quad 0.8090 .0 \quad 0.0 \quad 0.0$ 800100040.0
10.15
$\begin{array}{lllll}2 & 0.70 & 90.0 & 0.0 & 0.0\end{array}$ 900110035.0
10.10
$2 \quad 0.6390 .0 \quad 0.0 \quad 0.0$ 1100100035.0
10.10
$\begin{array}{lllll}2 & 0.65 & 90.0 & 0.0 & 0.0\end{array}$ $1300 \quad 90035.0$
10.10
$2 \quad 0.8090 .0 \quad 0.0 \quad 0.0$ 150080015.0
10.10
$\begin{array}{lllll}2 & 0.96 & 90.0 & 0.0 & 0.0\end{array}$ 170070015.0
\Four nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Five nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Six nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Seven nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Eight nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Nine nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert

## Parameters for SISIM - Aquitard

START OF PARAMETERS:
1
9
$\begin{array}{lllllllll}0.1 & 0.2 & 0.3 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.9\end{array}$
. 031 . 147 . 357 . 580 . 748 . 866 . 937 . 977 . 991
../data/SIS/AT_All.txt
1234
direct.ik
12034567
0
0.610 .540 .560 .530 .29
$-1.0 e 21$ 1.0e21
$0.0 \quad 1.0$
10.0
11.0
130.0
cluster.dat
30
0
sisim.dbg
OUTPUT\AQUITARDoutput\ATsisim_96-100.out 5
$225 \quad 13269500.0100 .0$
$70 \quad 282500.0 \quad 100.0$
$36 \quad 600.0 \quad 10.0$
48239
12
12
1
1
03
0
2000.02000 .050 .0
$0.0 \quad 0.0 \quad 0.0$
02.5

1
10.10

VARIOGRAMS
$2 \quad 0.9690 .0 \quad 0.0 \quad 0.0$
120090018.0
10.10
$20.9890 .0 \quad 0.0 \quad 0.0$
$800 \quad 900 \quad 30.0$
10.10
$20.8890 .0 \quad 0.0 \quad 0.0$
$\backslash 1=$ continuous(cdf), 0=categorical(pdf)
\number thresholds/categories
\thresholds / categories
\global cdf / pdf
$\backslash$ file with data
\columns for $X, Y, Z$, and variable
$\backslash$ file with soft indicator input
\columns for $X, Y, Z$, and indicators
$\backslash$ Markov-Bayes simulation ( $0=$ no, $1=y e s$ )
\calibration B(z) values
\trimming limits
\minimum and maximum data value
\lower tail option and parameter
\middle option and parameter
\upper tail option and parameter
$\backslash$ file with tabulated values
\columns for variable, weight
\debugging level: 0,1,2,3
\file for debugging output
$\backslash$ file for simulation output
\number of realizations
\nx,xmn,xsiz
\ny,ymn,ysiz
\nz,zmn,zsiz
\random number seed
\maximum original data for each kriging
\maximum previous nodes for each kriging
\maximum soft indicator nodes for kriging
\assign data to nodes? ( $0=$ no, $1=y e s$ )
\multiple grid search? ( $0=$ no,1=yes),num
\maximum per octant ( $0=$ not used)
\maximum search radii
\angles for search ellipsoid
$\backslash 0=$ full IK, 1=median approx. (cutoff)
\0=SK, 1=OK
\One nst, nugget effect AQUIFER
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Two nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Three nst, nugget effect
\it,cc,ang1,ang2,ang3

|  | 700 | 1000 | 38.0 |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
| 1 | 0.10 |  |  |  |
| 2 | 0.86 | 90.0 | 0.0 | 0.0 |
|  | 800 | 600 | 35.0 |  |
| 1 | 0.15 |  |  |  |
| 2 | 0.85 | 90.0 | 0.0 | 0.0 |
|  | 800 | 600 | 35.0 |  |
| 1 | 0.10 |  |  |  |
| 2 | 0.84 | 90.0 | 0.0 | 0.0 |
|  | 800 | 800 | 18.0 |  |
| 1 | 0.10 |  |  |  |
| 2 | 0.92 | 90.0 | 0.0 | 0.0 |
|  | 1200 | 900 | 12.0 |  |
| 1 | 0.75 |  |  |  |
| 2 | 0.80 | 90.0 | 0.0 | 0.0 |
|  | 800 | 800 | 15.0 |  |
| 1 | 0.58 |  |  |  |
| 2 | 0.96 | 90.0 | 0.0 | 0.0 |
|  | 1300 | 900 | 15.0 |  |

\a_hmax, a_hmin, a_vert
\Four nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Five nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Six nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Seven nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Eight nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert
\Nine nst, nugget effect
\it,cc,ang1,ang2,ang3
\a_hmax, a_hmin, a_vert

## APPENDIX B - FORTRAN PROGRAMS

## DETERMINE.for

```
C:\Documents and Settings\Lena\My Documents\...\Fortran_GSL2VMF\DETERMINE\DETERMINE_2015_12_17.f 1
PROGRAM DETERMINE
* --------------------------------------------------------------------
* Written by Larry Lemke and Lena Pappas Last Modified : 17 - Dec - 2015
*
* Modified 11 / 13 / 2012 to correct bug generating all aquifer cells
* ( }AQ=0 ) in first row and first column of every layer .
* Modified 1 / 20 / 2014 to eliminate - 3141 values in top row and last column
* of AQ . out file
*
* Modified 2 / 08 / 2014 to output CUBE file for SGeMS input ( for visualization )
* Modified 2 / 13 / 2014 to insert random aquifer or aquitard grid cell categories
* in cells that sit below Andy Frahm ' s lowest surface and the top of Joe Cypher ' s
* MODFLOW model bedrock surface .
*
* Modified 2 / 24 / 2014 to hardwire correction for aquifer material surrounding the
* following well screens : MW - 97 s , MW - 99 d , MW - 111
*
* Modified 3 / 3 / 2014 to correct bug in NKMIN and NKMAX calculation to account for
* rows in VMG files being written from back to front
* Modified 12 / 17 / 2015 to calculate percent aquifer along N - S profiles ( model
* coluns ) corresponding to " Walls " in WALLONE . f
*
* This program compares the elevation of VMODFLOW grid cells with the elevation
* of stratigraphic surfaces in a series of interpolated Surfer grid files to
* DETERMINE which layer the VMODFLOW grid cell corresponds to .
*
* After the layer number is determined , the grid cell can be categorized as an
* Aquifer ( 0 ) or Aquitard ( 1 ) or inactive cell (- 9999 )
*
* NB ! In the event that Andy Frahm ' s surface maps are shallower than the bedrock
* surface elevation embedded in the VMODFLOW grid file ( i . e . , active cells
* are present below the lowermost Frahm surface ) , an earlier version of
* DETERMINE assigned - 9999 values . These were subsequently ignored in
* GSL 2 VMFxx and therefore new values were not assigned ( default property
* value of 1 or 2 is retained ). The current version of DETERMINE identifies
* cells that sit between Andy ' s lowest surface and underlying bedrock and
* randomly assigns aquifer ( 0 ) or aquifer ( 1 ) values to the AQ array with a
* 2 / 3 chance for aquifer and 1 / 3 chance for aquitard ( the same proportion of
* aquifer and aquitard in Andy ' s larger deterministic model ).
*
* *** Variable Descriptions ***
*
* General Variables
* =================
* N , N 1 , N 2 , I , J , K = loop counter variables
* RNum = random number ( from 0 . 0 to 1 . 0 )
* RInt = random integer ( from 1 to 100 )
*
* Variables associated with original VMODFLOW Property and Grid Files
* =====================================================================
* NK = number of layers ( Z )
* NJ = number of columns ( X )
* NI = number of rows ( Y )
* X ( n ) = X coordinate of VMODFLOW Grid Cell
```

```
* \(\mathrm{Y}(\mathrm{n})=\mathrm{Y}\) coordinate of VMODFLOW Grid Cell
* \(Z(n)=Z\) coordinate of VMODFLOW Grid Cell
* ACTIVE ( X , Y , Z ) = array with active / inactive integer ; 1 = active 0 = inactive
* NKMINvmf , NKMAXvmf = first / last rows to be filled in VMG or VMP coords with
* Y ( rows ) counted from back to front
*
* Variables associated with Surfer Grids
* ==============================================
C: \Documents and Settings \Lena \My Documents \...\Fortran_GSL2VMF \DETERMINE \DETERMINE_2015_12_17.f 2
* NXs , NYs , NZs = number of X , Y , Z nodes in Surfer Grids
*
* Variables associated with GSLIB 3 D Simulation
* ============================================
* NX , NY , NZ = number of \(\mathrm{X}, \mathrm{Y}, \mathrm{Z}\) nodes in simulated gridc
* XMIN , YMIN , ZMIN = X , Y , Z coordinates of first node in simulated grid
* XSIZ , YSIZ , ZSIZ = X , Y, Z increment size ( constant ) in simulated grid
* XMAX , YMAX , ZMAX \(=\mathrm{X}, \mathrm{Y}, \mathrm{Z}\) coordinates of last node in simulated grid
*
* Variables associated with Fill Cells
* =====================================
* NJMIN , NKMIN = pointers to min ( first ) col / row / layer cell to be filled
* NJMAX , NKMAX = pointers to max ( last ) col / row / layer cell to be filled
*
* *** Declare Variables ***
IMPLICIT NONE
INTEGER N , N 1 , N 2 , I , J , K , P , Q , R
INTEGER NK , NJ , NI
INTEGER NX , NY , NZ
INTEGER NJMIN , NKMIN , NJMAX , NKMAX
INTEGER AQ , ACTIVE , RInt
INTEGER NKMINvmf , NKMAXvmf
INTEGER AQ 112 , \(A Q 128\), \(A Q 144\), AQ 160 , AQ 176 , \(A Q 192\), \(A Q 208\)
INTEGER AQ 224 , AQ 240 , AQ 254
INTEGER AT 112 , AT 128 , AT 144 , AT 160 , AT 176 , AT 192 , AT 208
INTEGER AT 224 , AT 240 , AT 254
REAL * \(8 \mathrm{Kx}, \mathrm{Ky}, \mathrm{Kz}, \mathrm{Y}, \mathrm{Z}, \mathrm{Xs}, \mathrm{Ys}, \mathrm{RNum}\)
REAL Zs 0 , Zs 1 , Zs 2 , Zs 3 , Zs 4 , Zs 5 , Zs 6 , Zs 7 , Zs 8
REAL N 2 G 112 , N 2 G 128 , N 2 G 144 , N 2 G 160 , N 2 G 176 , N 2 G 192 , N 2 G 208
REAL N 2 G 224 , N 2 G 240 , N 2 G 254
DOUBLE PRECISION X
REAL * 8 YMIN , ZMIN , YMAX , ZMAX , XSIZ , YSIZ , ZSIZ
DOUBLE PRECISION XMIN, XMAX
REAL * 8 NXs , NYs , NZs
CHARACTER ANSWER * 1
DIMENSION X ( 0 : 281 ) , Y ( 0 : 140 ) , Z ( 0 : 37 )
DIMENSION Xs ( \(0: 281\), 0 : 80 )
DIMENSION Ys ( 0 : 281 , 0 : 80 )
DIMENSION Zs 0 ( \(0: 281,0: 80\) )
DIMENSION Zs 1 ( \(0: 281\), \(0: 80\) )
DIMENSION Zs 2 ( 0 : 281 , \(0: 80\) )
DIMENSION Zs 3 ( 0 : 281, 0 : 80 )
DIMENSION Zs 4 ( 0 : 281 , 0 : 80 )
DIMENSION Zs 5 ( \(0: 281,0: 80\) )
DIMENSION Zs 6 ( 0 : 281 , 0 : 80 )
DIMENSION Zs 7 ( 0 : 281, 0 : 80 )
DIMENSION Zs 8 ( \(0: 281\), \(0: 80\) )
DIMENSION AQ ( \(0: 281\), \(0: 281\), \(0: 281\) ) , ACTIVE ( \(0: 281\), \(0: 281\), \(0: 281\) )
* *** Assign I / O files ***
*
* File 20 contains the input VMODFLOW Grid (. VMG ) file
* File 25 is the program parameter file
* File 50 is an output log for debugging write statements
* Files 61 through 68 contain the surfer (. DAT ) files
*
PRINT * , ' PROGRAM COMMENCES '
```

OPEN ( 20 , FILE = ' C : \ Documents and Settings \Lena \My Documents \Directe
1 d Study \ Fortran GSL 2 VMF \ DETERMINE \ seed DET . VMG ', STATUS = ' OLD ' )
PRINT * , ' FILE 20 OPENED '
OPEN ( 25 , FILE = ' C : \ Documents and Settings \Lena \My Documents \ Directed Stu
$\mathrm{C}: \backslash$ Documents and Settings \Lena \My Documents \...\Fortran_GSL2VMF \DETERMINE \DETERMINE_2015_12_17.f 3
1 dy \Fortran GSL 2 VMF \DETERMINE \DETERMINE . par ${ }^{\top}$, STATUS = ' OLD ' )
OPEN ( 50 , FILE $=$ ' C : \Documents and Settings \Lena \My Documents \ Directed Stu
1 dy \Fortran GSL 2 VMF \ DETERMINE \ DETERMINE 2015 . log ' )
OPEN ( 60 , FILE $=$ ' C : \ Documents and Settings \ Lena \My Documents \Directe
1 d Study \Fortran GSL 2 VMF \ DETERMINE \SurferSurfaces \Surface 0 . dat ', ST 2 ATUS = ' OLD ' )
OPEN ( 61 , FILE = ' C : \ Documents and Settings \ Lena \My Documents \ Directe 1 d Study \ Fortran GSL 2 VMF \ DETERMINE \ SurferSurfaces \Surface 1 . dat ', ST 2 ATUS = ' OLD ' )
OPEN ( 62 , FILE = ' C : \ Documents and Settings \ Lena \My Documents \ Directe 1 d Study \} Yortran GSL 2 VMF \ DETERMINE \ SurferSurfaces \Surface 2 . dat ', ST 2 ATUS = ' OLD ' )
OPEN ( 63 , FILE = ' C : \ Documents and Settings \ Lena \My Documents \Directe
1 d Study \ Fortran GSL 2 VMF \ DETERMINE \SurferSurfaces \Surface 3 . dat ', ST
2 ATUS = ' OLD ' )
OPEN ( 64 , FILE = ' C : \ Documents and Settings \ Lena \My Documents \Directe
1 d Study \Fortran GSL 2 VMF \ DETERMINE \SurferSurfaces \Surface 4 . dat ', ST
2 ATUS = ' OLD ' )
OPEN ( 65 , FILE = ' C : \ Documents and Settings \Lena \My Documents \Directe
1 d Study \Fortran GSL 2 VMF \ DETERMINE \SurferSurfaces \Surface 5 . dat ', ST
2 ATUS = ' OLD ' )
OPEN ( 66 , FILE = ' C : \ Documents and Settings \ Lena \My Documents \ Directe
1 d Study \ Fortran GSL 2 VMF \ DETERMINE \SurferSurfaces \Surface 6 . dat ', ST
2 ATUS = ' OLD ' )
PRINT * , ' FILE 66 OPENED '
OPEN ( 67 , FILE $=$ ' C : \ Documents and Settings \ Lena \My Documents \Directe
1 d Study \Fortran GSL 2 VMF \ DETERMINE \SurferSurfaces \Surface 7 . dat ', ST
2 ATUS = ' OLD ' )
PRINT * , ' FILE 67 OPENED '
OPEN ( 68 , FILE $=$ ' C : \ Documents and Settings \Lena \My Documents \Directe
1 d Study \ Fortran GSL 2 VMF \ DETERMINE \SurferSurfaces \Surface 8 . dat ', ST
2 ATUS = ' OLD ' )
PRINT * , ' FILE 68 OPENED '
*
*

* *** TASK 1 ************************ TASK $1^{* * * * * * * * * * * * * * * * * * * * * ~ T A S K ~} 1^{* * *}$
* 
* Read in VMODFLOW Grid (. VMG ) file info
* 

WRITE ( 50 , *)
WRITE ( 50 , *) " STARTING TASK 1 : Read in VMODFLOW Grid (. VMG ) file "
PRINT * , " STARTING TASK 1 : Read in VMODFLOW Grid (. VMG ) file "

* *** Note that. VMG files are written from left to right ( NJ ), front to
* back ( NI ) , and bottom to top ( NK ).
READ ( 20 , *) NJ
WRITE ( 50 , *) " NJ =" , NJ
DO $N=1$, $N J+1$ ! there is one more column line than the number of columns
READ ( 20 , *) X ( N )
WRITE ( 50 , 106 ) N , X ( N )
ENDDO
* 

READ ( 20 , *) NI
WRITE ( $50, *)$ " NI =" , NI
DO $N=1$, $N I+1$ ! there is one more row line than the number of rows
READ ( 20 , *) Y ( N )
WRITE ( 50 , 107 ) N , Y ( N )
ENDDO
*
READ ( 20 , *) NK
WRITE ( 50 , *) " NK =" , NK

```
DO N = 1 , NK + 1 ! there is one more layer line than the number of layers
READ ( 20 , *) Z ( N ) ! reads bottom layer first
WRITE ( 50 , 108 ) N , Z ( N )
ENDDO
C:\Documents and Settings\Lena\My Documents\...\Fortran_GSL2VMF\DETERMINE\DETERMINE_2015_12_17.f 4
* * Read Active Cell indicators from . VMG file
DO K = 1 , NK ! cycle slowest on Z ( layer ) ; layer 1 is bottom layer
DO I = NI , 1 , - 1 ! cycle next on Y
READ ( 20 , *) ( ACTIVE ( J , I , K ) , J = 1 , NJ ) ! cycle last on X
ENDDO
ENDDO
CLOSE ( 20 )
WRITE ( 50 , *) x ( NJ - 1 )
*
* **** TASK 2 ************************* TASK 2 ********************** TASK 2 *******
*
* This code assumes that there is a one - to - one correspondence between the GSLIB simulation
* grid and the portion of the VMODFLOW . VMG grid file that will be filled .
*
WRITE ( 50 , *)
WRITE ( 50, *) " TASK 2 "
PRINT * , " TASK 2 "
* Read GSLIB simulation grid parameters
READ ( 25 , *) NX , XMIN , XSIZ ! GSLIB coord indices : 1 to NX
READ ( 25 , *) NY , YMIN , YSIZ ! GSLIB coord indices : 1 to NY
READ ( 25 , *) NZ , ZMIN , ZSIZ ! GSLIB coord indices : 1 to NZ
Print * , " NX =" , NX
PRINT * , " NY =" , NY
PRINT * , " NZ =" , NZ
Print *
XMAX = XMIN + ( NX - 1 )* XSIZ
YMAX = YMIN + (NY - 1)* YSIZ
ZMAX = ZMIN + ( NZ - 1 )* ZSIZ
WRITE ( 50 , *) " NX = " , NX , " XSIZ = " , XSIZ
WRITE ( 50 , *) " NY = " , NY , " YSIZ = " , YSIZ
WRITE ( 50 , *) " NZ = " , NZ , " ZSIZ = " , ZSIZ
WRITE ( 50 , 109 ) XMIN , XMAX
WRITE ( 50 , 110 ) YMIN , YMAX
WRITE ( 50 , 111 ) ZMIN , ZMAX
*
* *** TASK 3 ************************ TASK 3 ********************** TASK 3 ***
*
* Read in SURFER (. DAT ) file info
* Note : This code assumes that there is a one - to - one correspondence between the Surfer
* grid and the portion of the VMODFLOW . VMG grid file that will be filled ( as well as the
* GSLIB simultaion grid ).
*
WRITE ( 50 , *)
WRITE ( 50, *) " STARTING TASK 3 : Read in SURFER (. DAT ) files "
PRINT * , " STARTING TASK 3 : Read in SURFER (. DAT ) files "
READ ( 25 , *) NXs ! surfer grid parameters
READ ( 25 , *) NYs ! surfer grid parameters
READ ( 25, *) NZs ! surfer grid parameters
WRITE ( 50 , *) ' NXs = ', NXs
WRITE ( 50 , *) ' NYs = ', NYs
WRITE ( 50 , *) ' NZs = ', NZs
*
* *** Note that . DAT files are written from left to right ( J ) , front to
* back ( K ) -- They cylce fastest on X , then on Y
DO K = 1 , NYs + 1
C:\Documents and Settings\Lena\My Documents\...\Fortran_GSL2VMF\DETERMINE\DETERMINE_2015_12_17.f 5
DO J = 1 , NXs + 1 ! cycles fastest on X , then Y
READ ( 60 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 0 ( J , K )
READ ( 61 , *) Xs ( J , K ), Ys ( J , K ), Zs 1 ( J , K )
```

```
READ ( 62 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 2 ( J , K )
READ ( 63 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 3 ( J , K )
READ ( 64 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 4 ( J , K )
READ ( 65 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 5 ( J , K )
READ ( 66 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 6 ( J , K )
READ ( 67 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 7 ( J , K )
READ ( 68 , *) Xs ( J , K ) , Ys ( J , K ) , Zs 8 ( J , K )
ENDDO
ENDDO
CLOSE ( 60 )
CLOSE ( 61 )
CLOSE ( 62 )
CLOSE ( 63 )
CLOSE ( 64 )
CLOSE ( 65 )
CLOSE ( 66 )
CLOSE ( 67 )
CLOSE ( 68 )
* *** TASK 4 ************************ TASK 4 ********************** TASK 4 ***
*
* Loop through VMODFLOW grid X coords and compare to GSLIB simulation X
* coordinate limits. Check to insure overlap between X coordinates and
* determine first and last VMODFLOW cell to be filled in X direction .
* ( NJMIN points to first fill cell and NJMAX points to last .)
* Similarly , loop through the Y coordinate direction .
*
WRITE ( 50 , *) " STARTING TASK 4 : Assign Counter Cells "
WRITE ( 50 , *) " NJ = " , NJ
WRITE ( 50 , *) " XMIN = " , XMIN
WRITE ( 50 , *) " X ( NJ + 1 )= " , X ( NJ + 1 )
IF ( XMIN . LT . X ( NJ + 1 ) ) THEN ! Tests to see if XMIN within VMODFLOW Grid
IF ( XMIN . GT . X ( 1 )) THEN ! Tests to see if XMIN within VMODFLOW Grid
DO N 1 = 1,NJ + 1
IF ( XMIN . LE . X ( N 1 )) THEN
NJMIN = N 1 ! Assigns X counter for first cell to be filled
GOTO 30
ELSE
CONTINUE
ENDIF
ENDDO
ELSE
* *** Need to replace first VMODFLOW cell with simulated values ***
NJMIN = 1
ENDIF
ELSE
PRINT * , " ERROR : No overlap between cells in X coordinate "
WRITE ( 50 , *) " XMIN ERROR : No X coordinate overlap in cells "
GOTO 9999
ENDIF
30 CONTINUE
DO N 2 = NJMIN , NJ + 1
c WRITE ( 50 , 116 ) N 2 , XMAX , X ( N 2 )
IF ( Xmax . LE . X ( N 2 )) then
GOTO 31
ENDIF
C:\Documents and Settings\Lena\My Documents\...\Fortran_GSL2VMF\DETERMINE\DETERMINE_2015_12_17.f 6
ENDDO
31 NJMAX = N 2 ! Assigns X counter for last cell to be filled
WRITE ( 50 , *) " LAST N 2 =" , N 2 , " NJMIN =" , NJMIN , " NJMAX =" , NJMAX
* Loop through VMODFLOW grid Y values ...
WRITE ( 50 , *) " NI = " , NI
WRITE ( 50 , *) " YMIN = " , YMIN
WRITE ( 50 , *) " Y ( NI + 1 )= " , Y ( NI + 1 )
IF ( YMIN . LT . Y ( NI + 1 )) THEN
IF ( YMIN . GT . Y ( 1 )) THEN
```

```
DO N 1 = 1 , NI + 1 ! Changed to N 1 = 1 , NI + 1 by LDL 03 / 03 / 2014
IF ( YMIN . LE . Y ( N 1 )) THEN
NKMIN = N 1 ! Assigns Y counter for first cell to be filled
NKMAXvmf = NI - N 1 ! Assigns Y counter for last cell to be filled
! Note : . VMG file counts Y rows from back to front
GOTO 32
ELSE
CONTINUE
ENDIF
ENDDO
ELSE
* *** Need to replace first VMODFLOW cell with simulated values ***
NKMIN = 1
ENDIF
ELSE
PRINT * , " ERROR : No overlap between cells in Y coordinate "
WRITE ( 50 , *) " YMIN ERROR : No Y coordinate overlap in cells "
GOTO 9999
ENDIF
32 CONTINUE
DO N 2 = NKMIN , NI + 1
C WRITE ( 50 , 117 ) N 2 , YMAX , Y ( N 2 )
IF ( YMAX . LE . Y ( N 2 )) THEN
GOTO 33
ENDIF
ENDDO
33 NKMAX = N 2
NKMINvmf = NI - N 2 ! Assign Y counter for first cell to be filled
! Note : . VMG file counts Y rows from back to front
WRITE ( 50 , *) " LAST N 2 =" , N 2 , " NKMIN =" , NKMIN , " NKMAX =" , NKMAX
WRITE ( 50, *) " Y ( N 2 ) = " , Y ( N 2 )
WRITE ( 50 , *) " NKMINvmf =" , NKMINvmf , " NKMAXvmf =" , NKMAXvmf
*
*
* *** TASK 5 ******************* TASK 5 ********************** TASK 5 ******
*
* Determine whether each cell to be filled corresponds to an ' AQUIFER ' or
* an ' AQUITARD ' layer . Note that Even numbered layers represent the base of
* an Aquifer in Andy Frahm ' s deterministic model (Odd numbered layers are
* the base of Aquitard layers ). Also note that all layers are not present in
* all locations !
*
* This code assumes that the grid increments for the VMODFLOW , SURFER , and
* GSLIB simulation files are the same .
* Indicator Variable Assignment :
* - 9999 = inactive cell ( below base of glacial sediments )
* 0 = Aquifer Layer
* 1 = Aquitard Layer
*
WRITE ( 50, *)
C:\Documents and Settings\Lena\My Documents\...\Fortran_GSL2VMF\DETERMINE\DETERMINE_2015_12_17.f 7
WRITE ( 50 , *)" START TASK 5 : Determine aquifer / aquitard for fill cells "
WRITE ( 50, *)
PRINT * , " STARTING TASK 5 : Determine aquifer / aquitard for fill cells "
* Fill all values in the AQ array with a default value of - 3141
* Note : AQ array contains indicator values for aquifer / aquitard / no fill
DO J = 0 , NJ + 1
DO K = 0, NI + 1
DO R = 0, NK + 1
AQ ( J , K , R )=- 3141
ENDDO
ENDDO
ENDDO
DO J = 1 , NXs ! Surfer Grid Dimensions
DO K = 1 , NYs
```

```
DO 22 R = 1 , NZs
* *** Note : Add 5 . 0 feet to shift to center of 10 foot thick VMODFLOW layers
IF (( Z ( R )+ 5 . 0 ). LT . Zs 0 ( J , K )) THEN
IF ( ACTIVE ( J + NJMIN - 1 , K + NKMIN - 1 , R ). eq . 1 ) THEN
c Check to see if there are any active cells in the VMODFLOW model that sit below
c Andy ' s basal surface . If so , assign aquifer or aquitard randomly to these cells .
CALL RANDOM NUMBER ( RNum )
RInt = INT ( RNUM * 100 . 0 )
IF ( RInt . LT . 67 ) THEN ! 2 / 3 of bulk model is aquifer
AQ ( J , K , R )= 0 ! assign aquifer
ELSE
AQ ( J , K , R )= 1 ! assign aquitard
ENDIF
ELSE
AQ ( J , K , R )=- 9999
ENDIF
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 1 ( J , K )) THEN
AQ ( J , K , R )= 0
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 2 ( J , K )) THEN
AQ ( J , K , R )= 1
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 3 ( J , K )) THEN
AQ ( J , K , R ) = 0
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 4 ( J , K )) THEN
AQ ( J , K , R )= 1
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 5 ( J , K )) THEN
AQ ( J , K , R )=0
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 6 ( J , K )) THEN
AQ ( J , K , R )= 1
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 7 ( J , K )) THEN
AQ ( J , K , R )=0
ELSEIF (( Z ( R )+ 5 . 0 ). LT . Zs 8 ( J , K )) THEN
AQ ( J , K , R )= 1
ELSE
AQ ( J , K , R )= 0
ENDIF
22 ENDDO
ENDDO
ENDDO
* Hardwire fix for aquifer material surrounding specific well screens
* MW - 97 s
Do J = 193 , 197
Do K = 55 , 58
AQ ( J , K , 17 )=0
AQ ( J , K , 16 )=0
Enddo
Enddo
C:\Documents and Settings\Lena\My Documents\...\Fortran_GSL2VMF\DETERMINE\DETERMINE_2015_12_17.f 8
* MW - 99 d
Do J = 180 , 185
Do K = 42, 47
AQ ( J , K , 11 )=0
Enddo
Enddo
* MW - 111
Do J = 218 , 225
Do K = 48, 54
AQ ( J , K , 16 )=0
AQ ( J , K , 15 )=0
Enddo
Enddo
WRITE ( 50 , *)
PRINT *
* *** Initialize aquifer and aquitard counters for individual wall locations
AQ 112 = 0
AQ 128 = 0
```

```
AQ 144 = 0
AQ 160 = 0
AQ 176 = 0
AQ 192 = 0
AQ 208 = 0
AQ 224=0
AQ 240 = 0
AQ 254 = 0
AT 112 = 0
AT 128=0
AT 144 = 0
AT 160 = 0
AT 176 = 0
AT 192 = 0
AT 208=0
AT 224=0
AT 240=0
AT 254 = 0
*
* *** TASK 6 ****************** TASK 6 ******************** TASK 6 ****
*
* Write output file .
*
4 5 ~ C O N T I N U E ~
WRITE ( 50 , *)
WRITE ( 50 , *)" STARTING TASK 6 : Write Output Files "
PRINT * , " STARTING TASK 6 : Write Output Files "
OPEN ( 51 , FILE = ' C : \ Documents and Settings \ Lena \ My Documents \ Directe
1 d Study \ Fortran GSL 2 VMF \ DETERMINE \ AQ 2015 . out ' )
OPEN ( 52 , FILE = ' C : \ Documents and Settings \ Lena \ My Documents \ Directe
1 d Study \ Fortran GSL 2 VMF \ DETERMINE \ Determine CUBE 2015 . out ' )
Write ( 52 , *) ' Deternmine CUBE . out '
Write ( 52 , *) ' 4 '
Write ( 52 , *) ' X '
Write ( 52 , *) ' Y '
Write ( 52 , *) ' Z '
Write ( 52 , *) ' Indicator '
DO R = 1 , NZ ! Z value Changed from NZ to NZ - 1 by LDL 8 / 6 / 12
! Changed back to NZ by LDL 2 / 8 / 14
DO Q = NKMIN , NKMAX ! Y value ( VMODFLOW Grid Coords )
DO P = NJMIN , NJMAX ! X value ( VMODFLOW Grid Coords )
WRITE ( 51 , 151 ) X ( P ) , Y ( Q ) , Z ( R ) , AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R )
WRITE ( 52 , 151 ) X ( P ) , Y ( Q ) , Z ( R ) , AQ ( P - NJMIN + 1, Q - NKMIN + 1 , R )
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! Count aquifer and aquitard cells at WALL }112\mathrm{ location
IF ( P . EQ . 112 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 112 = AQ 112 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 112 = AT 112 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL }112\mathrm{ location
IF ( P . EQ . 112 ) THEN
IF ( AQ ( P - NJMIN + 1, Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 112 = AQ 112 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 112 = AT 112 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL }128\mathrm{ location
IF ( P . EQ . 128 ) THEN
IF ( AQ ( P - NJMIN + 1, Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 128 = AQ 128 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1, R ). EQ . 1 ) THEN
```

```
AT 128 = AT 128 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 144 location
IF ( P . EQ . 144 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 144 = AQ 144 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 144 = AT 144 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 160 location
IF ( P . EQ . 160 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 160 = AQ 160 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 160 = AT 160 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 176 location
IF ( P . EQ . 176 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 176 = AQ 176 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 176 = AT 176 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 192 location
IF ( P . EQ . 192 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 192 = AQ 192 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 192 = AT 192 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 208 location
IF ( P . EQ . 208 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 208 = AQ 208 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 208 = AT 208 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 224 location
IF ( P . EQ . 224 ) THEN
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IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 224 = AQ 224 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 224 = AT 224 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 240 location
IF ( P . EQ . 240 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 240 = AQ 240 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
AT 240 = AT 240 + 1
ENDIF
ENDIF
! Count aquifer and aquitard cells at WALL 254 location
IF ( P . EQ . 254 ) THEN
IF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 0 ) THEN
AQ 254 = AQ 254 + 1
ELSEIF ( AQ ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 ) THEN
```

```
AT 254 = AT 254 + 1
ENDIF
ENDIF
ENDDO
ENDDO
ENDDO
N 2 G 112 = REAL ( AQ 112 )/ REAL ( AQ 112 + AT 112 )
N 2 G 128 = REAL ( AQ 128 )/ REAL ( AQ 128 + AT 128 )
N 2 G 144 = REAL ( AQ 144)/ REAL (AQ 144 + AT 144)
N 2 G 160 = REAL ( AQ 160 )/ REAL ( AQ 160 + AT 160 )
N 2 G 176 = REAL ( AQ 176 )/ REAL ( AQ 176 + AT 176 )
N 2 G 192 = REAL ( AQ 192)/ REAL ( AQ 192 + AT 192)
N 2 G 208 = REAL ( AQ 208 )/ REAL ( AQ 208 + AT 208 )
N 2 G 224 = REAL ( AQ 224 )/ REAL ( AQ 224 + AT 224)
N 2 G 240 = REAL ( AQ 240 )/ REAL ( AQ 240 + AT 240 )
N 2 G 254 = REAL ( AQ 254 )/ REAL (AQ 254 + AT 254)
PRINT *
PRINT *, ' N 2 G 112 = ', N 2 G }11
PRINT *,' N 2 G 128=',N 2 G 128
PRINT *, ' N 2 G 144 = ', N 2 G 144
PRINT *, 'N 2 G 160= ', N 2 G 160
PRINT *,' N 2 G 176 = ', N 2 G 176
PRINT *, ' N 2 G 192 = ', N 2 G }19
PRINT *, 'N 2 G 208= ', N 2 G 208
PRINT *, 'N 2 G 224 = ', N 2 G 224
PRINT *, 'N 2 G 240= ', N 2 G 240
PRINT *, 'N 2 G 254 = ', N 2 G 254
WRITE ( 50, *)
WRITE ( 50, *)' N 2 G 112 = ', N 2 G 112
WRITE ( 50 , *) ' N 2 G 128 = ', N 2 G 128
WRITE ( 50, *)' N 2 G 144 = ', N 2 G 144
WRITE ( 50, *) 'N 2 G 160 = ', N 2 G 160
WRITE ( 50, *) ' N 2 G 176 = ', N 2 G 176
WRITE ( 50, *) ' N 2 G 192 = ', N 2 G }19
WRITE ( 50 , *) ' N 2 G 208 = ', N 2 G 208
WRITE ( 50, *) 'N 2 G 224 = ', N 2 G 224
WRITE ( 50, *)' N 2 G 240 = ', N 2 G 240
WRITE ( 50, *) ' N 2 G 254 = ', N 2 G 254
WRITE (* , *)
WRITE ( 50 , *)
*
* --- Close output file and Close Number of Realization Do Loop
*
print * , " CLOSING OUTPUT FILES "
WRITE ( 50, *) " CLOSING OUTPUT FILES "
CLOSE ( 50 )
C:\Documents and Settings\Lena\My Documents\...\Fortran_GSL2VMF\DETERMINE\DETERMINE_2015_12_17.f 11
CLOSE ( 51 )
CLOSE ( 52 )
*
5 5 5 \text { Continue}
*
3 PRINT *
PRINT * , ' *** Continue ? ( Y / N ) '
READ * , ANSWER
IF (( ANSWER . EQ . ' N ' ). OR .( ANSWER . EQ . ' n ' )) THEN
STOP
ELSEIF (( ANSWER . EQ . ' Y ' ). OR .( ANSWER . EQ . ' y ' )) THEN
CONTINUE
ELSE
GOTO 3
ENDIF
PRINT *
PRINT * , ' NORMAL PROGRAM TERMINATION '
*
```

```
* *** Format Statements ****
106 FORMAT (" N = " , i 3 , " X ( N )=" , f 12 . 3 )
107 FORMAT (" N = " , i 3 , " Y ( N )=" , f 12 . 3 )
108 FORMAT (" N = " , i 3 , " Z ( N )=" , f 12 . 3 )
109 FORMAT (" XMIN = " , F 12 . 2 , T 25 , " XMAX = " , F 12 . 2 )
110 FORMAT (" YMIN = " , F 10. 2 , T 25 , " YMAX = " , F 10. 2 )
111 FORMAT (" ZMIN = " , F 10 . 2 , T 25 , " ZMAX = " , F 10 . 2 )
116 FORMAT (" N 2 =" , T 6 , I 3 , T 15 , " XMAX =" , T 20, F 12 . 2 , T 35 , "< = X ( N 2 )= " ,
F 12 . 2 )
117 FORMAT (" N 2 =" , T 6 , I 3 , T 15 , " YMAX =" , T 20, F 12 . 2 , T 35 , " < = Y ( N 2 )= " ,
F 12 . 2 )
151 FORMAT ( F 12. 2 , 3 X , F 10. 2 , 3 X , F 8 . 2 , 3 X , I 6 )
152 FORMAT ( I 1 )
9999 END
```


## GSL2VMF16.for

```
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 1
* ---------------------------------------------------------------------
PROGRAM GSL 2 VMF 16
* Written by Larry Lemke Last Modified : 13 - Nov - 2015
* Modified by Lena Pappas and Larry Lemke
*
* This program converts GSLIB simulatedfields of 3 D normalized ( 0 to 100 %) gamma values
* to hydraulic conductivity ( K ) fields ( cm / s ) in an output file formatted to replace
* the first part of a VMODFLOW formatted property (. VMP ) file .
*
* This is a streamlined version of Program GSL 2 VMF that assumes :
* The simulation grid size is equal to the VMODFLOW grid size . ( IMPORTANT !)
* Note , however , that GSLIB simulations are point - centered while the
* VMODFLOW grid definition is block - centered .
```



```
* The conversion to a . VMP file is accomplished through a series of 7 tasks :
* Task 1 : Read in initial VMODFLOW Property (. VMP ) file info .
* Task 2 : Read in VMODFLOW Grid (. VMG ) file info
* Task 3 : Read in GSLIB simulation SGSIM or SISIM gamma values for each cell
* and convert to K values .
*
* Note that for Lena ' s simulations , there is a 1 : 1 correspondence
* of GSLIB simulation and VMODFLOW grid cells . A separate program
* DETERMINE was used to categorize each filled grid cell as an
* Aquifer ( I = 0 ) or Aquitard ( I = 1 ) based on a deterministic hydrostratigraphic
* model , so that a value from the appropriate GSLIB simulation can be assigned .
* This file is called the AQ . out file and is opened as File 15 .
* Two additional indicator classes are included :
* I =- 3141 No replacement for these cells
* I =- 9999 Below layer 0 ( bedrock - inactive cell )
*
* The algorithm to convert gamma values to K values is based on conversion
* of normalized gamma values from well MW - 96 .
*
* Task 4 : Calculate means and variances for Aquifer and Aquitard cells
* Task 5 : Generate CONNEC 3 D CUBE indicator value files for current realization
* Indicator output files are generated using a K value threshold for :
* indicator 1 = permeable ; 0 = impermeable
* with grid cylcling fastest on Z then Y then X .
* Two versions are created with I = 1 for K > arithmetic mean and
* I = 1 for K > geometric mean .
* Task 6 : Group assigned K values into a user - defined number of
* property categories and reassign property values to each
* fill cell . Note that property categories are assigned soley
* on the basis of Kx = Ky values ( the Kz distribution is scaled from Kx ).
* Task 7 : Write an output file formatted for insertion ( substitution )
* into the first section of the VMODFLOW property (. VMP ) file .
*
*
* *** Variable Descriptions ***
*
* General Variables
* =================
* N , N 1 , N 2 ... N 6 = loop counter variables
* Dummy = Dummy variable
*
* Variables associated with original VMODFLOW Property and Grid Files
* ====================================================================
* P , Q , R = loop counter variables for cols ( X ) , rows ( Y ) , and layers ( Z )
* NK = number of layers ( Z )
```

* $\mathrm{NJ}=$ number of columns ( X )
* NI = number of rows ( $Y$ )
* NKP = original number of properties
* Ki ( n ) $=$ property index number
* Kx ( $n$ ) = Kx value ( midpoint of K values for property bin )
* KxMAX ( n ) = maximum K value for property bin
$\mathrm{C}: \backslash$ Documents and Settings \Lena \My Documents \Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 2
* Ky ( $n$ ) = Ky value
* Kz ( n ) = Kz value
* PROP = array containing property indices from original . VMP file into
* which updated K indices values are substituted for fill cells
* $X(\mathrm{n})=X$ coordinate of VMODFLOW Grid Cell
* $Y(n)=Y$ coordinate of VMODFLOW Grid Cell
* $Z(n)=Z$ coordinate of VMODFLOW Grid Cell
* KPXMIN = smallest pre - assigned Kx Property value
* KPXMAX = largest pre - assigned Kx Property value
* 
* Variables associated with GSLIB 3 D Simulation
* =============================================
* S , T , U = loop counter variables for cols ( X ) , rows (Y) , and layers ( Z )
* $N X$, $N Y$, $N Z=$ number of $X, Y, Z$ nodes in simulated grid
* XMIN , YMIN , ZMIN $=\mathrm{X}, \mathrm{Y}, \mathrm{Z}$ coordinates of first node in simulated grid
* XSIZ , YSIZ , ZSIZ = X , Y, Z increment size ( constant ) in simulated grid
* XMAX , YMAX , ZMAX = X , Y , Z coordinates of last node in simulated grid
* XSIM ( $\mathrm{x}, \mathrm{y}, \mathrm{z}$ ) , $\operatorname{YSIM}(\mathrm{x}, \mathrm{y}, \mathrm{z})$, ZSIM ( $\mathrm{x}, \mathrm{y}, \mathrm{z}$ ) = Arrays of simulation XYZ coords
* KSIM ( $\mathrm{x}, \mathrm{y}, \mathrm{z}$ ) = Array containing simulated K values
* 
* Variables associated with Fill Cells ( VMODFLOW coordinate indices )
* ====================================
* P , Q , R = loop counter variables for cols ( X ) , rows ( Y ) , and layers ( Z )
* NJMIN , NKMIN , NIMIN = pointers to min ( first ) col / row / layer cell to be filled
* NJMAX , NKMAX , NIMAX = pointers to max ( last ) col / row / layer cell to be filled
* NKMINvmf , NKMAXvmf = pointers to first / last fill cells in VMG ( Y back to front )
* FILLKxMIN $=$ minimum simulated $K x=K y$ value to be filled into a fill cell
* FILLKxMAX = maximum simulated $K x=K y$ value to be filled into a fill cell
* FILLKzMIN = minimum simulated Kz value to be filled into a fill cell
* FILLKzMAX = maximum simulated Kz value to be filled into a fill cell
* NEWPROPS = user - specified number of new property values to be assigned
* ANSWER = character value to allow user to manually input BOUND
* TALLY ( n ) = array to count number of KFILL values in KCLASS bins
* between FILLxMIN and FILLxMAX
* XCOUNT , YCOUNT , ZCOUNT = counts number of simulated cells equivalent to the
* current VMODFLOW cell to be filled
* FILLKx ( $\mathrm{x}, \mathrm{y}, \mathrm{z}$ ) = Array containing averaged $\mathrm{Kx}=\mathrm{Ky}$ values for fill cells
* FILLKz $(x, y, z)=$ Array containing averaged Kz values for fill cells
* GEOM = geometric average K - calculated using power averaging of K values
* SUM = sum of simulated K values used to calculate arithmetic average K
* MEAN = arithmetic average K - used for comparison with geometric mean
* alternately , assigned to vertical Kz
* HARM = harmonic average K - used for comparison with geometric mean
* PROP ( $x$, $y, z$ ) = Array containing original and fill cell property indices
* CASEID = identifies case number for power averaging routine ( task 5 )
* 
* KCLASS = Number of hydraulic conductivity classes
* KZHARMONIC = Logical Variabile controlling average vertical k assignment
* $\mathrm{t}=$ use harmonic mean
* $\mathrm{f}=\mathrm{use} 0.10$ * average horizontal perm
* RHOF = fluid ( water ) density at 15 degrees C ( kg / m ^ 3 )
* MEWF = fluid ( water ) dynamic viscosity at 15 degrees C (Ns / m ^ 2 )
* POR = uniform porosity ( hardwired at $36 \%$ )
* $\mathrm{g}=$ gravitational constant
* GLOBcount = integer count of number of filled cells for each realization
* GLOBsum = global sum of fill K values
* GLOBarith = global arithmetic mean
* GLOBgeom = global geometric mean
* GLOBharm = global harmonic mean
* IVFLAG = logical : t = IV included in IV 2 d 10 output file
* GLOBLNK = global sum of natural log of K fill values ( LNK values )
* MEANLNK = arithmetic average of LNK values
* VARLNK = variance of LNK values
* 
* VARMODFLAG = flag set to true if mean and variance $\ln (\mathrm{K})$ will be adjusted
* TARGMEAN = target mean ln ( K ) value ( ft / day )

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* TARGVAR = target variance ln ( K ) value
* MEANADJ = adjustment factor for mean $\ln (\mathrm{K})$ value
* VARADJ = adjustment factor for variance ln ( K )
* 
* XAQ , YAQ , ZAQ $=x$, $y$, and $z$ values from AQ file
* IAQ = indicator value from AQ file ( $0=$ aquifer , 1 = aquitard , - 9999 = bedrock )
* IND = array of aquifer ( 2 ) , aquitard ( 1 ) , or no change (- 1 ) indicator values
* 
* Variables associated SGS / SIS Cubes in indicator form for CONNEC 3 D
* =====================================
* CUBE - array of indicator values $1.0=$ aquifer , $2.0=$ aquitard , - $1.0=$ inactive cell
* CUBEcount $=$ number of cube cells in filled VMP file
* CUBEsum = sum of cube K values
* CUBEgeom = cube geometric mean
* CUBEarith = cube arithmetic mean
* CUBEoutfileA = output file name for indicator values with arith mean cutoff
* CUBEoutfileG = output file name for indicator values with geom mean cutoff
* KCUBE = holding array in GSLIB simulation coordinates for transformed K values
* CUBEGTA , CUBEGTG = count of cells with $\mathrm{K}>=$ Cube arithmetic / geometric means
* VMPcount , VMPsum , VMPgeom , VMParith = global vmp file metrics
* VMPAqcount , VMPAqsum , VMPAqgeom , VMPAqarith = vmp file aquifer metrics
* VMPAtcount , VMPAtsum , VMPAtgeom , VMPAtarith = vmp file aquitard metrics
* VMPAqmin , VMPAqmax , VMPAtmin , VMPAtmax = min max assigned aquifer / aquitard K values
* 
* *** Declare Variables ***

IMPLICIT NONE
INTEGER N , N 1 , N 2 , N 3 , N 4 , N 5 , N 6 , KCLASS , TEMP
INTEGER REALNUM , FIRST , RR , CURRENT , FIVECOUNT
INTEGER i , ii , iii
INTEGER NK , NJ , NI , NKP , Ki , PROP , TALLY
INTEGER S , T , U , NX , NY , NZ , IAQ
INTEGER P , Q , R , NJMIN , NIMIN , NKMIN , GLOBcount
INTEGER NJMAX , NIMAX , NKMAX , NEWPROPS , XCOUNT , YCOUNT , ZCOUNT
INTEGER XPOINT 1 , YPOINT 1 , ZPOINT 1 , XPOINT , YPOINT , ZPOINT
INTEGER AQCOUNT , ATCOUNT , XHARMCOUNT
INTEGER IND , PathCOUNT , XaqCOUNT , XatCOUNT , XskipCOUNT , Xnovalue
INTEGER CUBEcount , CUBE 2 , CUBEGTA , CUBEGTG
INTEGER VMPcount , VMPAqcount , VMPAtcount , TALLYTOT
INTEGER NKMINvmf , NKMAXvmf
REAL DUMMY , XaqPERCNT , XatPERCNT , SkipPERCNT
REAL CUBE
REAL * 8 Kx , Ky , Kz , KPXMIN , KPXMAX , Y , Z , KxMAX
REAL * 8 YMIN , ZMIN , YMAX , ZMAX , XSIZ , YSIZ , ZSIZ
REAL * 8 KSIM, YSIM, ZSIM, KSIM 1 , KSIM 0 , KSIM 1 K, KSIM 0 K
REAL * 8 FILLKxMIN , FILLKxMAX , FILLKzMIN , FILLKzMAX , FILLKx , FILLKz
REAL * 8 BOUND , GEOM , SUM , MEAN , HARM
REAL * 8 GLOBsum , GLOBarith , GLOBgeom , GLOBharm
REAL * 8 GLOBLNK , MEANLNK , VARLNK
REAL * 8 TARGVAR , TARGMEAN , LNFILLK , MEANADJ , VARADJ
REAL * 8 XAQ , YAQ , ZAQ
REAL * 8 AQSUM , AQARITH , AQGEOM , AQHARM , AQLNK , AQVARLNK , AQMEANLNK
REAL * 8 ATSUM , ATARITH , ATGEOM , ATHARM , ATLNK , ATVARLNK , ATMEANLNK
REAL * 8 XHARM , XHARMMIN , XHARMMAX , XHARMSUM , XHARMMEAN , AQVAL , ATVAL
DOUBLE PRECISION X , XMIN , XMAX , XSIM
REAL * 8 CUBEsum , CUBEarith , CUBEgeom , CUBEK
REAL * 8 VMPsum , VMPgeom , VMParith , VMPAqsum , VMPAqgeom , VMPAqarith

REAL * 8 VMPAtsum , VMPAtgeom , VMPAtarith
REAL * 8 VMPAqmin , VMPAqmax , VMPAtmin , VMPAtmax
CHARACTER DUMMIE * 24 , ANSWER * 1 , OUTPRE * 60 , str $* 8$, OUTFILE $* 65$
CHARACTER gamfile $1 * 65$, gamfile $0 * 65$, DATE * 24
CHARACTER CUBEoutfileA * 65 , CUBEoutfileg * 65
$\mathrm{C}: \backslash$ Documents and Settings \Lena $\backslash M y$ Documents $\backslash$ Directed Study $\backslash$ Fortran_GSL2VMF $\backslash$ GSL2VMF16.f 4
LOGICAL KZHARMONIC , IVFLAG , VARMODFLAG , UNIFORM
DIMENSION KI ( 280 )
DIMENSION KX ( 176 ) , KxMAX ( 176 ) , KY ( 176 ) , KZ ( 176 ) , TALLY ( 500 )
DIMENSION PROP ( $0: 280,0: 140,0: 36$ )
DIMENSION X ( $0: 281$ ) , $Y(0: 140), Z(0: 37)$
DIMENSION XSIM ( $0: 282,0: 140,0: 140), \operatorname{YSIM}(0: 282,0: 140,0: 140)$
DIMENSION ZSIM ( $0: 282$, $0: 140,0: 140$ ) $\operatorname{KSIM}(0: 280,0: 140$, $0: 140$ )
DIMENSION FILLKx ( $0: 280,0: 280,0: 280)$, FILLKz ( $0: 280,0: 140$, $0: 36$ )
DIMENSION LNFILLK ( 0 : 280, $0: 280$, $0: 280$ )
DIMENSION KSIM 1 ( $0: 280,0: 140,0: 140$ ) $\operatorname{KSIM} 0(0: 280,0: 140,0: 140)$
DIMENSION KSIM $1 \mathrm{~K}(0: 280,0: 140,0: 140)$, KSIM $0 \mathrm{~K}(0: 280$, $0: 140$, $0: 140)$
DIMENSION XHARM ( $1: 140$, $1: 50$ )
DIMENSION IND ( $0: 281,0: 140,0: 140$ ) , CUBEK ( $0: 281,0: 140$, $0: 140$ )
DIMENSION CUBE ( $0: 281,0: 140,0: 140)$ CUBE $2(0: 281,0: 140$, $0: 140)$

* *** I / O file Descriptions ***
* 
* File 10 contains the input VMODFLOW Property (. VMP ) file
* File 15 contains the aquifer / aquitard indicator file (from DETERMINE . for )
* File 20 contains the input VMODFLOW Grid (. VMG ) file
* File 25 is the parameter file
* File 30 contains the input GSLIB simulation file for aquifer data ( e . g . SGS . OUT )
* File 31 contains the input GSLIB simulation file for aquitard data ( e . g . SGS . OUT )
* File 40 is the formatted output file for ". VMP file " output
* File 41 contains indicator values based on arithmetic mean cutoff for
* postprocessing with CONNECT 3 D
* File 42 contains indicator values based on geometric mean cutoff for
* postprocessing with CONNECT 3 D
* File 50 is an output log for debugging write statements, summary statistics, and
* screening metrics
* File 51 accumulates a summary table of metrics for each realization processed
* File 52 is an output file with records from each individual $X$ flow pathway
* Files 60 and 61 are output files storing $K$ values for internal statistical analysis
* ( stats are calculated on realization K values within GSL 2 VMF )
* Files 62 and 63 are input files used to read $K$ values stored in files 60 and 61
* 

OPEN ( 10 , FILE = ' C : \ Documents and Settings \Lena \My Documents \ Directed Stu
1 dy \Fortran GSL 2 VMF \ seed. VMP ', STATUS = ' OLD ' )
OPEN ( 15 , FILE $=$ ' $C: \$ Documents and Settings \ Lena \My Documents \ Directe
1 d Study \ Fortran GSL 2 VMF \ DETERMINE \AQ . OUT ', STATUS = ' OLD ' )
OPEN ( 20 , FILE $=$ ' C : \ Documents and Settings \Lena \My Documents \Directe
1 d Study \Fortran GSL 2 VMF \ seed. VMG ', STATUS = ' OLD ' )
OPEN ( 25 , FILE $=$ ' C : \ Documents and Settings \Lena \My Documents \Directed Stu
1 dy \Fortran GSL 2 VMF \GSL 2 VMF 15 . par ', STATUS = ' OLD ' )
OPEN ( 50 , FILE $=$ ' C : \ Documents and Settings \ Lena \My Documents \Directed Stu
1 dy \Fortran GSL 2 VMF \OutputFiles \GSL 2 VMF 15 . log ' )
OPEN ( 51 , FILE $=$ ' $C: \$ Documents and Settings $\backslash$ Lena $\backslash$ My Documents $\backslash$ Directe
1 d Study \Fortran GSL 2 VMF \ OutputFiles \Summary Table . dat ',
2 Position = ' APPEND ' )
C

* *** Read data from paramater file ***

READ ( 25 , *) REALNUM
READ ( 25 , *) FIRST
CURRENT = FIRST - 1
READ ( 25 , *) UNIFORM
PRINT * , 'Uniform Heterogeneous Model Flag = ', Uniform
WRITE ( 50 , *) ' Uniform Heterogeneous Model Flag = ', Uniform
PRINT *
WRITE ( 50 , *)
READ ( $25, *)$ OUTPRE

```
print * , ' outpre = ', outpre
write ( 50, *) ' GSL 2 VMF output file record '
write ( 50, *)
ii = index ( outpre ,' ' )- 1
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READ ( 25 , *) gamfile 0
READ ( 25 , *) gamfile 1
OPEN ( 30 , FILE = gamfile 0 , STATUS = ' OLD ' ) ! GSLIB aquifer simulation
OPEN ( 31 , FILE = gamfile 1 , STATUS = ' OLD ' ) ! GSLIB aquitard simulation
write ( 50 , *) ' gamfile 1 = ', gamfile 1
write ( 50 , *) ' gamfile 0 = ', gamfile 0
write ( 50 , *) ' outpre = ', outpre
print * , ' gamfile 0 = ', gamfile 0
print * ,' gamfile 1 = ', gamfile 1
print * , ' GSL 2 VMF will process ', REALNUM ,' realizations '
write ( 50, *) ' GSL 2 VMF will process ', REALNUM,' realizations '
print * , ' The first realization number is ', FIRST
write ( 50 , *) ' The first realization number is ', FIRST
write ( 50, *)
2 print *
print * , ' *** Check your Parameter File ! '
print * , ' *** Are these correct ? Continue ( Y / N ) '
READ * , ANSWER
IF (( ANSWER . EQ . ' N ' ). OR .( ANSWER . EQ . ' n ' )) THEN
stop
ELSEIF (( ANSWER . EQ . ' Y ' ). OR .( ANSWER . EQ . ' y ' )) THEN
continue
ELSE
GOTO 2
ENDIF
*
* Read pointers to first ( min ) and last ( max ) col / row / layer cell to be filled
READ ( 25 , *) NJMIN
READ ( 25 , *) NJMAX
READ ( 25 , *) NKMIN
READ ( 25 , *) NKMAX
READ ( 25 , *) NIMIN
READ ( 25 , *) NIMAX
READ ( 25 , *) NKMINvmf
READ ( 25 , *) NKMAXvmf
*
* Read in GSLIB simulation domain coordinates
READ ( 25 , *) NX , XMIN , XSIZ
READ ( 25 , *) NY , YMIN , YSIZ
READ ( 25 , *) NZ , ZMIN , ZSIZ
Print * , " NX =" , NX
PRINT * , " NY =" , NY
PRINT * , " NZ =" , NZ
Print *
*
* Calculate associated maximimum GSLIB domain coordinates
XMAX = XMIN + ( NX - 1 )* XSIZ ! Point ( mesh ) centered grid
YMAX = YMIN + (NY - 1 )* YSIZ
ZMAX = ZMIN + ( NZ - 1 )* ZSIZ
WRITE ( 50 , *) " NX = " , NX , " XSIZ = " , XSIZ
WRITE ( 50 , *) " NY = " , NY , " YSIZ = " , YSIZ
WRITE ( 50 , *) " NZ = " , NZ , " ZSIZ = " , ZSIZ
WRITE ( 50 , 109 ) XMIN , XMAX
WRITE ( 50 , 110 ) YMIN , YMAX
WRITE ( 50 , 111 ) ZMIN , ZMAX
*
* Read flag to determine if harmonic averaging is used for Kz values
READ ( 25 , *) KZHARMONIC
*
* Read flag to determine if Variance and Mean LN ( K ) will be adjusted
```

```
READ ( 25 , *) VARMODFLAG
READ ( 25 , *) TARGVAR ! used only if VARMODFLAG = t
READ ( 25 , *) TARGMEAN ! used only if VARMODFLAG = t
*
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WRITE ( 50 , *)' VARMODFLAG = ', VARMODFLAG
WRITE ( 50, *)
Print * , ' VARMODFLAG = ', VARMODFLAG
Print *
*
* Read number of conductivity classes to be assigned
READ ( 25 , *) KCLASS
Print * , ' KCLASS = ', KCLASS
*
IF ( KCLASS . LT . 1 ) THEN
PRINT *
PRINT * , " ASSIGNED VALUE MUST BE AN INTEGER GREATER THAN 1 "
Print * , ' ERROR '
stop
ENDIF
*
IF ( KCLASS . GT . 175 ) THEN
PRINT *
PRINT * , " ASSIGNED VALUE MUST BE AN INTEGER LESS THAN 175 "
PRINT * , ' KCLASS = ', KCLASS
PRINT * , ' ERROR '
stop
ENDIF
*
*
* *** TASK 1 ************************ TASK 1 ********************** TASK 1 ***
*
* Read in initial VMODFLOW Property (. VMP ) file info
*
print * , ' Starting Task 1 : Read original VMODFLOW . VMP file '
WRITE ( 50 , *) " STARTING TASK 1 : Read original VMODFLOW . VMP file "
WRITE ( 50, *)
READ ( 10, 101 ) NK ! Number of layers ( Z )
READ ( 10 , 101 ) NJ ! Number of columns ( X )
READ ( 10 , 101 ) NI ! Number of rows ( Y )
READ ( 10 , 101 ) NKP ! Number of original K property classes
WRITE ( 50 , *) " NK =" , NK
WRITE ( 50, *) " NJ =" , NJ
WRITE ( 50 , *) " NI =" , NI
WRITE ( 50 , *) " NKP =" , NKP
*
* Find smallest and largest Kx values while reading in indices and K data
*
KPXMIN = 1000000 . 0
KPXMAX = 0 . 0
DO N = 1 , NKP
IF ( N . LE . 9 ) THEN
READ ( 10 , 102 ) Ki ( N ) , Kx ( N ) , Ky ( N ) , Kz ( N )
ELSE IF ( N . GE . 10 ) THEN
READ ( 10 , 103 ) Ki ( N ) , Kx ( N ) , Ky ( N ) , Kz ( N )
ENDIF
WRITE ( 50 , *) " N =" , N
WRITE ( 50, *) " Ki ( N )=" , Ki ( N )
WRITE ( 50 , *) " Kx ( N )=" , Kx ( N )
WRITE ( 50 , *) " Ky ( N )=" , Ky ( N )
WRITE ( 50 , *) " Kz ( N )=" , Kz ( N )
IF ( Kx ( N ). GT . KPXMAX ) THEN
KPXMAX = Kx ( N )
ENDIF
IF ( Kx ( N ). LT . KPXMIN ) THEN
```

```
KPXMIN = KX ( N )
ENDIF
ENDDO
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 7
**** Skip blank line in . VMP file
READ ( 10 , *)
* *** Read in Original Property Indice Values
* *** Note that . VMP files are written from left to right ( NJ ) , back ( NI )
* to front , and bottom to top ( NK ). Treatment of the Y coordinate ( I )
* variable is contrary to VMODFLOW User Manual Documentation for
* . VMP files . ***
DO R = 1 , NK
DO Q = NI , 1 , - 1
READ ( 10, *) ( PROP ( S , Q , R ) , S = 1 , NJ )
* WRITE ( 50 , 125 ) ( PROP ( S , Q , R ) , S = 1 , NJ )
ENDDO
* Skip Blank Line in . VMP file
READ ( 10 , *)
* WRITE ( 50 , *) " BLANK LINE SKIP "
ENDDO
*
*
CLOSE ( 10 )
* Read in maximum value for each new K property class from parameter file
Do N = 1 , KCLASS
READ ( 25, *) KxMAX ( NKP + N )
ENDDO
*
*
* *** TASK 2 ************************ TASK 2 ********************** TASK 2 ***
*
* Read in VMODFLOW Grid (. VMG ) file info
*
WRITE ( 50 , *)
WRITE ( 50 , *) " STARTING TASK 2 : Read in VMODFLOW Grid (. VMG ) file "
PRINT * , " STARTING TASK 2 : Read in VMODFLOW Grid (. VMG ) file "
* *** Note that . VMG files are written from left to right ( NJ ), front to
* back ( NI ) , and bottom to top ( NK ). Treatment of the Y ( I ) coordinate
* variable is consistent with VMODFLOW User Manual Documentation for
* . VMG files , however it is inconsistent with the direction in which
* . VMP elemental arrays are written for the Y ( I ) coordinate . ***
READ ( 20 , *) DUMMIE
DO N = 1 , NJ + 1
READ ( 20, *) X ( N )
ENDDO
READ ( 20 , *) DUMMIE
DO N = 1 , NI + 1
READ ( 20, *) Y ( N )
ENDDO
READ ( 20 , *) DUMMIE
DO N = 1, NK + 1
READ ( 20, *) Z ( N )
ENDDO
* *** TASK 3 ******************** TASK 3 ******************* TASK 3 *******
* Read in GSLIB simulation values and scale from gamma to K values *****
*
*
WRITE ( 50 , *)
WRITE ( 50 , *) " STARTING TASK 3 a : Gather GSLIB simulation info "
WRITE ( 50 , *)
PRINT * , " STARTING TASK 3 a : Read Gather GSLIB simulation info "
* Advance simulation file to first record and read in simulated gamma values
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* Note - This version assumes normalized gamma values are unitless
READ ( 30, *) DUMMIE
```

```
READ ( 30 , *) DUMMIE
READ ( 30 , *) DUMMIE
READ ( 31 , *) DUMMIE
READ ( 31 , *) DUMMIE
READ ( 31 , *) DUMMIE
*******************************************
* *** Loop through number of iterations ******************************************
*******************************************
FiveCount = 0 ! Counter used to cycle through groups of 5 realizations
DO 555 RR = 1 , REALNUM ! number of realizations to be processed
FiveCount = FiveCount + 1
Print * , ' FiveCount = ', FiveCount
IF ( FiveCount . GT . 5 ) THEN
FiveCount = 1
Print * , ' FiveCount = ', FiveCount
CLOSE ( 30 )
CLOSE ( 31 )
READ ( 25 , *) gamfile 0 ! GSLIB Aquifer Simulation Files ( 5 realizations )
READ ( 25 , *) gamfile 1 ! GSLIB Aquitard Simulation Files ( }5\mathrm{ realizations )
write (* , *) ' gamfile 1 = ', gamfile 1
write (* , *) ' gamfile 0 = ', gamfile 0
write ( 50 , *) ' gamfile 1 = ', gamfile 1
write ( 50 , *) ' gamfile 0 = ', gamfile 0
OPEN ( 30 , FILE = gamfile 0 , STATUS = ' OLD ' ) ! GSLIB aquifer simulation
OPEN ( 31 , FILE = gamfile 1 , STATUS = ' OLD ' ) ! GSLIB aquitard simulation
READ ( 30 , *) DUMMIE
READ ( 30 , *) DUMMIE
READ ( 30 , *) DUMMIE
READ ( 31 , *) DUMMIE
READ ( 31 , *) DUMMIE
READ ( 31 , *) DUMMIE
ENDIF
CALL FDATE ( DATE )
PRINT *
PRINT * , ' TODAY IS ', DATE
REWIND ( 15 ) ! Aquifer / Aquitard indicator file ( same for all realizations )
! Open files to store K values for statistical calculations for each realization
OPEN ( 60 , FILE = ' C : \ Documents and Settings \ Lena \ My Documents \ Di
1 rected Study \ Fortran GSL 2 VMF \ OutputFiles \ KSIM 0 K . dat ' ) ! aquifer
OPEN ( 61 , FILE = ' C : \ Documents and Settings \ Lena \ My Documents \ Di
1 rected Study \ Fortran GSL 2 VMF \ OutputFiles \ KSIM 1 K . dat ' ) ! aquitard
* *** Initialize variables for counts , averaging , and variance calculations ***
CURRENT = CURRENT + 1
GLOBsum = 0 . 0 ! Global values
GLOBgeom = 0 . 0
GLOBharm = 0 . 0
GLOBcount = 0
GLOBLNK = 0 . 0
AqSUM = 0 . 0 ! Aquifer only values
AqGEOM = 0 . 0
AqHARM = 0. 0
AqCOUNT = 0
AqLNK = 0 . 0
AqVARLNK = 0 . 0
AtSUM = 0 . 0 ! Aquitard only values
AtGEOM = 0 . 0
AtHARM = 0 . 0
AtCOUNT = 0
AtLNK = 0 . 0
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AtVARLNK = 0 . 0
DO N = 1 , NKP + KCLASS
TALLY ( N )=0
ENDDO
print *
```

```
print * ,' *** BEGINNING REALIZATION NUMBER ', CURRENT
print *
write ( 50 , *) ' ****** REALIZATION NUMBER ', CURRENT , ' *******
write ( 50 , *)
* ************* Read AQ . out and GSLIB files \(* * * * * * * * * * * * * * ~\)
DO \(U=1\), NZ ! layer ( Z ) ! layer 1 must be bottom layer
PRINT * , " CURRENTLY ON LAYER " , U
DO T = 1 , NY ! row ( Y ) ! reading from front to back
DO \(S=1\), NX ! column ( \(X\) ) ! reading from left to right
READ ( 15 , *) , XAQ , YAQ , ZAQ , IAQ ! Read from AQ . out file
! IAQ determines whether cell is aquifer \(I A Q=0\) or aquitard \(I A Q=1\)
READ ( \(30,{ }^{*}\) ) KSIM 0 ( S , T , U ) ! Aquifer values
* \(* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * ~+~\)
* CONVERT FROM NORMALIZED GAMMA TO K ( ft / d )
* Note - this version uses gamma values from MW - 96
* First , de - normalize the gamma data ( from \% to cpm )
* Second , convert from cpm to cm / s
* Third , convert from cm / s to ft / d
* Fourth , scale to range of observed values in aquifer samples
* ! convert to min and max gamma values of aquifer data set :
KSIM 0 K ( S , T , U ) \(=\) KSIM 0 ( S , T , U ) * ( 2726 . \(78-175\). 5 ) 175 . 5
KSIM 0 K ( S , T , U ) = 0. 00241 * EXP ( \(-0.00531 * \operatorname{KSIM} 0 \mathrm{~K}(\mathrm{~S}, \mathrm{~T}, \mathrm{U}))\) ! convert to cm / sec
KSIM 0 K ( S , T , U ) = KSIM \(0 \mathrm{~K}(\mathrm{~S}, \mathrm{~T}, \mathrm{U}) * 86400\). 0 / 2 . 54 / 12 . 0 ! convert to ft / day
* ! scale to range of observed values in aquifer samples :
KSIM 0 K ( S , T , U )=( KSIM 0 K ( S , T , U )- 0 . 00000352 )/( 2 . 690262 -
10 . 00000352 )* 98.4 - 0. 237 ) +0 . 237
aquifer zonation and improve VMODFLOW head
* ! Aquifer zonation implemented to improve calibration for downgradient wells
! ( MWs 111 , 102 , 97 , 98 , 99 , 82 )
! SGS Zonation ( 10 - MAR - 14 ): West of Col 127 x 10
! West of Col \(162 \times 5\)
! Else ( East of Col 162 ) x 1
! SIS Zonation ( 23 - Jun - 14 ) West of Col 127 x 10
! West of Col \(162 \times 1\)
! Else ( East of Col 162 ) x 1
IF ( S . LT . 127 ) THEN
KSIM 0 K ( S , T , U ) = KSIM 0 K ( S , T , U )* 10 . 0
ELSEIF ( S . LT . 162 ) THEN
KSIM 0 K ( S , T , U ) = KSIM \(0 \mathrm{~K}(\mathrm{~S}, \mathrm{~T}, \mathrm{U}\) )* 1 . 0 ! Changed from 5 . 0 to 1 . 0 ( LDL 23 - Jun -
14 )
ELSE
KSIM 0 K ( S , T , U )= KSIM 0 K ( S , T , U )* 1 . 0
ENDIF
*
IF ( KSIM 0 K ( S , T , U ). LT . 0 . 5 ) THEN ! truncate aquifer K at 0 . 51
KSIM 0 K ( S , T , U ) = 0.51
ENDIF
* **** Write Aquifer K values to output file for stat analysis
Write ( 60 , *) KSIM 0 K ( S , T , U )
```



```
READ ( 31 , *) KSIM 1 ( S , T , U ) ! Aquitard values
```



```
* CONVERT FROM NORMALIZED GAMMA TO K ( ft / d )
* Note - this version uses gamma values from MW - 96
* First , de - normalize the gamma data ( from \% to cpm )
* Second , convert from cpm to cm / s
C: \Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF \GSL2VMF16.f 10
* Third , convert from cm / s to ft / d
* ! convert to min and max gamma values of aquitard data set :
KSIM 1 K ( S , T , U ) = KSIM 1 ( S , T , U )* ( 2004 . 76 - 155 . 2 ) 155 . 2
KSIM \(1 \mathrm{~K}(\mathrm{~S}, \mathrm{~T}, \mathrm{U})=0.00241 * \operatorname{EXP}(-0.00531 * \operatorname{KSIM} 1 \mathrm{~K}(\mathrm{~S}, \mathrm{~T}, \mathrm{U}))\) ! convert to cm / sec
KSIM 1 K ( S , T , U )= KSIM 1 K ( S , T , U )* 86400 . 0 / 2 . 54 / 12 . 0 ! convert to ft / day
* ! scale to range of observed values in aquitard samples :
KSIM 1 K ( S , T , U )=( KSIM 1 K ( S , T , U )- 0 . 000163 )/( 2 . 9964 -
10 . 000163 )*( \(0.313-0\). 000716 ) + 0 . 000716
```

```
*
* Write Aquitard K values to output file for stat analysis
Write ( 61 , *) KSIM 1 K ( S , T , U )
* ************************************************************************
* Update Aquifer and Aquitard means, set CUBE flags for CONNEC 3 D
* *****************************************************************
IF (( IAQ . EQ . 0 )) THEN ! Aquifer Cell
KSIM ( S + NJMIN - 1 , T + NKMIN - 1 , U )= KSIM 0 K ( S , T , U ) ! VMODFLOW Grid Coords
IND ( S + NJMIN - 1, T + NKMIN - 1 , U )= 2 ! VMODFLOW Grid Coordinates
CUBEK ( S , T , U )= KSIM 0 K ( S , T , U ) ! GSLIB Simulation Coordinates
* *** Update the AQUIFER arithmetic , geometric , and harmonic means
AqSUM = AqSUM + KSIM 0 K ( S , T, U )
AqGEOM = AqGEOM + LOG ( KSIM 0 K ( S , T , U ))
AqHARM = AqHARM + KSIM 0 K ( S , T , U )**(- 1 . 0 )
AqLNK = AqLNK + LOG ( KSIM 0 K ( S , T , U ))
AqCOUNT = AqCOUNT + 1
* *** Set CUBE flag to 1 . 0 for aquifer
CUBE ( S , T , U ) = 1 . 0
ELSE IF ( IAQ . EQ . 1 ) THEN ! Aquitard Cell
KSIM ( S + NJMIN - 1 , T + NKMIN - 1 , U ) = KSIM 1 K ( S , T , U ) ! VMODFLOW Grid Coords
IND ( S + NJMIN - 1 , T + NKMIN - 1 , U )= 1 ! VMODFLOW Grid Coordinates
CUBEK ( S , T , U )= KSIM 1 K ( S , T , U ) ! GSLIB Simulation Coordinates
* *** Update the AQUITARD arithmetic , geometric , and harmonic means
AtSUM = AtSUM + KSIM 1 K ( S , T , U )
AtGEOM = AtGEOM + LOG ( KSIM 1 K ( S , T , U ))
AtHARM = AtHARM + KSIM 1 K ( S , T , U )**(- 1 . 0 )
AtLNK = AtLNK + LOG ( KSIM 1 K ( S , T, U ))
AtCOUNT = AtCOUNT + 1
* *** Set CUBE flag to 2 . 0 for aquitard
CUBE ( S , T , U ) = 2 . 0
ELSE ! Do not fill cell
KSIM ( S + NJMIN - 1 , T + NKMIN - 1 , U )=- 1 . 0 ! VMODFLOW Grid Coordinates
IND ( S + NJMIN - 1 , T + NKMIN - 1 , U )=- 1 ! VMODFLOW Grid Coordinates
CUBEK ( S , T , U )= 0 . 0 ! GSLIB Simulation Coordinates
! Should not be included in CubeArithMean or CubeGeomMean counts or calcs
* *** Set CUBE flag to - 1 . 0 for inactive cell
CUBE ( S , T , U ) = - 1 . 0
ENDIF
XSIM ( S + NJMIN - 1 , T + NKMIN - 1 , U ) = XMIN + ( S - 1 )* XSIZ
YSIM ( S + NJMIN - 1 , T + NKMIN - 1 , U ) = YMIN + ( T - 1 )* YSIZ
ZSIM ( S + NJMIN - 1, T + NKMIN - 1, U ) = ZMIN + (U - 1 )* ZSIZ
ENDDO
ENDDO
ENDDO
Print * , " End of Do Loop "
CLOSE ( 60 )
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 11
CLOSE ( 61 )
*
* *** TASK 4 ************************ TASK 4 *********************** TASK 4 *******
*
*
* *** Calculate Means and Variances for Aquifer and Aquitard cells
WRITE ( 50 , *) , ' Starting Task 4 '
WRITE ( 50 , *)
PRINT * , ' Starting Task 4 '
PRINT *
PRINT * , ' AQCOUNT = ', AqCOUNT
PRINT * , ' ATCOUNT = ', AtCOUNT
WRITE ( 50 , *) ,' AQCOUNT = ', AqCOUNT
WRITE ( 50 , *) ,' ATCOUNT = ', AtCOUNT
WRITE ( 50 , *) ,' % AQUIFER = ', REAL ( AqCOUNT )/ REAL ( AqCOUNT + AtCOUNT )* 100 .
WRITE ( 50 , *),' % AQUITARD = ', REAL ( AtCOUNT )/ REAL (AqCOUNT + AtCOUNT )* 100 .
PRINT * , '% AQUIFER = ', REAL (AqCOUNT )/ REAL ( AqCOUNT + AtCOUNT )* 100 . 0
PRINT * , ' % AQUITARD = ', REAL ( AtCOUNT )/ REAL (AqCOUNT + AtCOUNT )* 100 . 0
```

```
* Initialize values to track largest and smallest K values assigned
FILLKxMIN = 1000000 . 0
FILLKxMAX = 0 . 0
FILLKzMIN = 1000000 . 0
FILLKzMAX = 0 . 0
*
******************************************************************************
* Loop through VMODFLOW cells to be filled with simulated values
* Decision Rule : If a simulation grid node falls on a VMODFLOW cell lower
* boundary , the simulation grid value is included. If the simulation grid
* node falls on a VMODFLOW cell upper boundary , it is not included ( it
* will be included in the next VMODFLOW cell ).
WRITE ( 50 , *) " NKMIN , NKMAX = " , NKMIN , NKMAX
WRITE ( 50 , *) " NJMIN , NJMAX = " , NJMIN , NJMAX
*
DO R = 1 , 36 ! Layer ( Z ) ! Changed from R = 1 , 35 to R = 1 , 36 by LDL 2 / 19 / 2014
DO Q = NKMIN , NKMAX ! Row ( Y )
DO P = NJMIN , NJMAX ! Column ( X )
*
* *** Assign averaged K value to KFILL array
IF ( KSIM ( P , Q , R ). GT . 0 . 0 ) THEN
FILLKx ( P , Q , R ) = KSIM ( P , Q , R )
! Apply Kv : Kh ratio
IF ( KZHARMONIC ) THEN
FILLKz ( P , Q , R ) = HARM !!! Undefined at this point !!!
ELSE
FILLKz ( P , Q , R ) = FILLKx ( P , Q , R )* 0 . 10 ! 10 : 1 Kx : Kz scaling factor
ENDIF
* *** Update minimum and maximum fill K variable trackers
IF ( FILLKx ( P , Q , R ). LT . FILLKxMIN )
+ FILLKxMIN = FILLKx ( P , Q , R )
IF ( FILLKx ( P , Q , R ). GT . FILLKxMAX )
+ FILLKxMAX = FILLKx ( P , Q , R )
IF ( FILLKz ( P , Q , R ). LT . FILLKzMIN )
+ FILLKzMIN = FILLKz ( P , Q , R )
IF ( FILLKz ( P , Q , R ). GT . FILLKzMAX )
+ FILLKzMAX = FILLKz ( P , Q , R )
*
* *** Update the global arithmetic , geometric , and harmonic means
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 12
GLOBsum = GLOBsum + FILLKx ( P , Q , R )
GLOBgeom = GLOBgeom + LOG ( FILLKx ( P , Q , R ))
GLOBharm = GLOBharm + FILLKx ( P , Q , R )**(- 1 . 0 )
GLOBLNK = GLOBLNK + LOG ( FILLKx ( P , Q , R ))
GLOBcount = GLOBcount + 1
ENDIF
*
22 ENDDO
21 ENDDO
20 ENDDO
* *** Report minimum and maximum fill values
WRITE ( 50 , 301 ) FILLKxMIN
WRITE ( 50 , 302 ) FILLKxMAX
WRITE (* , 301 ) FILLKxMIN
WRITE (*, 302 ) FILLKxMAX
*
* *** Calculate Arithmetic , Geometric , and Harmonic Means
*
GLOBarith = GLOBsum / REAL ( GLOBcount )
GLOBgeom = EXP ( GLOBgeom / REAL ( GLOBcount ))
GLOBharm =( GLOBharm / REAL ( GLOBcount ))**(- 1 . 0 )
MEANLNK = GLOBLNK / REAL ( GLOBcount )
*
AqARITH = AqSUM / REAL ( AqCOUNT )
```

```
AqGEOM = EXP ( AqGEOM / REAL ( AqCOUNT ))
AqHARM =( AqHARM / REAL ( AqCOUNT ) )**(- 1 . 0 )
AqMEANLNK = AqLNK / REAL ( AqCOUNT )
AtARITH = AtSUM / REAL ( AtCOUNT )
AtGEOM = EXP ( AtGEOM / REAL ( AtCOUNT ))
AtHARM =( AtHARM / REAL ( AtCOUNT ))**(- 1 . 0 )
AtMEANLNK = AtLNK / REAL ( AtCOUNT )
* Calculate Global Variance ln ( K )
VARLNK = 0 . d 0
DO R = 1 , 35 ! Layer ( Z )
DO Q = NKMIN , NKMAX ! Row ( Y )
DO P = NJMIN , NJMAX ! Column ( X )
IF ( FILLKx ( P , Q , R ). GT . 0 . 0 ) THEN
VARLNK = VARLNK + ( LOG ( FILLKX ( P , Q , R ))- MEANLNK )** 2 . 0
ENDIF
ENDDO
ENDDO
ENDDO
VARLNK = VARLNK / REAL ( GLOBcount ) ! Global
* **** Calculate variance for Aquifer and Aquitard cells independently
OPEN ( 62 , FILE = ' C : \ Documents and Settings \ Lena \ My Documents \ Directed Stu
1 dy \ Fortran GSL 2 VMF \ OutputFiles \ KSIM 0 K . dat ', STATUS = ' OLD ' )
DO N = 1 , AqCOUNT
READ ( 62 , *) AqVAL
AqVARLNK = AqVARLNK + ( LOG ( AqVAL )- AqMEANLNK )** 2 . 0
ENDDO
CLOSE ( 62 )
AqVARLNK = AQVARLNK / REAL ( AQCOUNT ) ! Aquifer
OPEN ( 63 , FILE = ' C : \ Documents and Settings \ Lena \ My Documents \ Directed Stu
1 dy \ Fortran GSL 2 VMF \ OutputFiles \ KSIM 1 K . dat ', STATUS = ' OLD ' )
DO N = 1 , AtCOUNT
READ ( 63 , *) AtVAL
AtVARLNK = AtVARLNK + ( LOG ( AtVAL )- AtMEANLNK )** 2 . 0
ENDDO
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 13
CLOSE ( 63 )
AtVARLNK = ATVARLNK / REAL ( ATCOUNT ) ! Aquitard
* *** Report Arithmetic , Geometric , and Harmonic Means , and LNK values
WRITE (* , *)
WRITE (* , *) ' GLOBcount = ', GLOBcount
WRITE (* , *) ' GLOBAL ARITHMETIC MEAN = ', GLOBarith
WRITE (* , *) ' GLOBAL GEOMETRIC MEAN = ', GLOBgeom
WRITE (* , *) ' GLOBAL HARMONIC MEAN = ', GLOBharm
WRITE (* , *) ' MEAN of LNK = ', MEANLNK
WRITE (* , *) ' GLOBAL VARIANCE of LNK = ', VARLNK
WRITE (* , *)
WRITE ( 50 , *)
WRITE ( 50 , *) ' GLOBcount = ', GLOBcount
WRITE ( 50 , *) ' GLOBAL ARITHMETIC MEAN = ', GLOBarith
WRITE ( 50 , *) ' GLOBAL GEOMETRIC MEAN = ', GLOBgeom
WRITE ( 50 , *) ' GLOBAL HARMONIC MEAN = ', GLOBharm
WRITE ( 50 , *) ' MEAN of LNK = ', MEANLNK
WRITE ( 50 , *) ' GLOBAL VARIANCE of LNK = ', VARLNK
WRITE ( 50, *)
WRITE (* , *) ' AqCOUNT = ', AqCOUNT
WRITE (* , *) ' AQUIFER ARITHMETIC MEAN = ', AqARITH
WRITE (* , *) ' AQUIFER GEOMETRIC MEAN = ', AqGEOM
WRITE (* , *) ' AQUIFER HARMONIC MEAN = ', AqHARM
WRITE (* , *) ' AQUIFER MEAN LNK = ', AqMEANLNK
WRITE (* , *) ' AQUIFER VARIANCE LN ( K ) = ', AqVARLNK
WRITE (* , *)
WRITE ( 50 , *) ' AqCOUNT = ', AqCOUNT
WRITE ( 50 , *) ' AQUIFER ARITHMETIC MEAN = ', AqARITH
WRITE ( 50 , *) ' AQUIFER GEOMETRIC MEAN = ', AqGEOM
WRITE ( 50 , *) ' AQUIFER HARMONIC MEAN = ', AqHARM
```

```
WRITE ( 50 , *) ' AQUIFER MEAN LNK = ', AqMEANLNK
WRITE ( 50 , *) ' AQUIFER VARIANCE LN ( K ) = ', AqVARLNK
WRITE ( 50 , *)
WRITE (* , *) ' AtCOUNT = ', AtCOUNT
WRITE (* , *) ' AQUITARD ARITHMETIC MEAN = ', AtARITH
WRITE (* , *) ' AQUITARD GEOMETRIC MEAN = ', AtGEOM
WRITE (* , *) ' AQUITARD HARMONIC MEAN = ', AtHARM
WRITE (* , *) ' AQUITARD MEAN LNK = ', AtMEANLNK
WRITE (* , *) ' AQUITARD VARIANCE LN ( K ) = ', AtVARLNK
WRITE (* , *)
WRITE ( 50 , *) ' AtCOUNT = ', AtCOUNT
WRITE ( 50 , *) ' AQUITARD ARITHMETIC MEAN = ', AtARITH
WRITE ( 50 , *) ' AQUITARD GEOMETRIC MEAN = ', AtGEOM
WRITE ( 50 , *) ' AQUITARD HARMONIC MEAN = ', AtHARM
WRITE ( 50 , *) ' AQUITARD MEAN LNK = ', AtMEANLNK
WRITE ( 50, *) ' AQUITARD VARIANCE LN ( K ) = ', AtVARLNK
WRITE ( 50, *)
* *** TASK 5 ********************** TASK 5 ********************* TASK 5 ****
* ********* Generate CUBE indicator value files for CONNEC 3 D *************
*
WRITE ( 50 , *) ' STARTING TASK 5 : CONNEC 3 D Cube indicator files '
WRITE ( 50, *)
Print * ,' STARTING TASK 5 : CONNEC 3 D Cube indicator files '
Print *
*
* *** Create File Names for CONNECT 3 D postprocessing file output ***
* This assigns the value of current to the string " str " and then creates a corresponding
* " outfile " string with a file name incremented for each realization number .
* CUBEoutfiles similarly incremented for A = arithmetic and G = geometric mean indicators
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 14
IF ( CURRENT . LT . 10) THEN ! Note : hardwired for SGS or SIS
write ( str ,' ( I 1 ) ' ) CURRENT
outfile = outpre ( 1 : ii )// '_ 0 ' // str ( 1 : 1 )// ' . VMP '
c CUBEoutfileA = ' SGS A 0 ' // str ( 1 : 1 )// ' . dat '
c CUBEoutfileG = ' SGS G 0 ' // str ( 1 : 1 )// ' . dat
CUBEoutfileA = ' SIS A 0 ' // str ( 1 : 1 )// ' . dat '
CUBEoutfileG = ' SIS G 0 ' // str ( 1 : 1 )// ' . dat '
ELSEIF ( CURRENT . LT . 100 ) THEN ! Note : hardwired for SGS or SIS
write ( str ,' ( I 2 ) ' ) CURRENT
outfile = outpre ( 1 : ii )// '_' // str ( 1 : 2 )// ' . VMP '
c CUBEoutfileA = ' SGS A ' // str ( 1 : 2 )// ' . dat '
c CUBEoutfileG = ' SGS G ' // str ( 1 : 2 )// ' . dat '
CUBEoutfileA = ' SIS A ' // str ( 1 : 2 )// ' . dat '
CUBEoutfileG = ' SIS G ' // str ( 1 : 2 )// ' . dat '
ELSE ! Note : hardwired for SGS or SIS
write ( str ,' ( I 3 ) ' ) CURRENT
outfile = outpre ( 1 : ii )// '_' // str ( 1 : 3 )// ' . VMP '
c CUBEoutfileA = ' SGS A ' // str ( 1 : 3 )// ' . dat
c CUBEoutfileG = ' SGS G ' // str ( 1 : 3 )// ' . dat '
CUBEoutfileA = ' SIS A ' // str ( 1 : 3 )// ' . dat '
CUBEoutfileG = ' SIS G ' // str ( 1 : 3 )// ' . dat '
ENDIF
Print * , " outfile = " , outfile
Print * , " CUBEoutfileA = " , CUBEoutfileA
Print * , " CUBEoutfileG = " , CUBEoutfileG
Write ( 50 , *) " outfile = " , outfile
Write ( 50 , *) " CUBEoutfileA = " , CUBEoutfileA
Write ( 50 , *) " CUBEoutfileG = " , CUBEoutfileG
PRINT *
OPEN ( 41 , FILE = CUBEoutfileA )
OPEN ( 42 , FILE = CUBEoutfileG )
*
c Initialize CUBE variables
*
CUBEcount = 0
```

```
CUBEsum = 0. 0
CUBEgeom = 0 . 0
CUBEGTA = 0
CUBEGTG = 0
Do U = 1 , NZ ! cycle fastest on X , slowest on Z
Do T = 1 , NY
Do S = 1 , NX
If ( CUBE ( S , T , U ). GT . 0 . 0 ) THEN ! Cube ( STU ) > 0 = active model cell
CUBEsum = CUBEsum + CUBEK ( S , T , U )
CUBEgeom = CUBEgeom + LOG ( CUBEK ( S , T , U ))
CUBEcount = CUBEcount + 1
ENDIF
ENDDO
ENDDO
ENDDO
CUBEarith = CUBEsum / REAL ( CUBEcount )
CUBEgeom = EXP ( CUBEgeom / REAL ( CUBEcount ))
PRINT * , ' CUBEcount ', CUBEcount
PRINT * , ' CUBEarith = ', CUBEarith
PRINT * , ' CUBEgeom = ', CUBEgeom
WRITE ( 50 , *) ' CUBEcount = ', CUBEcount
WRITE ( 50 , *) ' CUBEarith = ', CUBEarith
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 15
WRITE ( 50 , *) ' CUBEgeom = ', CUBEgeom
DO S = 1 , NX ! CONNEC 3 D cycles fastest on Z then Y then X
DO T = 1 , NY
DO U = 1, NZ - 1 ! Top layer is ignored
IF ( CUBE ( S , T , U ). GT . 0 ) THEN
IF ( CUBEK ( S , T , U ). GT . CUBEarith ) THEN
WRITE ( 41 , 522 ) 1
CUBE 2 ( s , t ,u )= 1
CUBEGTA = CUBEGTA + 1
ELSE
WRITE ( 41 , 522 ) 0
CUBE 2 ( s , t , u )= 0
ENDIF
IF ( CUBEK ( S , T , U ). GT . CUBEgeom ) THEN
WRITE ( 42, 522 ) 1
CUBEGTG = CUBEGTG + 1
ELSE
WRITE ( 42 , 522 ) 0
ENDIF
ELSE
WRITE ( 41 , 522 ) 0
WRITE ( 42 , 522 ) 0
ENDIF
ENDDO
ENDDO
ENDDO
Print * , ' CUBEGTA count = ', CUBEGTA
Print * , ' CUBEGTG count = ', CUBEGTG
WRITE ( 50 , *) ' CUBEGTA count = ', CUBEGTA
WRITE ( 50 , *) ' CUBEGTG count = ', CUBEGTG
*
CLOSE ( 41 )
CLOSE ( 42 )
*
c Write GSLIB formatted output file for input into SGeMS for visualization purposes
*
OPEN ( 43 , File =" GSLIB Cube out . dat ")
Write ( 43 , *) " GSLIB Cube out . dat "
Write ( 43, *) 4
Write ( 43 , *) " X "
Write ( 43 , *) " Y "
```

```
Write ( 43 , *) " Z "
Write ( 43 , *) " Indicator "
*
*
DO U = 1 , NZ - 1 ! GSLIB cycles fastest on X then Y then Z ; top layer ignored
DO T = 1 , NY
DO S = 1 ,NX
Write ( 43 , 407 ) ( xmin +( S - 1 )* xsiz ) , ( ymin +( T - 1 )* ysiz ) ,
+( zmin +( U - 1 )* zsiz ) , CUBE 2 ( S , T , U )
ENDDO
ENDDO
ENDDO
*
CLOSE ( 43 )
*
* ***
* *** TASK 6 ********************* TASK 6 ********************** TASK 6 ****
*
* Group assigned K values into a user - defined number of property
* categories and reassign property values to each fill cell .
*
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WRITE ( 50 , *)
WRITE ( 50, *) ' STARTING TASK 6 a : Assign . VMP Property Indice Values '
WRITE ( 50 , *)
Print *
Print * , ' STARTING TASK 6 a : Assign . VMP Property Indice Values '
Print *
*
*
* Assign Property Indice Values
Write ( 50 , *) ' N ', 'Kxmax ( n ) ', ' Kxmax ( n - 1 ) ', ' Kx ( n ) '
Kx ( NKP + 1 ) = KxMax ( NKP + 1 )/ 2 . 0 ! Assumes lower bound of KClass bin is zero
Write ( 50, 351 ) 2 , Kxmax ( 2 ) , Kxmax ( 1 ) , kx ( 2 )
DO N = NKP + 2 , NKP + KCLASS
Kx (N )=( KxMax ( N )+ KxMax ( N - 1 ))/ 2 . 0 ! Avg of upper and lower bounds
Write ( 50, 351 ) N , Kxmax ( n ) , Kxmax ( n - 1 ) , kx ( n )
ENDDO
*
* *** TASK 6 b ****************** TASK 6 b ********************* TASK 6 b ****
*
45 CONTINUE
WRITE ( 50, *)
WRITE ( 50 , *)" STARTING TASK 6 b : Determine Property Indices "
WRITE ( 50 , *)
PRINT * , "STARTING TASK 6 b : Determine Property Indices "
*
* Determine appropriate K Bin and assign corresponding property indice
TALLYTOT = 0
DO R = NIMIN , NIMAX ! Layer ( Z )
DO Q = NKMIN , NKMAX ! Row ( Y )
DO P = NJMIN , NJMAX ! Column ( X )
IF ( FILLKx ( P , Q , R ). GT . 0 . 0 ) THEN ! Cell will be filled
IF ( FILLKx ( P , Q , R ). LE . KxMax ( 2 )) THEN
PROP ( P , Q , R )= 1 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 3 )) THEN
PROP ( P , Q , R ) = 2 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 4 )) THEN
PROP ( P , Q , R )= 3 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 5 )) THEN
PROP ( P , Q , R )= 4 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 6 )) THEN
PROP ( P , Q , R )= 5 + NKP ! 6
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 7 )) THEN
```

```
PROP ( P , Q , R )= 6 + NKP ! 7
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 8 )) THEN
PROP ( P , Q , R )= 7 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 9 )) THEN
PROP ( P , Q , R ) = 8 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 10 )) THEN
PROP ( P , Q , R )= 9 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 11 )) THEN
PROP ( P , Q , R ) = 10 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 12 )) THEN
PROP ( P , Q , R )= 11 + NKP ! 12
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 13 )) THEN
PROP ( P , Q , R )= 12 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 14 )) THEN
PROP ( P , Q , R )= 13 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 15 )) THEN
PROP ( P , Q , R )= 14 + NKP ! 15
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 16 )) THEN
PROP ( P , Q , R )= 15 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 17 )) THEN
PROP ( P , Q , R )= 16 + NKP
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ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 18 )) THEN
PROP ( P , Q , R )= 17 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 19 )) THEN
PROP ( P , Q , R ) = 18 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 20 )) THEN
PROP ( P , Q , R )= 19 + NKP ! 20
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 21 )) THEN
PROP ( P , Q , R )= 20 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 22 )) THEN
PROP ( P , Q , R )= 21 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 23 )) THEN
PROP ( P , Q , R )= 22 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 24 )) THEN
PROP ( P , Q , R )= 23 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 25 )) THEN
PROP ( P , Q , R )= 24 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 26 )) THEN
PROP ( P , Q , R )= 25 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 27 )) THEN
PROP ( P , Q , R )= 26 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 28 )) THEN
PROP ( P , Q , R )= 27 + NKP ! 28
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 29 )) THEN
PROP ( P , Q , R )= 28 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 30 )) THEN
PROP ( P , Q , R ) = 29 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 31 )) THEN
PROP ( P , Q , R )= 30 + NKP ! 31
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 32 )) THEN
PROP ( P , Q , R )= 31 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 33 )) THEN
PROP ( P , Q , R )= 32 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 34 )) THEN
PROP ( P , Q , R )= 33 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 35 )) THEN
PROP ( P , Q , R ) = 34 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 36 )) THEN
PROP ( P , Q , R )= 35 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 37 )) THEN
PROP ( P , Q , R )= 36 + NKP
ELSEIF ( FIlLKx ( P , Q , R ). LE . KxMax ( 38 )) THEN
PROP ( P , Q , R )= 37 + NKP
ELSEIF ( FILLKx ( P , Q , R ). LE . KxMax ( 39 )) THEN
```

```
PROP ( P , Q , R ) = 38 + NKP
ELSE
PROP ( P , Q , R )= 39 + NKP
ENDIF
TALLY ( PROP ( P , Q , R ))= TALLY ( PROP ( P , Q , R ))+ 1
TALLYTOT = TALLYTOT + 1
! Check for out of bounds K property classes
IF ( PROP ( P , Q , R ). GE . KCLASS + NKP ) THEN
PROP ( P , Q , R ) = KCLASS + NKP
ENDIF
IF ( PROP ( P , Q , R ). LE . 0 ) THEN
PROP ( P , Q , R ) = 1
ENDIF
ENDIF
ENDDO ! next col ( X )
ENDDO ! next row ( Y )
ENDDO ! next layer ( Z )
PRINT * , ' TallyTot = ', tallyTot
C:\Documents and Settings\Lena\My Documents\Directed Study\Fortran_GSL2VMF\GSL2VMF16.f 18
WRITE ( 50 , *) ' TallyTot = ', tallyTot
*
* *** TASK 6 c ******************* TASK 6 c ******************** TASK 6 c ****
*
WRITE ( 50 , *)
WRITE ( 50 , *)" START TASK 6 c : Scale and Report Prop Indice K values "
WRITE ( 50, *)
PRINT * , " STARTING TASK 6 c : Scale and Report Prop Indice K Values "
* Property Value Scaling
DO N =( NKP + 1 ) , ( NKP + KCLASS )
Ki ( N ) = N
Kx ( N ) = Kx ( N )* 10. 0 ! Scaling factor added to agree with pump test K values .
Ky ( N )= Kx ( N ) ! Set Ky = Kx
Kz ( N ) = Kx ( N )/ 10 . 0 !!! Default Kx : Kz = 10 : 1
ENDDO
DO N = 1 , NKP + KCLASS
WRITE (* , 311 ) N , TALLY ( N ) , Kx ( N )
WRITE ( 50 , 311 ) N , TALLY ( N ) , Kx ( N )
ENDDO
WRITE ( 50 , *)
print * , " N = " , N
PRINT * , ' GLOBCOUNT = ', GLOBCOUNT
WRITE ( 50 , *) ' GLOBCOUNT = ', GLOBCOUNT
WRITE ( 50, *) ' The total number of pre - assigned properties is : ', NKP
WRITE ( 50 , *) ' KPxMIN = ', KPxMIN
WRITE ( 50 , *) ' KPxMAX = ', KPxMAX
WRITE ( 50, *)
PRINT * , ' The total number of pre - assigned properties is : ', NKP
PRINT * , ' KPxMIN = ', KPXMIN
PRINT * , ' KPxMAX = ', KPXMAX
PRINT *
WRITE ( 50 , 306 ) FILLKxMIN
WRITE ( 50 , 308) FILLKxMAX
WRITE (* , 306 ) FILLKxMIN
WRITE (* , 308 ) FILLKxMAX
WRITE ( 50 , *)
55 PRINT *
NEWPROPS = KCLASS
PRINT * , ' VALUE FOR NEWPROPS IS ', NEWPROPS
WRITE ( 50 , *)
WRITE ( 50 , *) " VALUE FOR NEWPROPS IS " , NEWPROPS
WRITE ( 50, *)
WRITE ( 50, *)
*
* *** TASK 6 d ******************* TASK 6 d ******************** TASK 6 d ****
*
```

```
WRITE ( 50 , *)
WRITE ( 50 , *)" STARTING TASK 6 d : Compute and Report VMP values "
WRITE ( 50 , *)
PRINT * , " STARTING TASK 6 d : Compute and Report VMP Values "
VMPcount = 0
VMPsum = 0 . 0
VMPgeom = 0 . 0
VMPAqcount = 0
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VMPAqsum = 0 . 0
VMPAqgeom = 0 . 0
VMPAqarith = 0 . 0
VMPAtcount = 0
VMPAtsum = 0 . 0
VMPAtgeom = 0 . 0
VMPAtarith = 0 . 0
VMPAqmin = 1 . 1 E 99
VMPAqmax = 0 . 0
VMPAtmin = 1 . 1 E 99
VMPAtmax = 0 . 0
Do U = 1, NZ ! cycle fastest on X , slowest on Z
Do T = 1 , NY
Do S = 1 , NX
If ( CUBE ( S , T , U ). EQ . 1 . 0 ) THEN ! Deterministic Aquifer Model Cell
VMPcount = VMPcount + 1
VMPsum = VMPsum + Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
VMPgeom = VMPgeom + LOG ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )))
VMPAqcount = VMPAqcount + 1
VMPAqsum = VMPAqsum + Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
VMPAqgeom = VMPAqgeom + LOG ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )))
If ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )). LT . VMPAqmin ) THEN
VMPAqmin = Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
ENDIF
IF ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )). GT . VMPAqmax ) THEN
VMPAqmax = Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
ENDIF
ELSEIF ( CUBE ( S , T , U ). EQ . 2 . 0 ) THEN ! Deterministic Aquitard Cell
VMPcount = VMPcount + 1
VMPsum = VMPsum + Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
VMPgeom = VMPgeom + LOG ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )))
VMPAtcount = VMPAtcount + 1
VMPAtsum = VMPAtsum + Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
VMPAtgeom = VMPAtgeom + LOG ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )))
If ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )). LT . VMPAtmin ) THEN
VMPAtmin = Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
ENDIF
IF ( Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U )). GT . VMPAtmax ) THEN
VMPAtmax = Kx ( PROP ( S + NJMIN - 1 , T + NKMIN - 1 , U ))
ENDIF
ENDIF
ENDDO
ENDDO
ENDDO
VMParith = VMPsum / REAL ( VMPcount )
VMPAqarith = VMPAqsum / REAL ( VMPAqcount )
VMPAtarith = VMPAtsum / REAL ( VMPAtcount )
VMPgeom = EXP ( VMPgeom / REAL ( VMPcount ))
VMPAqgeom = EXP ( VMPAqgeom / REAL ( VMPAqcount ))
VMPAtgeom = EXP ( VMPAtgeom / REAL ( VMPAtcount ))
PRINT * , ' VMPcount ', VMPcount
PRINT * , ' VMParith = ', VMParith
PRINT * , ' VMPgeom = ', VMPgeom
WRITE ( 50 , *)' VMPcount = ', VMPcount
WRITE ( 50 , *) ' VMParith = ', VMParith
WRITE ( 50 , *) ' VMPgeom = ', VMPgeom
```

```
PRINT *
PRINT * , ' VMPAqcount ', VMPAqcount
PRINT * , ' VMPAqarith = ', VMPAqarith
PRINT * , ' VMPAqgeom = ', VMPAqgeom
WRITE ( 50 , *) ' VMPAqcount = ', VMPAqcount
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WRITE ( 50 , *) ' VMPAqarith = ', VMPAqarith
WRITE ( 50 , *) ' VMPAqgeom = ', VMPAqgeom
PRINT *
PRINT * , ' VMPAtcount ', VMPAtcount
PRINT * , ' VMPAtarith = ', VMPAtarith
PRINT * , ' VMPAtgeom = ', VMPAtgeom
WRITE ( 50 , *) ' VMPAtcount = ', VMPAtcount
WRITE ( 50 , *) ' VMPAtarith = ', VMPAtarith
WRITE ( 50 , *) ' VMPAtgeom = ', VMPAtgeom
PRINT *
PRINT * , ' VMPAqmin = ', VMPAqmin
PRINT * , ' VMPAqmax = ', VMPAqmax
PRINT * , ' VMPAtmin = ', VMPAtmin
PRINT * , ' VMPAtmax = ', VMPAtmax
WRITE ( 50 , *)
WRITE ( 50 , *) ' VMPAqmin = ', VMPAqmin
WRITE ( 50 , *) ' VMPAqmax = ', VMPAqmax
WRITE ( 50 , *) ' VMPAtmin = ', VMPAtmin
WRITE ( 50 , *) ' VMPAtmax = ', VMPAtmax
* Write out metrics for current realization
*
c WRITE ( 51 , 51 ) ! header write statement ( use only once )
WRITE ( 51 , 52 ) OUTFILE , DATE , GLOBARITH , VMPARITH , GLOBGEOM ,
1 VMPGEOM , AqARITH , VMPaqArith , AqGEOM , VMPaqGeom ,
2 AtARITH , VMPatArith , AtGEOM , VMPatGeom
*
*
* *** TASK 7 ************************ TASK 7 ********************** TASK 7 ***
*
* write an output file formatted for insertion ( substitution )
* into the first section of the VMODFLOW property (. VMP ) file .
*
WRITE ( 50 , *)
WRITE ( 50 , *) " STARTING TASK 7 "
PRINT * , " STARTING TASK 7 : Writing output file "
PRINT * , " Outfile = " , OUTFILE
WRITE ( 50 , *) " Outfile = " , OUTFILE
OPEN ( 40 , FILE = OUTFILE )
IF ( NK . LT . 10 ) THEN
WRITE ( 40 , 401 ) NK
ELSEIF ( NK . LT . 100 ) THEN
WRITE ( 40 , 402 ) NK
ELSE
WRITE ( 40 , 403 ) NK
ENDIF
IF ( NJ . LT . 10 ) THEN
WRITE ( 40 , 401 ) NJ
ELSEIF ( NJ . LT . 100 ) THEN
WRITE ( 40 , 402 ) NJ
ELSE
WRITE ( 40 , 403 ) NJ
ENDIF
IF ( NI . LT . 10 ) THEN
WRITE ( 40 , 401 ) NI
ELSEIF ( NI . LT . 100 ) THEN
WRITE ( 40 , 402 ) NI
ELSE
WRITE ( 40 , 403 ) NI
```

```
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ENDIF
IF (( NKP + NEWPROPS ). LT . 10 ) THEN
WRITE ( 40 , 401 ) NKP + NEWPROPS
ELSEIF (( NKP + NEWPROPS ). LT . 100 ) THEN
WRITE ( 40 , 402 ) NKP + NEWPROPS
ELSE
WRITE ( 40 , 403 ) NKP + NEWPROPS
ENDIF
*
* Write Property Indices and associated Kx , Ky , Kz values
DO N = 1 , NKP + NEWPROPS
IF ( N . LT . 10 ) THEN
WRITE ( 40 , 102 ) Ki ( N ) , Kx ( N ) , Ky ( N ) , Kz ( N )
ELSEIF ( N . LT . 100 ) THEN
WRITE ( 40, 103 ) Ki (N ) , Kx ( N ) , Ky (N ) , Kz ( N )
ELSE
WRITE ( 40 , 104 ) Ki ( N ) , Kx ( N ) , Ky ( N ) , Kz ( N )
ENDIF
ENDDO
* Write blank line
WRITE ( 40, *)
* Write K Property index matrix , stepping sequentially through rows , columns ,
* and layers. Use a single line for all Property indices associated with an
* individual row and leave a blank line before moving up to the next layer .
*
IF ( UNIFORM ) THEN
print * , ' UNIFORM HETEROGENEOUS MODEL '
write ( 50 , *) ' UNIFORM HETEROGENEOUS MODEL '
DO R = NIMIN , NIMAX ! ( Z )
DO Q = NKMIN , NKMAX ! ( Y )
DO P = NJMIN , NJMAX ! ( X )
IF ( CUBE ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 1 . 0 ) THEN ! AQUIFER
PROP ( P , Q , R )= 22 ! Populate with Property 22
ELSE IF ( CUBE ( P - NJMIN + 1 , Q - NKMIN + 1 , R ). EQ . 2 . 0 ) THEN ! AQUITARD
PROP ( P , Q , R )= 4 ! Populate with Proerty 4
ELSE
PROP ( P , Q , R )= 1
ENDIF
ENDDO
ENDDO
ENDDO
ELSE
print * ,' NONUNIFORM HETEROGENEOUS MODEL '
write ( 50 , *) ' NONUNIFORM HETEROGENEOUS MODEL '
ENDIF
DO R = 1 , NK ! Layer 1 must be bottom layer
DO Q = NI , 1 , - 1 ! writes from back to front ( Y )
DO S = 1 , NJ ! writes from left to right ( X )
IF ( PROP ( S , Q , R ). LE . 9 ) THEN
Write ( 40 , 219 , ADVANCE =" NO ") PROP ( S , Q , R )
ELSE IF ( PROP ( S , Q , R ). LE . 99 ) THEN
Write ( 40 , 220 , ADVANCE =" NO ") PROP ( S , Q , R )
ELSE
Write ( 40 , 221 , ADVANCE =" NO ") PROP ( S , Q , R )
ENDIF
ENDDO
WRITE ( 40 , 122 ) ! blank space
ENDDO
WRITE ( 40 , *) ! blank line
ENDDO
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* --- Close output file and Close Number of RealizationS Do Loop
*
CLOSE ( 40 )
```

```
print * , " ClOSING OUTPUT FILE FOR REALIZATION " , CURRENT
PRINT *
WRITE ( 50 , *) " ClOSING OUTPUT FILE FOR REALIZATION " , CURRENT
WRITE ( 50, *)
WRITE ( 50, *)
WRITE ( 50 , *)
*
*
5 5 5 \text { Continue}
*
ClOSE ( 25 ) ! CloSe PARAMETER FILE
CLOSE ( 50 ) ! CLOSE LOG FILE
CLOSE ( 51 ) ! CLOSE SUMMARY TABLE FILE
*
*
PRINT *
PRINT * ,' NORMAL PROGRAM TERMINATION '
pause
*
* *** Format Statements ****
51 FORMAT (" OUTFILE " , T 20 , " DATE " , T 46 , " GLOBarith " , T 61 , " VMParith " , T 76 ,
2 " GLOBgeom " , T 91 , " VMPgeom " , T 106 , " AQarith " , T 121 , " VMPaqArith " , T 136 ,
3 " AQgeom " , T 151 , " VMPaqGeom " , T 166 , " ATarith " , T 181 , " VMPatArith " , T 196 ,
4 " ATgeom " , T 211 , " VMPAtgeom ")
52 FORMAT ( A 16 , T 20 , A 24 , T 45 , E 12 . 5 , T 60 , E 12 . 5 , T 75 , E 12 . 5 , T 90 , E 12 .
5, T 105,
2 E 12. 5 , T 120, E 12. 5 , T 135, E 12 . 5 , T 150, E 12. 5 , T 165 , E 12 . 5 , T 180,
3 E 12. 5, T 195, E 12. 5 , T 210, E 12 . 5 )
53 format (" OUTFILE " , T 20 , " DATE ")
101 FORMAT ( I 4 )
102 FORMAT ( I 1 , 3 ( 1 X , E 12 . 5 ))
103 FORMAT ( I 2 , 3 ( 1 X , E 12 . 5 ))
104 FORMAT ( I 3 , 3 ( 1 X , E 12 . 5 ))
106 FORMAT (" N = " , I 3 , 2 X , " X ( N )= " , F 12 . 3 )
107 FORMAT (" N = " , I 3 , 2 X , " Y ( N )= " , F 12 . 3 )
108 FORMAT (" N = " , I 3 , 2 X , " Z ( N )= " , F 12 . 3)
109 FORMAT (" XMIN = " , F 12 . 2 , T 25 , " XMAX = " , F 12 . 2 )
110 FORMAT (" YMIN = " , F 10 . 2 , T 25 , " YMAX = " , F 10 . 2)
111 FORMAT (" ZMIN = " , F 10 . 2 , T 25 , " ZMAX = " , F 10 . 2 )
112 FORMAT (" XPOINT 1 =" , T 10 , I 4 , T 25 , " YPOINT 1 =" , T 35 , I 4 , T 50 ,
1 " ZPOINT 1 =" , T 60, I 4 )
113 FORMAT (" HARMONIC MEAN :" , T 25 , F 10 . 3 )
114 FORMAT (" GEOMETRIC MEAN :" , T 25 , F 10 . 3)
115 FORMAT (" ARITHETIC MEAN :" , T 25 , F 10 . 3)
116 FORMAT (" N 2 =" , T 6 , I 3 , T 15 , " XMAX =" , T 20, F 12 . 2 , T 35 , " < X ( N 2 )= " , F
12. 2)
117 FORMAT (" N 2 =" , T 6 , I 3 , T 15 , " YMAX =" , T 20, F 12 . 2 , T 35 , " < Y ( N 2 )= " , F
12 . 2 )
118 FORMAT (" N 2 =" , T 6 , I 3 , T 15 , " ZMAX =" , T 20, F 12 . 2 , T 35 , " < Z ( N 2 )= " , F
12 . 2 )
122 FORMAT ()
125 FORMAT ( 120 ( I 2 , 1 X ))
130 FORMAT ( 1 x )
219 FORMAT ( I 1 , 1 X )
220 FORMAT ( I 2 , 1 X )
221 FORMAT ( I 3 , 1 X )
301 FORMAT ( ' FILLKx , yMIN = ', E 10 . 4 )
3 0 2 ~ F O R M A T ~ ( ~ ' ~ F I L L K x ~ , ~ y M A X ~ = ~ ' , ~ E ~ 1 0 ~ . ~ 4 ~ ) ~
303 FORMAT (' Initial MEAN LN ( K ) ', 1 x , F 8 . 4 , 2 x ,' VAR LN ( K ) ', 1 x , F 8 . 4 )
304 FORMAT ( ' Target MEAN LN ( K ) ', 1 x , F 8 . 4 , 2 x ,' VAR LN ( K ) ', 1 x , F 8 . 4 )
305 FORMAT ( ' Adjusted MEAN LN ( K ) ', 1 x , F 8 . 4 , 2 x ,' VAR LN ( K ) ', 1 x , F 8 . 4 )
306 FORMAT ( ' Unscaled FILLKx , yMIN = ', f 12 . 6 )
308 FORMAT ( ' Unscaled FILLKx , yMAX = ', f 12 . 3)
310 FORMAT ( ' BIN NUMBER ', I 3 , 1 x ,' TALLY ', I 4 , 1 x ,' TALLY 2 ', I 4 , 1 x ,
+' MIDPOINT ', F 9 . 5 )
```

```
311 FORMAT ( ' BIN NUMBER ', I 3 , 1 x ,' TALLY ', I 6 , 1 x ,' MIDPOINT ', F 9 . 4 )
351 FORMAT ( I 3 , 2 x , F 9 . 5 , 2 x , F 9 . 5 , 2 x , F 9. 5 )
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4 0 1 ~ F O R M A T ~ ( ~ I ~ 1 ~ ) ~
4 0 2 ~ F O R M A T ~ ( ~ I ~ 2 ~ ) ~
4 0 3 ~ F O R M A T ~ ( ~ I ~ 3 ~ ) ~
4 0 4 ~ F O R M A T ~ ( ~ I ~ 4 ~ ) ~
405 FORMAT ( ' REALIZATION ', 1 X , I 3 , 1 X ,' XHARMMIN ', 1 X , E 12 . 6 , 1 X ,' XHARMMAX ',
+1 X, E 12. 6, 1 X ,' XHARMMEAN ', 1 X , E 12 . 6 , 1 X,' ( ft / d ) ' )
406 FORMAT ( ' REALIZATION ', 1 X , I 3 , 1 X ,' AVERAGE K ', 1 X , F 8 . 4 , 1 X ,' MEANLNK ',
+ 1 X , F 8 . 4 , 1 X ,' VARIANCE LNK ', 1 X , F 8 . 4 , 1 X ,' ( ft / d ) ' )
407 FORMAT ( F 12. 2 , 2 X , F 12. 2 , 2 X , F 12. 2 , 2 X , I 1 )
522 FORMAT ( I 1 )
9999 END
```


## WALL.for

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PROGRAM WALLONE

* Written by Larry Lemke and Lena Pappas Last Modified : December 072015
* 
* This program compiles particle location data in nine 2 D planes east of the source area
* and west of the Huron River for one hundred MODPATH. mpF output files into a 2 D
* array ( WALL ) to be used in statistical analysis. Backtracking of particle tracking
* is disregarded in this program , and particles are only counted once per wall intersection .
* 
* Program modified to count particles terminating in internal sinks corresponding to
* the ( Allen Creek ) drain boundatry
* Program modified to add coordinate locations to particle distributions within
* the 2 D walls
* 
* Program modified to generate output for Wagner Road ( WALL 112 ).
* 
* Program modified on Dec 72015 to hold fixed the I and K positions of particles
* exiting the model at positions west of the eastern most wall ( WALL 254 )
* 
* *** Variable Descriptions ***
* 
* General Variables
* ==================
* I , J , K = coordinate variables
* 
* Variables associated with MODPATH . mpF Files
* ============================================
* INPRE = MODPATH file name prefix for input file
* PARTNUM = Particle Number
* $X=$ Particle location $X$ coordinate
* $Y=$ Particle location $Y$ coordinate
* LOCZ = Particle location Z coordinate within the Modflow cell
* GLOBZ = Global particle coordinate in the $Z$ direction
* TIME = cumulative tracking time ( days )
* J = J column index of cell containing the particle ( x )
* $I=I$ row index of cell containing the particle ( y )
* K = K layer index of cell containing the particle ( z )
* TIMESTEP = Cumulative MODFLOW timestep number
* PARTNUMLAST = particle number from prior line of.$m p F$ output file
* ILAST , JLAST , KLAST $=\mathrm{I}$, J , K values from prior line of . mpF file
* JMAX = variable to track largest J value ( farthest eastward progression
* of current particle ( min value for JMAX = 112 at line source )
* 
* Variables associated with MODPATH . VMG File
* =============================================
* INPRE = MODPATH file name prefix for input file
* NCOL , NROW , NLAY = number of columns , rows , layers in VMODFLOW grid
* COL ( J ) = x coordinate of each column boundary
* ROW ( I ) = y coordinate of each row boundary
* LAY ( K ) = z coordinate of each layer boundary
* 
* Variables associated with WALL ARRAYS
* ====================================
* IMIN , IMAX = Range of I indices in the north / south direction
* COLUMNS = Number of columns in the wall array
* COUNT = Number of Modpath realizations read
* WALL 128 COUNT = number of particles passing through WALL 128 , etc .

```
* Y 128 MIN , Y 128 MAX = min and max Y value in WALL 128 , etc .
* Y 128 SUM = sum of Y values for all particles passing through WALL 128 , etc .
* Y 128 MEAN = mean of Y values for particles passing through WALL 128 , etc .
* Y 128 SIGMA = standard deviation of \(Y\) values for particles in WALL 128 , etc .
*
* *** Declare Variables ***
```

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IMPLICIT NONE
INTEGER NCOL , NROW , NLAY
INTEGER I , J , K , N , ii , JMAX , DRAINCOUNT
INTEGER IMIN , IMAX , COLUMNS
INTEGER WALL 128 , WALL 144 , WALL 160 , WALL 176 , WALL 192 , WALL 208 , WALL 224
INTEGER WALL 240 , WALL 254 , WALL 112 , COUNT , C , PARTNUM , TIMESTEP
INTEGER WALL 128 COUNT, WALL 144 COUNT, WALL 160 COUNT, WALL 176 COUNT
INTEGER WALL 192 COUNT, WALL 208 COUNT, WALL 224 COUNT, WALL 240 COUNT
INTEGER WALL 254 COUNT, WALL 112 COUNT
INTEGER PARTNUMLAST , ILAST , JLAST , KLAST
CHARACTER DUMMY * 2 , INPRE * 24 , INFILE * 80 , str * 3 , INFILE 2 * 120
REAL * $8 \mathrm{X}, \mathrm{Y}$, LOCZ , GLOBZ , TIME
REAL * 8 YAVG , ZAVG , COL , ROW , LAY
REAL * 8 Y 112 MIN , Y 112 MAX , Y 112 SUM , Y 112 MEAN , Y 112 SIGMA
REAL * 8 Y 128 MIN , Y 128 MAX , Y 128 SUM , Y 128 MEAN , Y 128 SIGMA
REAL * 8 Y 144 MIN , Y 144 MAX , Y 144 SUM , Y 144 MEAN , Y 144 SIGMA
REAL * 8 Y 160 MIN , Y 160 MAX , Y 160 SUM , Y 160 MEAN, Y 160 SIGMA
REAL * 8 Y 176 MIN , Y 176 MAX , Y 176 SUM , Y 176 MEAN , Y 176 SIGMA
REAL * 8 Y 192 MIN, Y 192 MAX, Y 192 SUM, Y 192 MEAN, Y 192 SIGMA
REAL * 8 Y 208 MIN , Y 208 MAX , Y 208 SUM, Y 208 MEAN, Y 208 SIGMA
REAL * 8 Y 224 MIN , Y 224 MAX , Y 224 SUM , Y 224 MEAN , Y 224 SIGMA
REAL * 8 Y 240 MIN , Y 240 MAX , Y 240 SUM , Y 240 MEAN , Y 240 SIGMA
REAL * 8 Y 254 MIN , Y 254 MAX , Y 254 SUM , Y 254 MEAN , Y 254 SIGMA
REAL * 8 Z 112 MIN, Z 112 MAX, Z 112 SUM, Z 112 MEAN, Z 112 SIGMA
REAL * 8 Z 128 MIN, Z 128 MAX, Z 128 SUM, Z 128 MEAN , Z 128 SIGMA
REAL * 8 Z 144 MIN , Z 144 MAX , Z 144 SUM , Z 144 MEAN , Z 144 SIGMA
REAL * 8 Z 160 MIN, Z 160 MAX, Z 160 SUM, Z 160 MEAN, Z 160 SIGMA
REAL * 8 Z 176 MIN , Z 176 MAX , Z 176 SUM , Z 176 MEAN , Z 176 SIGMA
REAL * 8 Z 192 MIN, Z 192 MAX, Z 192 SUM, Z 192 MEAN, Z 192 SIGMA
REAL * 8 Z 208 MIN, Z 208 MAX, Z 208 SUM, Z 208 MEAN, Z 208 SIGMA
REAL * 8 Z 224 MIN , Z 224 MAX , Z 224 SUM, Z 224 MEAN , Z 224 SIGMA
REAL * 8 Z 240 MIN, Z 240 MAX, Z 240 SUM, Z 240 MEAN, Z 240 SIGMA
REAL * 8 Z 254 MIN, Z 254 MAX , Z 254 SUM , Z 254 MEAN , Z 254 SIGMA
DIMENSION COL ( 300 ) , ROW ( 300 ) , LAY ( 50 )
DIMENSION WALL 112 ( 0 : 132 , 0 : 36 )
DIMENSION WALL 128 ( $0: 132,0: 36$ )
DIMENSION WALL 144 ( $0: 132$, $0: 36$ )
DIMENSION WALL 160 ( $0: 132$, $0: 36$ )
DIMENSION WALL 176 ( $0: 132$, $0: 36$ )
DIMENSION WALL 192 ( $0: 132$, $0: 36$ )
DIMENSION WALL 208 ( $0: 132$, $0: 36$ )
DIMENSION WALL 224 ( $0: 132,0: 36$ )
DIMENSION WALL 240 ( $0: 132$, $0: 36$ )
DIMENSION WALL 254 ( $0: 132$, $0: 36$ )
DIMENSION DRAINCOUNT ( 0 : 105 )

* *** Assign I / O files ***
* 
* File 20 is the program parameter file
* File 25 contains the input MODPATH (. mpf ) files
* File 30 is seed . VMG
* File 50 is an output log for debugging write statements
* File 60 is the formatted output file for WALL 128
* File 61 is the formatted output file for WALL 144
* File 62 is the formatted output file for WALL 160
* File 63 is the formatted output file for WALL 176
* File 64 is the formatted output file for WALL 192
* File 65 is the grid file ( y , z , particle \# ) for WALL 128
* File 66 is the grid file ( y , z , particle \# ) for WALL 144

```
* File 67 is the grid file ( y , z , particle # ) for WALL 160
* File 68 is the grid file ( y , z , particle # ) for WALL 176
* File 69 is the grid file ( y , z , particle # ) for WALL }19
* File 71 is the formatted output file for WALL 208
* File 72 is the formatted output file for WALL }22
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* File 73 is the formatted output file for WALL }24
* File 74 is the formatted output file for WALL }25
* File 75 is the grid file ( y , z , particle # ) for WALL }20
* File 76 is the grid file ( y , z , particle # ) for WALL 224
* File 77 is the grid file ( y , z , particle # ) for WALL 240
* File 78 is the grid file ( y , z , particle # ) for WALL 254
* File 80 is the formatted output file for WALL }11
* File 81 is the grid file ( y , z , particle # ) for WALL }11
*
OPEN ( 20 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ WALL . pa
1r ', STATUS = ' OLD ' )
OPEN ( 50 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE RunLog ' )
*
* *** TASK 1 ************************ TASK 1 ********************** TASK 1 ***
*
* Read in the parameter file information
*
WRITE ( 50 , *)
WRITE ( 50 , *) " STARTING TASK 1 : Read in parameter file "
PRINT * , " STARTING TASK 1 : Read in paratmeter file "
READ ( 20 , *) COUNT
WRITE ( 50 , *) " Number of Modpath Realizations =" , COUNT
PRINT * , " Number of Modpath Realizations =" , COUNT
READ ( 20, *) IMIN , IMAX
WRITE ( 50, *) " IMIN =" , IMIN , " IMAX =" , IMAX
COLUMNS = IMAX - IMIN + 1
READ ( 20 , *) INPRE
WRITE ( 50 , *) " Modpath file prefix is " , INPRE
PRINT * , " Modpath file prefix is " , INPRE
write ( 50 , *)
ii = index ( inpre ,' ' )- 1
CLOSE ( 20 )
OPEN ( 30 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ seed . VMG ' )
READ ( 30, *) NCOL
DO J = 1 , NCOL + 1
READ ( 30 , *) COL ( J )
ENDDO
READ ( 30, *) NROW
DO I = NROW + 1 , 1 , - 1 ! Read from north to south
READ ( 30 , *) ROW ( I )
ENDDO
READ ( 30 , *) NLAY
DO K = 1, NLAY + 1
READ ( 30, *) LAY ( K )
ENDDO
CLOSE ( 30 )
*
* **** TASK 2 ************************ TASK 2 ********************** TASK 2 *******
*
WRITE ( 50 , *)
WRITE ( 50, *) " Starting TASK 2 "
PRINT * , " TASK 2 - reading Modpath Files "
C Initialize Variables
WALL }112\mathrm{ Count = 0
WALL }128\mathrm{ Count = 0
WALL 144 Count = 0
WALL }160\mathrm{ Count = 0
```

```
WALL 176 Count = 0
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WALL }192\mathrm{ Count = 0
WALL }208\mathrm{ Count = 0
WALL 224 Count = 0
WALL 240 Count = 0
WALL 254 Count = 0
Y 112 MIN =( ROW ( IMAX ) + ROW ( IMAX - 1 ))/ 2 . 0 ! Set min equal to max Y coodinate
Y 128 MIN =( ROW ( IMAX ) + ROW ( IMAX - 1))/ 2 . 0
Y 144 MIN =( ROW ( IMIN ) + ROW ( IMIN + 1 ))/ 2 . 0
Y 160 MIN =( ROW ( IMIN ) + ROW ( IMIN + 1))/ 2 . 0
Y 176 MIN =( ROW ( IMIN )+ ROW ( IMIN + 1 ))/ 2 . 0
Y 192 MIN =( ROW ( IMIN )+ ROW ( IMIN + 1 ))/ 2 . 0
Y 208 MIN =( ROW ( IMIN )+ ROW ( IMIN + 1))/ 2 . 0
Y 224 MIN =( ROW ( IMIN )+ ROW ( IMIN + 1 ))/ 2 . 0
Y 240 MIN =( ROW ( IMIN ) + ROW ( IMIN + 1))/ 2 . 0
Y 254 MIN =( ROW ( IMIN )+ ROW ( IMIN + 1 ))/ 2 . 0
Y 112 MAX =( ROW ( IMIN ) + ROW ( IMIN + 1 ))/ 2 . 0 ! Set max equal to min Y coodinate
Y 128 MAX =( ROW ( IMIN ) + ROW ( IMIN + 1 ))/ 2 . 0
Y 144 MAX =( ROW ( IMAX ) + ROW ( IMAX - 1 ))/ 2 . 0
Y 160 MAX =( ROW ( IMAX ) + ROW ( IMAX - 1))/ 2 . 0
Y 176 MAX =( ROW ( IMAX ) + ROW ( IMAX - 1 ))/ 2 . 0
Y 192 MAX =( ROW ( IMAX )+ ROW ( IMAX - 1 ))/ 2 . 0
Y 208 MAX =( ROW ( IMAX )+ ROW ( IMAX - 1))/ 2 . 0
Y 224 MAX =( ROW ( IMAX ) + ROW ( IMAX - 1 ))/ 2 . 0
Y 240 MAX =( ROW ( IMAX )+ ROW ( IMAX - 1))/ 2 . 0
Y 254 MAX =( ROW ( IMAX ) + ROW ( IMAX - 1 ))/ 2 . 0
Z 112 MIN =( LAY ( NLAY ) + LAY (NLAY - 1))/ 2 . 0 ! Set min equal to max z coodinate
Z 128 MIN =( LAY ( NLAY ) + LAY ( NLAY - 1 ))/ 2 . 0
Z 144 MIN =( LAY ( NLAY ) + LAY ( NLAY - 1 ))/ 2 . 0
Z 160 MIN =( LAY ( NLAY )+ LAY ( NLAY - 1 ))/ 2 . 0
Z 176 MIN =( LAY ( NLAY ) + LAY ( NLAY - 1 ))/ 2 . 0
Z 192 MIN =( LAY ( NLAY ) + LAY ( NLAY - 1 ))/ 2 . 0
Z 208 MIN =( LAY ( NLAY ) + LAY ( NLAY - 1 ))/ 2 . 0
Z 224 MIN =( LAY ( NLAY )+ LAY ( NLAY - 1 ))/ 2 . 0
Z 240 MIN =( LAY ( NLAY ) + LAY (NLAY - 1 ))/ 2 . 0
Z 254 MIN =( LAY ( NLAY ) + LAY ( NLAY - 1 ))/ 2 . 0
Z 112 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0 ! Set max equal to min Z coodinate
Z 128 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Z 144 MAX =( LAY ( 1 )+ LAY ( 2 ))/ 2 . 0
Z 160 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Z 176 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Z 192 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Z 208 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Z 224 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Z 240 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Z 254 MAX =( LAY ( 1 ) + LAY ( 2 ))/ 2 . 0
Y 112 SUM = 0 . 0
Y 128 SUM = 0 . 0
Y 144 SUM = 0. 0
Y 160 SUM = 0 . 0
Y 176 SUM = 0 . 0
Y 192 SUM = 0 . 0
Y 208 SUM = 0 . 0
Y 224 SUM = 0 . 0
Y 240 SUM = 0 . 0
Y 254 SUM = 0 . 0
Y 112 SIGMA = 0 . 0
Y 128 SIGMA = 0 . 0
Y 144 SIGMA = 0 . 0
Y 160 SIGMA = 0 . 0
Y 176 SIGMA = 0 . 0
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Y 192 SIGMA = 0 . 0
Y 208 SIGMA = 0.0
```

```
Y 224 SIGMA = 0 . 0
Y 240 SIGMA = 0 . 0
Y 254 SIGMA = 0 . 0
Z 112 SUM = 0 . 0
Z 128 SUM = 0 . 0
Z 144 SUM = 0 . 0
Z 160 SUM = 0 . 0
Z 176 SUM = 0 . 0
Z 192 SUM = 0 . 0
Z 208 SUM = 0 . 0
Z 224 SUM = 0 . 0
Z 240 SUM = 0 . 0
Z 254 SUM = 0 . 0
Z 112 SIGMA = 0 . 0
Z 128 SIGMA = 0 . 0
Z 144 SIGMA = 0 . 0
Z 160 SIGMA = 0 . 0
Z 176 SIGMA = 0 . 0
Z 192 SIGMA = 0 . 0
Z 208 SIGMA = 0 . 0
Z 224 SIGMA = 0 . 0
Z 240 SIGMA = 0 . 0
Z 254 SIGMA = 0 . 0
Print * ,' WALL }112\mathrm{ Count = ', WALL }112\mathrm{ Count
Write ( 50, *), 'WALL }112\mathrm{ Count = ', WALL }112\mathrm{ Count
Print *,''WALL }128\mathrm{ Count = ', WALL 128 Count
Write ( 50, *), ' WALL }128\mathrm{ Count = ', WALL }128\mathrm{ Count
Print *, ' WALL 144 Count = ', WALL 144 Count
Write ( 50, *), 'WALL 144 Count = ', WALL 144 Count
Print * , ' WALL 160 Count = ', WALL 160 Count
Write ( 50 , *), 'WALL 160 Count = ', WALL 160 Count
Print * , ' WALL 176 COUNT = ', WALL 176 COUNT
Write ( 50 , *) , ' WALL 176 COUNT = ', WALL }176\mathrm{ COUNT
Print * ,' WALL }192\mathrm{ Count = ', WALL 192 Count
Write ( 50 , *) , ' WALL }192\mathrm{ Count = ', WALL }192\mathrm{ Count
Print *, ' WALL 208 Count = ', WALL 208 Count
Write ( 50 , *) , ' WALL }208\mathrm{ Count = ', WALL }208\mathrm{ Count
Print * ,' WALL 224 Count = ', WALL 224 Count
Write ( 50 , *), 'WALL 224 Count = ', WALL 224 Count
Print * , ' WALL 240 COUNT = ', WALL }240\mathrm{ COUNT
Write ( 50 , *), 'WALL }240\mathrm{ COUNT = ', WALL }240\mathrm{ COUNT
Print * , ' WALL 254 Count = ', WALL 254 Count
Write ( 50, *),' WALL 254 Count = ', WALL 254 Count
DO C = 1 , COUNT ! read 100 realizations
PRINT * , ' Reading Realization Number ', C
WRITE ( 50 , *) ' Reading Realization Number ', C
DRAINCOUNT ( C )= 0 ! Initialize Counter Variable
* This assigns the value of current realization to the string " str " and then creates
* a corresponding " outfile " string with a file name incremented for each realization number .
IF ( C . LT . 10 ) THEN ! single digit
write ( str ,' ( I 1 ) ' ) C
infile = inpre ( 1 : ii )// ' 00 ' // str ( 1 : 1 )// ' . mpF '
ELSEIF ( C . LT . 100 ) THEN ! double digit
write ( str ,' ( I 2 ) ' ) C
infile = inpre ( 1 : ii )// ' 0 ' // str ( 1 : 2 )// ' . mpF '
ELSE ! three digits
write ( str ,' ( I 3 ) ' ) C
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infile = inpre ( 1 : ii )// str ( 1 : 3 )// ' . mpF '
ENDIF
Print * , " infile = " , infile
Write ( 50 , *) " infile = " , infile
INFILE 2 = 'C : \ Documents and Settings \ Lena \ Desktop \' // inpre ( 1 : i
1 i )// '_,MPF Files \' // infile
PRINT * ,', Infile 2 = ', Infile 2
```

```
OPEN ( 25 , File = INFILE 2 )
JMAX = 111 ! Initialize at J = X particle release point at
! one cell west of line source at Wagner Rd
READ ( 25 , *) DUMMY
88 CONTINUE
READ ( 25 , *) PARTNUM , X , Y , LOCZ , GLOBZ , TIME , J , I , K , TIMESTEP
C
c *** Test for next or final particle
IF (( PARTNUM . GT . PARTNUMLAST ). OR . ( PARTNUM . EQ .- 9999 )) THEN
c *** Test for particle termination in drain
IF (( ILAST . GE . 49 ). AND .( ILAST . LE . 129 )) THEN
IF (( JLAST . GE . 166 ). AND . ( JLAST . LE . 260 )) THEN
IF (( KLAST . GE . 5 ). AND .( KLAST . LE . 20 )) THEN
DRAINCOUNT ( C )= DRAINCOUNT ( C ) + }
ENDIF
ENDIF
ENDIF
c *** Test for particle termination prior to final WALL }25
IF ( JLAST . LE . 208 ) THEN ! Assign Particle Position to subsquent walls
PRINT * , ' 208 TEST '
PRINT * , ' REALIZ = ', C ,' PARTNUM = ', PARTNUMLAST ,' JLAST = ', JLAST
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 208 ( I , K ) = WALL 208 ( I , K ) + 1
WALL }208\mathrm{ COUNT = WALL }208\mathrm{ COUNT + 1
WALL 224 ( I , K ) = WALL 224 ( I , K )+ 1
WALL }224\mathrm{ COUNT = WALL }224\mathrm{ COUNT + 1
WALL 240 ( I , K ) = WALL 240 ( I , K )+ 1
WALL }240\mathrm{ COUNT = WALL }240\mathrm{ COUNT + 1
WALL 254 ( I , K )= WALL 254 ( I , K )+ 1
WALL 254 COUNT = WALL 254 COUNT + 1
ENDIF
ELSEIF (( JLAST . GT . 208 ). AND .( JLAST . LE . 224 )) THEN
! Assign Particle Position to subsquent walls
print * ,' 224 TEST '
PRINT * ,' REALIZ = ', C ,' PARTNUM = ', PARTNUMLAST ,' JLAST = ', JLAST
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 224 ( I , K ) = WALL 224 ( I , K ) + 1
WALL }224\mathrm{ COUNT = WALL }224\mathrm{ COUNT + 1
WALL 240 ( I , K )= WALL 240 ( I , K )+ 1
WALL }240\mathrm{ COUNT = WALL }240\mathrm{ COUNT + 1
WALL 254 ( I , K )= WALL 254 ( I , K )+ 1
WALL 254 COUNT = WALL 254 COUNT + 1
ENDIF
ELSEIF (( JLAST . GT . 224 ). AND .( JLAST . LE . 240 )) THEN ! Assign Particle Position to
subsquent walls
PRINT * , ' 240 TEST '
PRINT * , ' REALIZ = ', C ,' PARTNUM = ', PARTNUMLAST ,' JLAST = ', JLAST
IF (( I . GE . IMIN ). AND .( I . LE . IMAX )) THEN
WALL 240 ( I , K ) = WALL 240 ( I , K )+ 1
WALL }240\mathrm{ COUNT = WALL }240\mathrm{ COUNT + 1
WALL 254 ( I , K )= WALL 254 ( I , K )+ 1
WALL 254 COUNT = WALL }254\mathrm{ COUNT + 1
ENDIF
ELSEIF (( JLAST . GT . 240 ). AND . ( JLAST . LE . 254 )) THEN ! Assign Particle Position to last
wall
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PRINT * , ' 254 TEST '
PRINT * , ' REALIZ = ', C ,' PARTNUM = ', PARTNUMLAST ,' JLAST = ', JLAST
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 254 ( I , K ) = WALL 254 ( I , K ) + 1
WALL 254 COUNT = WALL 254 COUNT + 1
ENDIF
ENDIF
JMAX = 111 ! Reset JMAX Counter to particle line source location behind Wagner Rd
ENDIF
```

```
IF ( PARTNUM . EQ .- 9999 ) THEN ! Final particle has been reached
GOTO 889 ! Exit Loop
ENDIF
C
IF (( J . EQ . 112 ). AND .( JMAX . LT . 112 )) THEN
! J = 112 is the index for the column for Wagner Road
! Therefore , a new particle has been encountered in the . MPF file
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 112 ( I , K ) = WALL 112 ( I , K ) + 1
WALL }112\mathrm{ COUNT = WALL }112\mathrm{ COUNT + 1
ENDIF
ENDIF
C
IF ( J . GT . JMAX ) THEN ! Particle has advanced downgradient
IF ( J . EQ . 128 ) THEN ! J = 128 is the index for the column where WALL 128 is located
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 128 ( I , K )= WALL 128 ( I , K )+ 1
WALL }128\mathrm{ COUNT = WALL }128\mathrm{ COUNT + 1
ENDIF
ENDIF
C
IF ( J . EQ . 144 ) THEN ! J = 144 is the index for the column where WALL 144 is located
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 144 ( I , K )= WALL 144 ( I , K )+ 1
WALL }144\mathrm{ COUNT = WALL }144\mathrm{ COUNT + 1
ENDIF
ENDIF
C
IF ( J . EQ . 160 ) THEN ! J = 160 is the index for the column where WALL 160 is located
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 160 ( I , K ) = WALL 160 ( I , K ) + 1
WALL }160\mathrm{ COUNT = WALL 160 COUNT + 1
ENDIF
ENDIF
C
IF ( J . EQ . 176 ) THEN ! J = 176 is the index for the column where WALL 176 is located
IF (( I . GE . IMIN ). AND .( I . LE . IMAX )) THEN
WALL 176 ( I , K ) = WALL 176 ( I , K ) + 1
WALL }176\mathrm{ COUNT = WALL 176 COUNT + 1
ENDIF
ENDIF
C
IF ( J . EQ . 192 ) THEN ! J = 192 is the index for the column where WALL 192 is located
IF (( I . GE . IMIN ). AND .( I . LE . IMAX )) THEN
WALL 192 ( I , K ) = WALL 192 ( I , K )+ 1
WALL }192\mathrm{ COUNT = WALL }192\mathrm{ COUNT + 1
ENDIF
ENDIF
C
IF ( J . EQ . 208 ) THEN ! J = 208 is the index for the column where WALL 208 is located
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 208 ( I , K ) = WALL 208 ( I , K )+ 1
WALL }208\mathrm{ COUNT = WALL }208\mathrm{ COUNT + 1
C print * ,' rEAL = ', C ,' PART = ', PARTNUM ,' J = ', J ,' JLAST = ', JLAST
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ENDIF
ENDIF
C
IF ( J . EQ . 224 ) THEN ! J = 224 is the index for the column where WALL 224 is located
IF (( I . GE . IMIN ). AND . ( I . LE . IMAX )) THEN
WALL 224 ( I , K )= WALL 224 ( I , K )+ 1
WALL }224\mathrm{ COUNT = WALL }224\mathrm{ COUNT + 1
ENDIF
ENDIF
```

```
C
IF ( J . EQ . 240 ) THEN ! J = 240 is the index for the column where WALL 240 is located
IF (( I . GE . IMIN ). AND .( I . LE . IMAX )) THEN
WALL 240 ( I , K )= WALL 240 ( I , K )+ 1
WALL 240 COUNT = WALL 240 COUNT + 1
ENDIF
ENDIF
c
IF ( J . EQ . 254 ) THEN ! J = 254 is the index for the column where WALL 254 is located
IF (( I . GE . IMIN ). AND .( I . LE . IMAX )) THEN
WALL 254 ( I , K )= WALL 254 ( I , K )+ 1
WALL 254 COUNT = WALL 254 COUNT + 1
ENDIF
ENDIF
ENDIF
IF ( J . GT . JMAX ) THEN
JMAX = J
ENDIF
PARTNUMLAST = PARTNUM
ILAST = I
JLAST = J
KLAST = K
GOTO 888
89 CONTINUE
PRINT * , C , ' realizations completed '
Write ( 50 , *) C , ' realizations completed '
Print * ,' WALL }112\mathrm{ Count = ', WALL }112\mathrm{ Count
Write ( 50 , *) , ' WALL }112\mathrm{ Count = ', WALL }112\mathrm{ Count
Print * , ' WALL }128\mathrm{ Count = ', WALL }128\mathrm{ Count
Write ( 50 , *) , ' WALL }128\mathrm{ Count = ', WALL }128\mathrm{ Count
Print * , ' WALL }144\mathrm{ Count = ', WALL }144\mathrm{ Count
Write ( 50 , *) , ' WALL 144 Count = ', WALL 144 Count
Print * , ' WALL }160\mathrm{ Count = ', WALL 160 Count
Write ( 50 , *) , ' WALL }160\mathrm{ Count = ', WALL }160\mathrm{ Count
Print * , ' WALL }176\mathrm{ COUNT = ', WALL }176\mathrm{ COUNT
Write ( 50 , *) , ' WALL }176\mathrm{ COUNT = ', WALL }176\mathrm{ COUNT
Print * , ' WALL }192\mathrm{ Count = ', WALL }192\mathrm{ Count
Write ( 50 , *), ' WALL }192\mathrm{ Count = ', WALL }192\mathrm{ Count
Print * , ' WALL 208 Count = ', WALL 208 Count
Write ( 50 , *) , ' WALL }208\mathrm{ Count = ', WALL }208\mathrm{ Count
Print * , 'WALL }224\mathrm{ Count = ', WALL 224 Count
Write ( 50 , *) , ' WALL 224 Count = ', WALL 224 Count
Print * ,' WALL 240 COUNT = ', WALL 240 COUNT
Write ( 50 , *) , ' WALL }240\mathrm{ COUNT = ', WALL }240\mathrm{ COUNT
Print * , ' WALL 254 Count = ', WALL 254 Count
Write ( 50 , *), ' WALL 254 Count = ', WALL 254 Count
Print * , ' DrainCount = ', DRAINCOUNT ( C )
Write ( 50 , *) ' DrainCount = ', DRAINCOUNT ( C )
Print *
Write ( 50 , *)
ENDDO
*
* *** TASK 3 ************************ TASK 3 *********************** TASK 3 ***
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*
* Write output files
*
WRITE ( 50 , *)
WRITE ( 50, *) " STARTING TASK 3 : Write output files and compute stats "
PRINT * , "STARTING TASK 3 : Write output files and compute stats "
OPEN ( 80 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 112 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
c *** Write file with number of particles counted in each wall cell
WRITE ( 80 , 100 ) ( WALL 112 ( I , K ) , I = IMIN , IMAX )
```

```
ENDDO
CLOSE ( 80 )
OPEN ( 60 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 128 . out ' )
DO K = 36, 1, - 1 ! layers 36 to 1 written from top to bottom , respectively
c *** Write file with number of particles counted in each wall cell
WRITE ( 60 , 100 ) ( WALL 128 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 60 )
OPEN ( 61 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 144 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 61 , 100 ) ( WALL 144 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 61 )
OPEN ( 62 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 160 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 62 , 100 ) ( WALL 160 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 62 )
OPEN ( 63 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 176 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 63 , 100 ) ( WALL 176 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 63 )
OPEN ( 64 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 192 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 64 , 100 ) ( WALL 192 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 64 )
OPEN ( 71 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 208 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 71 , 100 ) ( WALL 208 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 71 )
OPEN ( 72 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 224 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 72 , 100 ) ( WALL 224 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 72 )
OPEN ( 73 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
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1 WallONE 240 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 73 , 100 ) ( WALL 240 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 73 )
OPEN ( 74 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WallONE 254 . out ' )
DO K = 36 , 1 , - 1 ! layers 36 to 1 written from top to bottom , respectively
WRITE ( 74 , 100 ) ( WALL 254 ( I , K ) , I = IMIN , IMAX )
ENDDO
CLOSE ( 74 )
* ***** Print Grid Files ( Counts and Y , Z Coordinates ) for each Wall
OPEN ( 81 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 112 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0 ! coodinate for center of cell
ZAVG =( LAY ( K )+ LAY ( K + 1 ))/ 2 . 0 ! coodinate for center of cell
```

```
WRITE ( 81 , 165 ) YAVG , ZAVG , WALL 112 ( I , K )
IF ( WALL 112 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 112 MIN ) THEN ! Check for Y minimum
Y 112 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 112 MAX ) THEN ! Check for Y maximum
Y 112 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 112 MIN ) THEN ! Check for Z minimum
Z 112 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 112 MAX ) THEN ! Check for Z maximum
Z 112 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 112 SUM = Y 112 SUM + YAVG * WALL 112 ( I , K ) ! Add to sum
Z 112 SUM = Z 112 SUM + ZAVG * WALL 112 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE ( 81 )
OPEN ( 65 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 128 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0 ! coodinate for center of cell
ZAVG =( LAY ( K ) + LAY ( K + 1 ))/ 2 . 0 ! coodinate for center of cell
WRITE ( 65 , 165 ) YAVG , ZAVG , WALL 128 ( I , K )
IF ( WALL 128 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 128 MIN ) THEN ! Check for Y minimum
Y 128 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 128 MAX ) THEN ! Check for Y maximum
Y 128 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 128 MIN ) THEN ! Check for Z minimum
Z 128 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 128 MAX ) THEN ! Check for Z maximum
Z 128 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 128 SUM = Y 128 SUM + YAVG * WALL 128 ( I , K ) ! Add to sum
Z 128 SUM = Z 128 SUM + ZAVG * WALL 128 ( I , K ) ! Add to sum
ENDIF
ENDDO
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ENDDO
CLOSE ( 65 )
OPEN ( 66 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 144 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K ) + LAY ( K + 1 ))/ 2 . 0
WRITE ( 66 , 165 ) YAVG , ZAVG , WALL 144 ( I , K )
IF ( WALL 144 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 144 MIN ) THEN ! Check for Y minimum
Y 144 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 144 MAX ) THEN ! Check for Y maximum
Y 144 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 144 MIN ) THEN ! Check for Z minimum
Z 144 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 144 MAX ) THEN ! Check for Z maximum
```

```
Z 144 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 144 SUM = Y 144 SUM + YAVG * WALL 144 ( I , K ) ! Add to sum
Z 144 SUM = Z 144 SUM + ZAVG * WALL 144 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE ( }66\mathrm{ )
OPEN ( 67 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 160 . OUT ' )
DO K = 36, 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K )+ LAY ( K + 1 ))/ 2 . 0
WRITE ( 67 , 165 ) YAVG , ZAVG , WALL 160 ( I , K )
IF ( WALL 160 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 160 MIN ) THEN ! Check for Y minimum
Y 160 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 160 MAX ) THEN ! Check for Y maximum
Y 160 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 160 MIN ) THEN ! Check for Z minimum
Z 160 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 160 MAX ) THEN ! Check for Z maximum
Z 160 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 160 SUM = Y 160 SUM + YAVG * WALL 160 ( I , K ) ! Add to sum
Z 160 SUM = Z 160 SUM + ZAVG * WALL 160 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE ( 67 )
OPEN ( 68 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 176 . OUT ' )
DO K = 36, 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K )+ LAY ( K + 1 ))/ 2 . 0
WRITE ( 68 , 165 ) YAVG , ZAVG , WALL 176 ( I , K )
IF ( WALL 176 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 176 MIN ) THEN ! Check for Y minimum
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Y 176 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 176 MAX ) THEN ! Check for Y maximum
Y 176 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 176 MIN ) THEN ! Check for Z minimum
Z 176 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 176 MAX ) THEN ! Check for Z maximum
Z 176 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 176 SUM = Y 176 SUM + YAVG * WALL 176 ( I , K ) ! Add to sum
Z 176 SUM = Z 176 SUM + ZAVG * WALL 176 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE ( 68 )
OPEN ( 69 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 192 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
```

```
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K ) + LAY ( K + 1 ))/ 2 . 0
WRITE ( 69 , 165 ) YAVG , ZAVG , WALL 192 ( I , K )
IF ( WALL 192 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 192 MIN ) THEN ! Check for Y minimum
Y 192 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 192 MAX ) THEN ! Check for Y maximum
Y 192 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 192 MIN ) THEN ! Check for Z minimum
Z 192 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 192 MAX ) THEN ! Check for Z maximum
Z 192 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 192 SUM = Y 192 SUM + YAVG * WALL 192 ( I , K ) ! Add to sum
Z 192 SUM = Z 192 SUM + ZAVG * WALL 192 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE (69 )
OPEN ( 75 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 208 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K ) + LAY ( K + 1 ))/ 2 . 0
WRITE ( 75 , 165 ) YAVG , ZAVG , WALL 208 ( I , K )
IF ( WALL 208 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 208 MIN ) THEN ! Check for Y minimum
Y 208 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 208 MAX ) THEN ! Check for Y maximum
Y 208 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 208 MIN ) THEN ! Check for Z minimum
Z 208 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 208 MAX ) THEN ! Check for Z maximum
Z 208 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 208 SUM = Y 208 SUM + YAVG * WALL 208 ( I , K ) ! Add to sum
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Z 208 SUM = Z 208 SUM + ZAVG * WALL 208 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE ( 75 )
OPEN ( 76 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 224 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I ) + ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K )+ LAY ( K + 1 ))/ 2 . 0
WRITE ( 76 , 165 ) YAVG , ZAVG , WALL 224 ( I , K )
IF ( WALL 224 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 224 MIN ) THEN ! Check for Y minimum
Y 224 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 224 MAX ) THEN ! Check for Y maximum
Y 224 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 224 MIN ) THEN ! Check for Z minimum
Z 224 MIN = ZAVG ! Assign new Z minimum
```

```
ENDIF
IF ( ZAVG . GT . Z 224 MAX ) THEN ! Check for Z maximum
Z 224 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 224 SUM = Y 224 SUM + YAVG * WALL 224 ( I , K ) ! Add to sum
Z 224 SUM = Z 224 SUM + ZAVG * WALL 224 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE (76 )
OPEN ( 77 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 240 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K ) + LAY ( K + 1 ))/ 2 . 0
WRITE ( 77 , 165 ) YAVG , ZAVG , WALL 240 ( I , K )
IF ( WALL 240 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 240 MIN ) THEN ! Check for Y minimum
Y 240 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 240 MAX ) THEN ! Check for Y maximum
Y 240 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 240 MIN ) THEN ! Check for Z minimum
Z 240 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 240 MAX ) THEN ! Check for Z maximum
Z 240 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 240 SUM = Y 240 SUM + YAVG * WALL 240 ( I , K ) ! Add to sum
Z 240 SUM = Z 240 SUM + ZAVG * WALL 240 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE ( 77 )
OPEN ( 78 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ Output \
1 WALLONE GRID 254 . OUT ' )
DO K = 36 , 1 , - 1 ! Top layer to bottom layer
DO I = IMIN , IMAX ! North to south
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY (K ) + LAY ( K + 1 ))/ 2 . 0
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WRITE ( 78 , 165 ) YAVG , ZAVG , WALL 254 ( I , K )
IF ( WALL 254 ( I , K ). GT . 0 ) THEN
IF ( YAVG . LT . Y 254 MIN ) THEN ! Check for Y minimum
Y 254 MIN = YAVG ! Assign new Y minimum
ENDIF
IF ( YAVG . GT . Y 254 MAX ) THEN ! Check for Y maximum
Y 254 MAX = YAVG ! Assign new Y maximum
ENDIF
IF ( ZAVG . LT . Z 254 MIN ) THEN ! Check for Z minimum
Z 254 MIN = ZAVG ! Assign new Z minimum
ENDIF
IF ( ZAVG . GT . Z 254 MAX ) THEN ! Check for Z maximum
Z 254 MAX = ZAVG ! Assign new Z maximum
ENDIF
Y 254 SUM = Y 254 SUM + YAVG * WALL 254 ( I , K ) ! Add to sum
Z 254 SUM = Z 254 SUM + ZAVG * WALL 254 ( I , K ) ! Add to sum
ENDIF
ENDDO
ENDDO
CLOSE ( 78 )
* ***** Calculate Y and Z Standard Deviations ****
Y 112 MEAN = Y 112 SUM / WALL }112\mathrm{ COUNT
```

```
Y 128 MEAN = Y 128 SUM / WALL 128 COUNT
Y 144 MEAN = Y 144 SUM / WALL 144 COUNT
Y 160 MEAN = Y 160 SUM / WALL 160 COUNT
Y 176 MEAN = Y 176 SUM / WALL 176 COUNT
Y 192 MEAN = Y }192\mathrm{ SUM / WALL }192\mathrm{ COUNT
Y 208 MEAN = Y 208 SUM / WALL 208 COUNT
Y 224 MEAN = Y 224 SUM / WALL 224 COUNT
Y 240 MEAN = Y 240 SUM / WALL 240 COUNT
Y 254 MEAN = Y 254 SUM / WALL 254 COUNT
Z 112 MEAN = Z 112 SUM / WALL 112 COUNT
Z 128 MEAN = Z 128 SUM / WALL 128 COUNT
Z 144 MEAN = Z 144 SUM / WALL 144 COUNT
Z 160 MEAN = Z 160 SUM / WALL 160 COUNT
Z 176 MEAN = Z 176 SUM / WALL 176 COUNT
Z 192 MEAN = Z 192 SUM / WALL }192\mathrm{ COUNT
Z 208 MEAN = Z 208 SUM / WALL 208 COUNT
Z 224 MEAN = Z 224 SUM / WALL 224 COUNT
Z 240 MEAN = Z 240 SUM / WALL 240 COUNT
Z 254 MEAN = Z 254 SUM / WALL 254 COUNT
DO K = 1 , NLAY ! Loop through model layers
DO I = IMIN , IMAX ! Loop through model rows in each ' wall '
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0
ZAVG =( LAY ( K ) + LAY ( K + 1 ))/ 2 . 0
IF ( WALL 112 ( I , K ). GT . 0 ) THEN
DO N = 1 , WALL 112 ( I , K )
Y 112 SIGMA = Y 112 SIGMA +( YAVG - Y 112 MEAN )** 2 . 0
Z 112 SIGMA = Z 112 SIGMA +( ZAVG - Z 112 MEAN )** 2 . 0
ENDDO
ENDIF
IF ( WALL 128 ( I , K ). GT . 0 ) THEN
DO N = 1 , WALL 128( I , K )
Y 128 SIGMA = Y 128 SIGMA +( YAVG - Y 128 MEAN )** 2 . 0
Z 128 SIGMA = Z 128 SIGMA +( ZAVG - Z 128 MEAN )** 2 . 0
ENDDO
ENDIF
IF ( WALL 144 ( I , K ). GT . 0 ) THEN
DO N = 1 , WALL 144 ( I , K )
Y 144 SIGMA = Y 144 SIGMA +( YAVG - Y 144 MEAN )** 2 . 0
Z 144 SIGMA = Z 144 SIGMA +( ZAVG - Z 144 MEAN )** 2 . 0
ENDDO
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ENDIF
IF ( WALL 160 ( I , K ). GT . 0 ) THEN
DO N = 1 , WALL 160 ( I , K )
Y 160 SIGMA = Y 160 SIGMA +( YAVG - Y 160 MEAN )** 2 . 0
Z 160 SIGMA = Z 160 SIGMA +( ZAVG - Z 160 MEAN )** 2 . 0
ENDDO
ENDIF
IF ( WALL 176 ( I , K ). GT . 0 ) THEN
DO N = 1 , WALL 176 ( I , K )
Y 176 SIGMA = Y 176 SIGMA +( YAVG - Y 176 MEAN )** 2 . 0
Z 176 SIGMA = Z 176 SIGMA +( ZAVG - Z 176 MEAN )** 2 . 0
ENDDO
ENDIF
IF ( WALL 192 ( I , K ). GT . 0 ) THEN
DO N = 1 , WALL 192 ( I , K )
Y 192 SIGMA = Y 192 SIGMA +( YAVG - Y 192 MEAN )** 2 . 0
Z 192 SIGMA = Z 192 SIGMA +( ZAVG - Z 192 MEAN )** 2 . 0
ENDDO
ENDIF
IF ( WALL 208 ( I , K ). GT . 0 ) THEN
DO N = 1 , WALL 208 ( I , K )
Y 208 SIGMA = Y 208 SIGMA +( YAVG - Y 208 MEAN )** 2 . 0
Z 208 SIGMA = Z 208 SIGMA +( ZAVG - Z 208 MEAN )** 2 . 0
ENDDO
```

ENDIF
IF ( WALL 224 ( I , K ). GT . 0 ) THEN
DO $N=1$, WALL 224 ( I , K )
Y 224 SIGMA $=$ Y 224 SIGMA +( YAVG - Y 224 MEAN )** 2 . 0
Z 224 SIGMA = Z 224 SIGMA +( ZAVG - Z 224 MEAN )** 2 . 0
ENDDO
ENDIF
IF ( WALL 240 ( I , K ). GT . 0 ) THEN
DO $N=1$, WALL 240 ( I , K )
Y 240 SIGMA $=$ Y 240 SIGMA +( YAVG - Y 240 MEAN )** 2 . 0
Z 240 SIGMA $=$ Z 240 SIGMA +( ZAVG - Z 240 MEAN )** 2 . 0
ENDDO
ENDIF
IF ( WALL 254 ( I , K ). GT . 0 ) THEN
DO $N=1$, WALL 254 ( I , K )
Y 254 SIGMA $=$ Y 254 SIGMA $+($ YAVG - Y 254 MEAN $) * * 2$. 0
Z 254 SIGMA = Z 254 SIGMA +( ZAVG - Z 254 MEAN )** 2 . 0
ENDDO
ENDIF
ENDDO
ENDDO
Y 112 SIGMA = SQRT ( Y 112 SIGMA / WALL 112 COUNT )
Y 128 SIGMA = SQRT ( Y 128 SIGMA / WALL 128 COUNT )
Y 144 SIGMA = SQRT ( Y 144 SIGMA / WALL 144 COUNT )
Y 160 SIGMA = SQRT ( Y 160 SIGMA / WALL 160 COUNT )
Y 176 SIGMA = SQRT ( Y 176 SIGMA / WALL 176 COUNT )
Y 192 SIGMA = SQRT ( Y 192 SIGMA / WALL 192 COUNT )
Y 208 SIGMA = SQRT ( Y 208 SIGMA / WALL 208 COUNT )
Y 224 SIGMA = SQRT ( Y 224 SIGMA / WALL 224 COUNT )
Y 240 SIGMA = SQRT ( Y 240 SIGMA / WALL 240 COUNT )
Y 254 SIGMA = SQRT ( Y 254 SIGMA / WALL 254 COUNT )
Z 112 SIGMA = SQRT ( Z 112 SIGMA / WALL 112 COUNT )
Z 128 SIGMA = SQRT ( Z 128 SIGMA / WALL 128 COUNT )
Z 144 SIGMA = SQRT ( Z 144 SIGMA / WALL 144 COUNT )
Z 160 SIGMA = SQRT ( Z 160 SIGMA / WALL 160 COUNT )
Z 176 SIGMA = SQRT ( z 176 SIGMA / WALL 176 COUNT )
Z 192 SIGMA = SQRT ( Z 192 SIGMA / WALL 192 COUNT )
Z 208 SIGMA = SQRT ( Z 208 SIGMA / WALL 208 COUNT )
Z 224 SIGMA = SQRT ( Z 224 SIGMA / WALL 224 COUNT )
Z 240 SIGMA = SQRT ( Z 240 SIGMA / WALL 240 COUNT )
$\mathrm{C}: \$ Documents and Settings \Lena \Desktop\WALL\VisualStudioSolution\WALLONE_FIXED_2015_12_07.f 16
Z 254 SIGMA = SQRT ( Z 254 SIGMA / WALL 254 COUNT )

* ***** Write Out Count and Calculated Values *****

WRITE ( 50 , *)
WRITE ( 50 , *) " Number of Particles Exiting in the Drain "
PRINT * , ' Realization Draincount '
DO C = 1 , COUNT
WRITE ( 50 , 101 ) C , DRAINCOUNT ( C )
PRINT * , C , DRAINCOUNT ( C )
ENDDO
WRITE ( 50 , *)
WRITE ( 50 , 103 ) " Wall Number " , " YIMN " , " YMAX " , " YMEAN " , " Y STD DEV "
WRITE ( 50 , 102 ) " Wagner Rd " , Y 112 MIN , Y 112 MAX , Y 112 MEAN , Y 112 SIGMA WRITE ( 50 , 102 ) " WALL 128 " , Y 128 MIN , Y 128 MAX , Y 128 MEAN , Y 128 SIGMA WRITE ( 50 , 102 ) " WALL 144 " , Y 144 MIN , Y 144 MAX , Y 144 MEAN , Y 144 SIGMA WRITE ( 50 , 102 ) " WALL 160 " , Y 160 MIN , Y 160 MAX , Y 160 MEAN , Y 160 SIGMA WRITE ( 50 , 102 ) " WALL 176 " , Y 176 MIN , Y 176 MAX , Y 176 MEAN , Y 176 SIGMA WRITE ( 50 , 102 ) " WALL 192 " , Y 192 MIN , Y 192 MAX , Y 192 MEAN , Y 192 SIGMA WRITE ( 50 , 102 ) " WALL 208 " , Y 208 MIN , Y 208 MAX , Y 208 MEAN , Y 208 SIGMA WRITE ( 50 , 102 ) " WALL 224 " , Y 224 MIN , Y 224 MAX , Y 224 MEAN , Y 224 SIGMA WRITE ( 50 , 102 ) " WALL 240 " , Y 240 MIN , Y 240 MAX , Y 240 MEAN , Y 240 SIGMA WRITE ( 50 , 102 ) " WALL 254 " , Y 254 MIN , Y 254 MAX , Y 254 MEAN , Y 254 SIGMA
WRITE ( 50 , *)
WRITE ( $\left.50,{ }^{*}\right)$
WRITE ( 50 , 103 ) " Wall Number " , " ZIMN " , " ZMAX " , " ZMEAN " , " Z STD DEV "

```
WRITE ( 50 , 102 ) " Wagner Rd " , z 112 MIN , z 112 MAX , z 112 MEAN , z 112 SIGMA
WRITE ( 50 , 102 ) " WALL 128 " , Z 128 MIN , Z 128 MAX , Z 128 MEAN , Z 128 SIGMA
WRITE ( 50 , 102 ) " WALL 144 " , Z 144 MIN , Z 144 MAX , Z 144 MEAN , Z 144 SIGMA
WRITE ( 50 , 102 ) " WALL 160 " , Z 160 MIN , Z 160 MAX , Z 160 MEAN , Z 160 SIGMA
WRITE ( 50 , 102 ) " WALL 176 " , Z 176 MIN , Z 176 MAX , Z 176 MEAN , Z 176 SIGMA
WRITE ( 50 , 102 ) " WALL 192 " , Z 192 MIN , Z 192 MAX , Z 192 MEAN , Z 192 SIGMA
WRITE ( 50 , 102 ) " WALL 208 " , Z 208 MIN , Z 208 MAX , Z 208 MEAN , Z 208 SIGMA
WRITE ( 50, 102 ) " WALL 224 " , Z 224 MIN, Z 224 MAX , Z 224 MEAN , Z 224 SIGMA
WRITE ( 50 , 102 ) " WALL 240 " , Z 240 MIN , Z 240 MAX , Z 240 MEAN , Z 240 SIGMA
WRITE ( 50 , 102 ) " WALL 254 " , Z 254 MIN , Z 254 MAX , Z 254 MEAN , Z 254 SIGMA
PAUSE
WRITE ( 50 , *)
WRITE ( 50 , *) " Successful Program Termination "
CLOSE ( 50 )
100 FORMAT ( 113 ( I 5 , 1 X ))
101 FORMAT ( I 3 , 2 X , I 4 )
102 FORMAT ( 2 X , A 9 , T 15 , F 8 . 1 , T 30, F 8 . 1 , T 45 , F 8 . 1 , T 60, F 8 . 1 )
103 FORMAT ( A 11 , T 15 , A 4 , T 30, A 4 , T 45 , A 5 , T 60 , A 9 )
165 FORMAT ( F 10. 1 , 2 X , F 7 . 1 , 2 X , I 6 )
9999 END
```


## POLYPATH.for

```
C:\Documents and Settings\Lena\Desktop\WALL\VisualStudioSolution\POLYPATH.f 1
* -------------------------------------------------------------------------
PROGRAM POLYPATH
* Written by Larry Lemke and Lena Pappas Last Modified : November 20 2015
*
* This program compiles MODPATH particle location data from multiple realizations into a single
* pathline density map ( XY Plane )
* *** Variable Descriptions ***
*
* General Variables
* ==================
* I , J , K = coordinate variables
*
* Variables associated with MODPATH . mpF Files
* ============================================
* INPRE = MODPATH file name prefix for input file
* PARTNUM = Particle Number
* X = Particle location X coordinate
* Y = Particle location Y coordinate
* LOCZ = Particle location Z coordinate within the Modflow cell
* GLOBZ = Global particle coordinate in the Z direction
* TIME = cumulative tracking time ( days )
* J = J column index of cell containing the particle ( x )
* I = I row index of cell containing the particle ( y )
* K = K layer index of cell containing the particle ( z )
* TIMESTEP = Cumulative MODFLOW timestep number
* PARTNUMLAST = particle number from prior line of . mpF output file
* ILAST , JLAST , KLAST = I , J , K values from prior line of . mpF file
* JMAX = variable to track largest J value ( farthest eastward progression
* of current particle ( min value for JMAX = 112 at line source )
*
* Variables associated with MODPATH . VMG File
* =============================================
* INPRE = MODPATH file name prefix for input file
* NCOL , NROW , NLAY = number of columns , rows , layers in VMODFLOW grid
* COL ( J ) = x coordinate of each column boundary
* ROW ( I ) = y coordinate of each row boundary
* LAY ( K ) = z coordinate of each layer boundary
*
* Variables associated with WALL ARRAYS
* =====================================
* IMIN , IMAX = Range of I indices in the north / south direction
* COLUMNS = Number of columns in the xy array
* COUNT = Number of Modpath realizations read
* PARTNUM = partical number
*
* *** Declare Variables ***
IMPLICIT NONE
INTEGER PATHCOUNT
INTEGER NCOL , NROW , NLAY , COUNT
INTEGER C , I , J , K , N , ii
INTEGER IMIN , IMAX , COLUMNS
INTEGER PARTNUM , TIMESTEP , PARTNUMLAST , ILAST , JLAST , KLAST
CHARACTER DUMMY * 2, INPRE * 24, INFILE * 80, str * 3, INFILE 2 * 120
REAL * 8 X , Y , Z , LOCZ , GLOBZ , TIME
REAL * 8 YAVG , XAVG , COL , ROW , LAY
DIMENSION COL ( 300 ) , ROW ( 300 ) , LAY ( 50 )
DIMENSION PATHCOUNT ( 0 : 300 , 0 : 300 )
```

```
* *** Assign I / O files ***
*
* File 20 is the program parameter file
* File 25 contains the input MODPATH (. mpf ) files
* File 30 is seed . VMG
C:\Documents and Settings\Lena\Desktop\WALL\VisualStudioSolution\POLYPATH.f 2
* File 50 is an output log
* File 65 is the formatted output file for grid information
*
OPEN ( 20, FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ PolyPat
1 h \ PolyPath . par ', STATUS = ' OLD ' )
OPEN ( 50 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ PolyPat
1 h \ Output \ PolyPath RunLog ' )
*
*
* *** TASK 1 ************************ TASK 1 ********************** TASK 1 ***
*
* Read in the parameter file information
*
WRITE ( 50 , *)
WRITE ( 50 , *) " STARTING TASK 1 : Read in parameter file "
PRINT * , " STARTING TASK 1 : Read in paratmeter file "
READ ( 20 , *) COUNT
WRITE ( 50 , *) " Number of Modpath Realizations =" , COUNT
PRINT * , " Number of Modpath Realizations =" , COUNT
READ ( 20 , *) IMIN , IMAX
WRITE ( 50 , *) " IMIN =" , IMIN , " IMAX =" , IMAX
COLUMNS = IMAX - IMIN + 1
READ ( 20 , *) INPRE
WRITE ( 50 , *) " Modpath file prefix is " , INPRE
PRINT * , " Modpath file prefix is " , INPRE
write ( 50 , *)
ii = index ( inpre ,' ' )- 1
CLOSE ( 20)
OPEN ( 30 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ seed . VMG ' )
READ ( 30, *) NCOL
DO J = 1 , NCOL + 1
READ ( 30 , *) COL ( J )
ENDDO
READ ( 30 , *) NROW
DO I = NROW + 1 , 1, - 1 ! Read from north to south
READ ( 30 , *) ROW ( I )
ENDDO
READ ( 30, *) NLAY
DO K = 1 , NLAY + 1
READ ( 30, *) LAY ( K )
ENDDO
CLOSE ( 30 )
*
* **** TASK 2 *********************** TASK 2 *********************** TASK 2 *******
*
WRITE ( 50 , *)
WRITE ( 50 , *) " Starting TASK 2 "
PRINT * , " TASK 2 - reading Modpath Files "
C Initialize Variables
DO I = 1 , NROW
DO J = 1 , NCOL
PATHCOUNT ( J , I )= 0
ENDDO
ENDDO
KLAST = 0
PARTNUMLAST = 0
DO C = 1 , COUNT ! read 100 realizations
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PRINT * , ' Reading Realization Number ', C
```

```
WRITE ( 50 , *) ' Reading Realization Number ', C
* This assigns the value of current realization to the string " str " and then creates
* a corresponding " infile " string with a file name incremented for each realization number .
IF ( C . LT . 10 ) THEN ! single digit
write ( str ,' ( I 1 ) ' ) C
infile = inpre ( 1 : ii )// ' 00 ' // str ( 1 : 1 )// ' . mpF '
ELSEIF ( C . LT . 100 ) THEN ! double digit
write ( str ,' ( I 2 ) ' ) C
infile = inpre ( 1 : ii )// ' 0 ' // str ( 1 : 2 )// ' . mpF '
ELSE ! three digits
write ( str,' ( I 3 ) ' ) C
infile = inpre ( 1 : ii )// str ( 1 : 3 )// ' . mpF '
ENDIF
Print * , " infile = " , infile
Write ( 50 , *) " infile = " , infile
INFILE 2 = ' C : \ Documents and Settings \ Lena \ Desktop \' // inpre ( 1 : i
1 i )// '_ MPF Files \' // infile
PRINT * ,'' Infile 2 = ', Infile 2
OPEN ( 25 , File = INFILE 2 )
READ ( 25 , *) DUMMY
888 CONTINUE
READ ( 25 , *) PARTNUM , X , Y , LOCZ , GLOBZ , TIME , J , I , K , TIMESTEP
C
c *** Test for next or final particle
IF ( PARTNUM . EQ .- 9999 ) GOTO 889 ! proceed to next realization
IF (( K . EQ . KLAST ). OR .( PARTNUM . GT . PARTNUMLAST )) THEN
c *** Add to counter at new particle position
PATHCOUNT ( J , I )= PATHCOUNT ( J , I )+ 1
ENDIF
KLAST = K
PARTNUMLAST = PARTNUM
GOTO }88
8 8 9 ~ C O N T I N U E ~
ENDDO
*
* *** TASK 3 ************************ TASK 3 *********************** TASK 3 ***
*
* ***** Write Grid File ( Counts and X , Y Coordinates )
OPEN ( 65 , FILE = ' C : \ Documents and Settings \ Lena \ Desktop \ WALL \ PolyPat
1 h \ Output \ PolyPath XY Grid . OUT ' )
c DO I = IMIN , IMAX ! Rows in Y coordinate direction ( north to south )
DO I = 1 , NROW ! Rows in Y coordinate direction ( north to south )
DO J = 1 , NCOL ! Columns in X coordinate direction ( west to east )
YAVG =( ROW ( I )+ ROW ( I + 1 ))/ 2 . 0 ! coodinate for center of cell
XAVG =( COL ( J )+ COL ( J + 1 ))/ 2 . 0 ! coodinate for center of cell
WRITE ( 65 , 165 ) XAVG , YAVG , PATHCOUNT ( J , I )
ENDDO
ENDDO
CLOSE ( 65 )
PAUSE
WRITE ( 50 , *)
WRITE ( 50 , *) " Successful Program Termination "
CLOSE ( 50)
165 FORMAT ( F 10. 1 , 2 X , F 10 . 1 , 2 X , I 6 )
9999 END
```


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# ABSTRACT <br> INTEGRATION OF DETERMINISTIC AND STOCHASTIC MODELS IN A 1,4-DIOXANE CONTAMINATED GLACIAL AQUIFER SYSTEM, WASHTENAW COUNTY, MICHIGAN 

by

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August 2016

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Hybrid models incorporating stochastic variability within a deterministic hydrostratigraphic framework provide an effective way to assess uncertainty in flow and transport model predictions. This study evaluated the distribution of groundwater flow and contaminant transport pathways in two ensembles of spatially variable hydraulic conductivity (K) distributions. The models comprised a $360 \mathrm{ft}-$ thick sequence of Pleistocene glacial sediments in in an approximately $8 \mathrm{mi}^{2}$ area across Washtenaw County, Michigan. Conditioned K fields were generated using Sequential Gaussian Simulation (SGS) and Sequential Indicator Simulation (SIS) constructed using indicator classes based on natural gamma ray logs from 77 monitoring wells. K fields were modeled independently for aquifer and aquitard materials and subsequently embedded within a 3D MODFLOW model constructed using a deterministic framework of eight aquifer and aquitard layers.

MODPATH was used to track the pathways of 100 particles released as line sources at five depth intervals with documented 1,4-dioxane concentrations along the boundary of the contaminant source area. Pathways for 100 realizations of each ensemble were combined to produce maps and cross sections showing the frequency of particles passing through model cells downgradient of the line source and upgradient of the hypothesized groundwater discharge location along the Huron River approximately 8 km from the line source. Differences in the spatial distribution of particle pathways
observed between the SIS and SGS ensembles were observed, and compared to distribution resulting from deterministic modeling. Results revealed channelization and dispersion patterns downgradient are influenced by several factors, including model type, distance from source, dispersion orientation, head differentials, and percentage of aquifer and aquitard material.

## AUTOBIOGRAPHICAL STATEMENT

My post-secondary education began at Schoolcraft College, where I was awarded the Presidential Academic Scholarship to attend Wayne State University. I received dual Bachelor of Science degrees from Wayne State University in Biology and Environmental Science in 2007. From there, I pursued a career as an environmental consultant at an international firm where I expanded the knowledge base received through Wayne State through experience. I rejoined Wayne State under fellowship to complete a Master's of Science in Geology, and am pleased to present this thesis to the College of Liberal Arts and Sciences. Since that time, I have resumed a career as a geologist at a national consulting firm. I look forward to applying the knowledge gained during this recent tenure to regional pollution issues to help improve quality of life in the area.

