GRP Model MODFLOW-USG Input/Output File Readme

Some components of the GRP Model use features of MODFLOW-USG that have not yet been fully implemented in Groundwater Vistas Version 8. These included Horizontal Flow Barrier (HFB) package inputs for a Voronoi mesh, saving of immobile domain output concentrations and mass fluxes to binary output files, and specification of model cells subject to dual-domain processes. These limitations are overcome with the following steps:

1. ***SMC_Faults_11Lyr.hfb*** is the HFB package input file developed for the Voronoi mesh, and it is generated by using the Python script ***CreateHFB_DisLpf.py*** which reads the model's DIS and LPF package input files to calculate the HFB package hydraulic characteristic values for each node pair on either side of a fault as listed in the file ***SMC_BasinFaultNodes.csv***. After using Groundwater Vistas to create model input files, both ***CreateHFB_DisLpf.py*** and ***SMC_BasinFaultNodes.csv*** need to be copied to the directory with the model input files. ***CreateHFB_DisLpf.py*** needs to be executed to create ***SMC_Faults_11Lyr.hfb.*** Finally, the reference to the HFB package input needs to be updated in the MODFLOW-USG .nam file, replacing the name of the .hfb file referenced in the .nam file created by Groundwater Vistas as indicated below.

   ```
   HFB6 52 1. SMC_Faults_11Lyr.hfb
   ```

2. Saving of immobile domain output concentrations and specification of specification of model cells subject to dual-domain processes are both set in the Dual-Porosity Transport (DPT) package input file (.dpt file) by copying the contents of the file ***Dual_Domain_Header_AllChinleSAG_SaveConCcb_11Lays.dpt*** over the first line of the .dpt file created by Groundwater Vistas. This file contains a new header line that species that immobile domain concentrations will be saved on Fortran unit number 133 and mass fluxes will be saved on Fortran unit number 96. Further, the contents of ***Dual_Domain_Header_AllChinleSAG_SaveConCcb_11Lays.dpt*** sets the value of **ICBNDIMFLG** to 1 to indicate that values of **ICBNDIM** will be provided to specify which cells are subject to dual-domain processes, followed by the **ICBNDIM** arrays themselves. After replacing the first line in the .dpt input file, simply save the updated file. Then a final step in saving the immobile domain concentrations and mass fluxes is to add additional lines in the .nam file specifying the output file names for Fortran unit numbers 133 and 96:

   ```
   DATA(BINARY) 133 <MODFLOW-USG_RootFilename>_IMM.con
   DATA(BINARY) 96 <MODFLOW-USG_RootFilename>_IMM.ccb
   ```

   Where `<MODFLOW-USG_RootFilename>` represents the MODFLOW-USG root filename, e.g., ***HMC_Grants_2002-2019_Calib_U*** for the uranium calibration simulation files. The practice followed for the GRP Model has been to use the same root filename as the mobile domain concentration output file but add "_IMM" to indicate this file is the immobile domain concentration outputs.

For simulation of molybdenum with powellite precipitation, an initial simulation is run without powellite precipitation. When this simulation is complete ***PowellitePCB_Concs.py*** is executed on the output concentrations from the binary output (.con) file and designated model node locations of powellite

precipitation in ***PowellitePCB_RegNodeList.txt*** to generate ***PowellitePCB_ConcsToImport.csv*** with information to import to Groundwater Vistas as specified concentration cells to be used with the MODFLOW-USG Prescribed Concentration package.

Since the GRP Model transport concentration units are input and output as mg/ft^3 because of the non-linear sorption isotherm, the output binary concentration files (.con) must be converted back to units of mg/L to be compared with analytical data, generate concentration contours, etc. The Python script ***USG_Con_ConvUnits.py*** was developed to accomplish this task. The practice for the GRP Model has been to add "_mgft3" to the end of the mobile and immobile domain output .con files after the completion of each simulation to indicate these files are in units of mg/ft$_3$. Then in ***USG_Con_ConvUnits.py*** the name of the file to convert from mg/ft^3 is specified as the variable "inconfile" (line 29 of the script) and the name of the converted output file (i.e., now without the "_mgft3" at the end of the root name in units of mg/L is specified as the variable "outconfile" (line 30 of the script).

```
inconfile = 'HMC_Grants_200YrPred_NoFurtherCollInj_U_mgft3.con'
outconfile = 'HMC_Grants_200YrPred_NoFurtherCollInj_U.con'
```

Save the script and execute it, and the converted output file will be produced.

The MODFLOW-USG model calibration simulation files input and output files along with their corresponding Groundwater Vistas files and Python processing scripts and ancillary files are provided in .zip archive format.

- **HMC_Grants_2002-2019_Calib_Mo_PrePowellite.zip** - molybdenum calibration period to generate powellite Prescribed Concentration package inputs
- **HMC_Grants_2002-19_Calib_Mo.zip** - molybdenum calibration 2002-2019
- **HMC_Grants_2002-19_Calib_U.zip** - uranium calibration 2002-2019