Introduction to Groundwater Modelling with Modflow and FloPy

Haili Jia

Council for Geoscience, South Africa

Jul, 2020

Council for Geoscience

Disclaimer

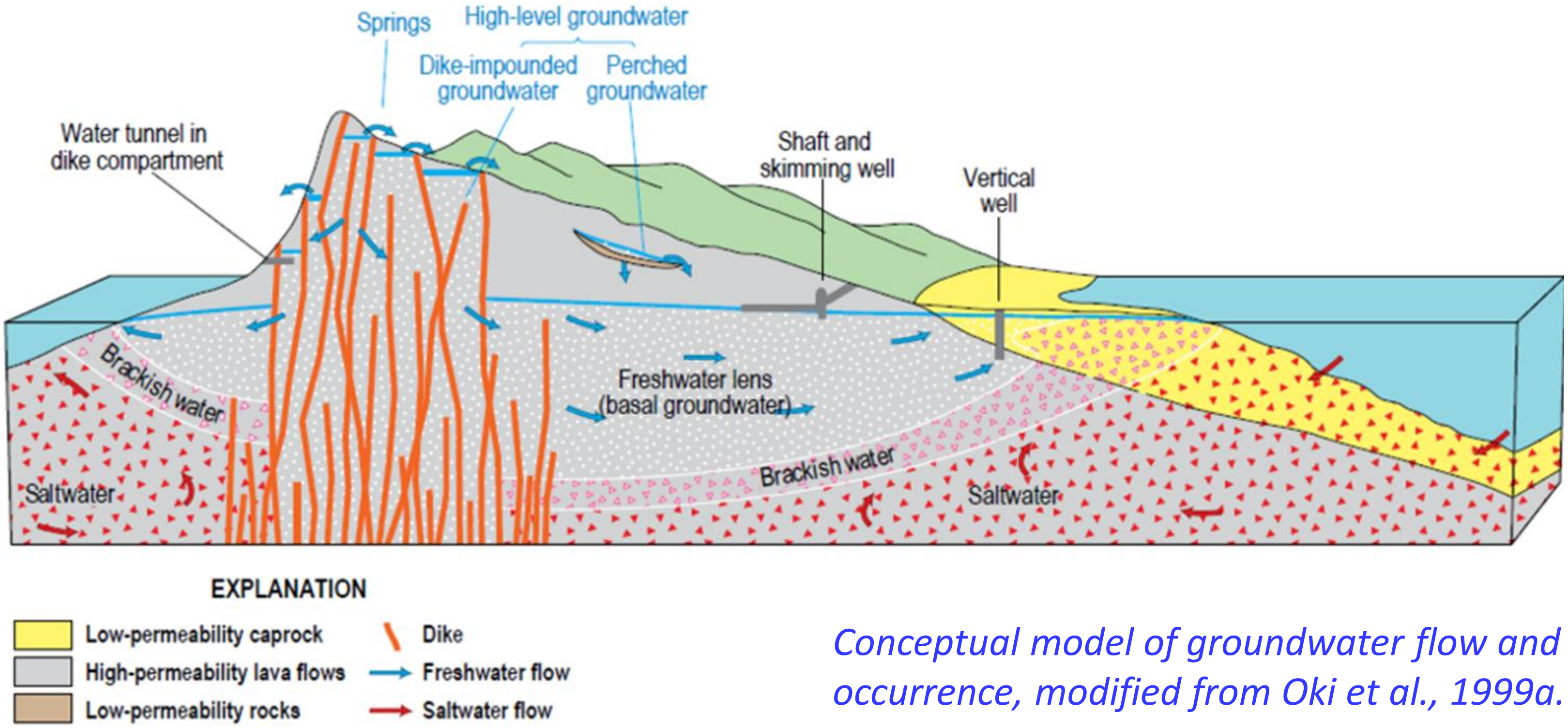
The information contained in these documents is the sole property of the Council for Geoscience and all rights are reserved. The information is intended solely for the recipient and is confidential. Any use of this information by any person, including the recipient, and any further dissemination or disclosure of the information, either in whole or in part, is prohibited except with the prior written consent of the Council for Geoscience. The opinions expressed are in good faith and while every care has been taken in preparing these documents, the Council for Geoscience makes no representations and gives no warranties of whatever nature in respect of these documents, including, but not limited to, the accuracy or completeness of any information, facts and/or opinions contained therein. The Council for Geoscience, its Board, employees and agents cannot be held liable for the use of and reliance on the opinions, estimates, forecasts and findings in these documents.

Overview of the Webinar

- Groundwater model
- Introduction to MODFLOW
- Introduction to FloPy
- Tutorial on FloPy

Groundwater Model

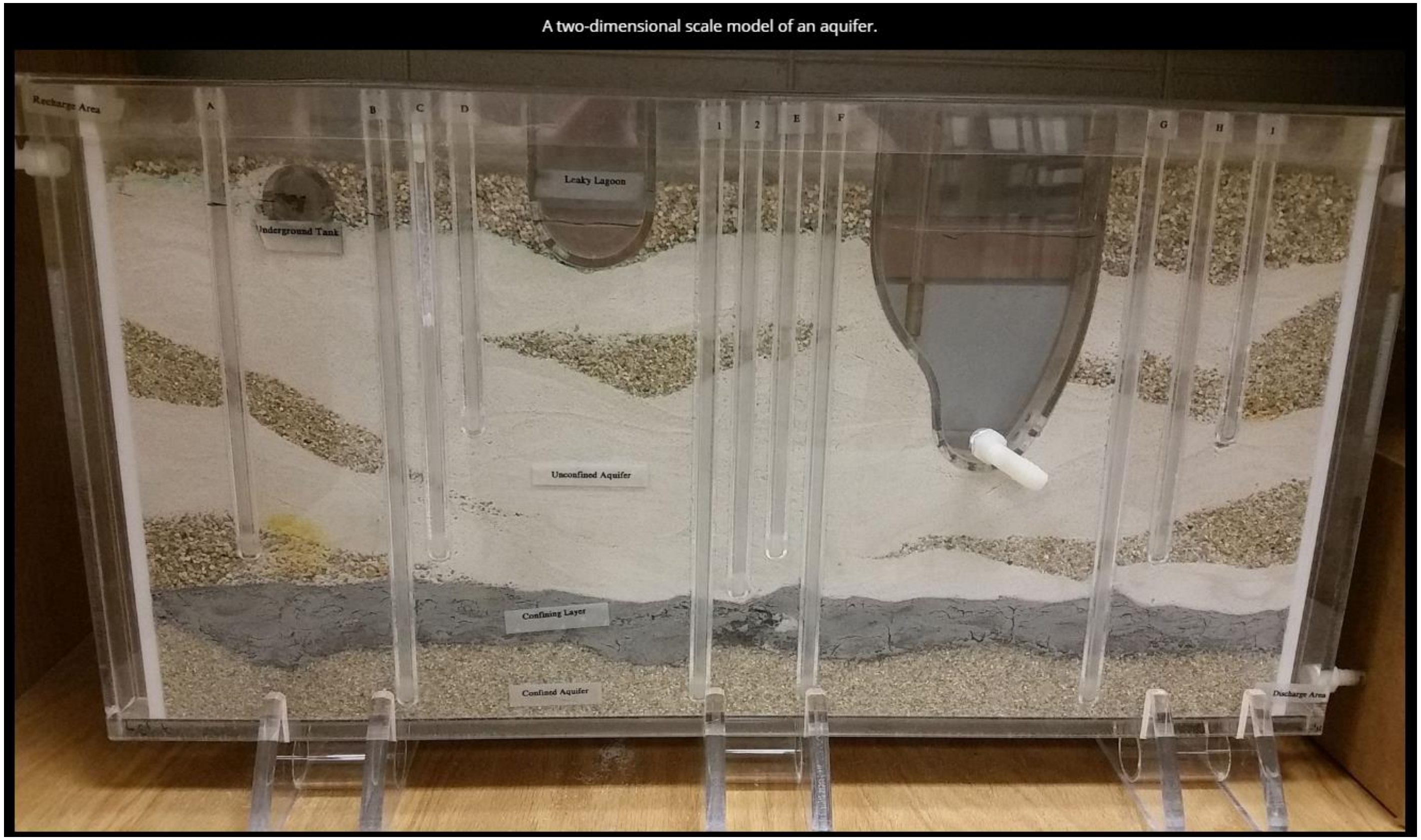
- A simplification of a real-world groundwater system, it can be:
  - Conceptual model
  - Physical scale model
  - Analog model
  - Mathematical model
    - Analytical model
    - Numerical model



Conceptual model of groundwater flow and occurrence, modified from Oki et al., 1999a.

Conceptual model

Descriptive representation of the groundwater system, can include geological and hydrological conditions, important hydrogeological processes, boundaries, parameters…



https://www.wikiwand.com/en/Hydrological_model#

Physical scale model

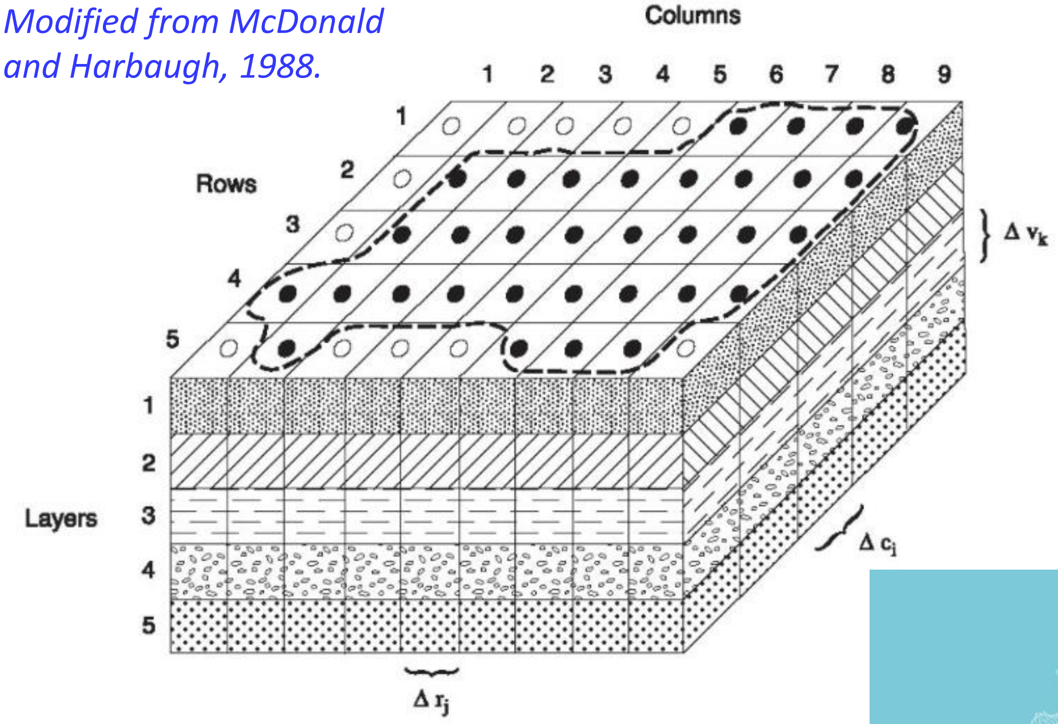
Scale model of groundwater flow system, commonly a scaled experimental setup to demonstrate aquifer setting and behavior.

Analog model

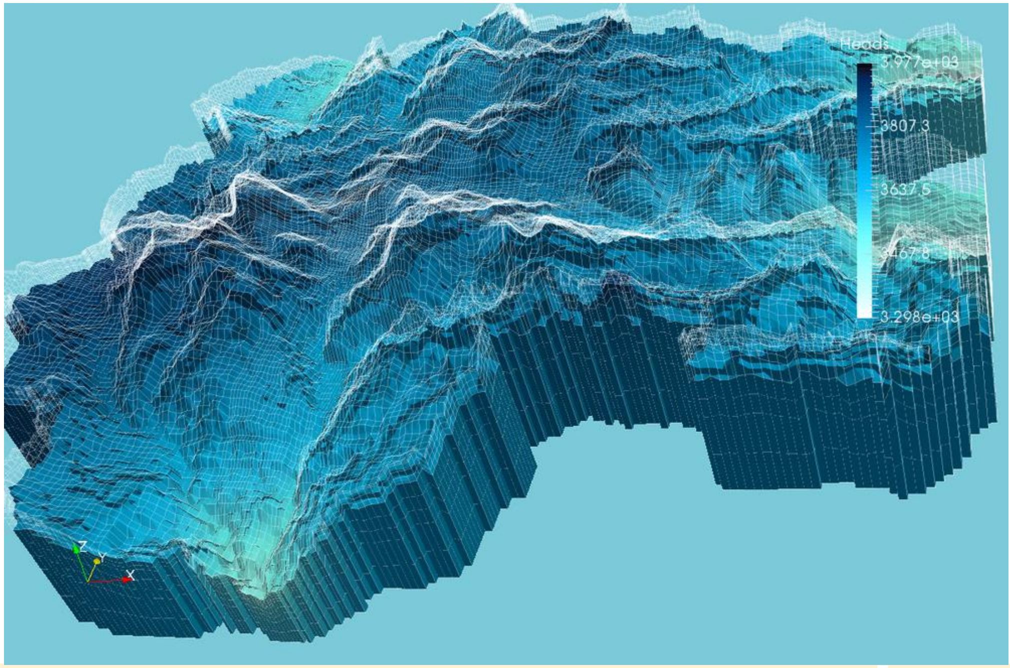
Electrical current flow through a circuit board to represent groundwater flow system.

https://darcylecture2016.wordpress.com/2016/02/20/test/photo-15/

Modified from McDonald and Harbaugh, 1988.



From Hatari labs



3D numerical groundwater model

The groundwater flow domain is discretized into cells, horizontally and vertically. Numerical solution to be calculated by computer. Two methods:

- Finite difference
- Finite element

Numerical Groundwater Model – Purpose

- Predictive purpose
  - to predict aquifer response to external stresses such as pumping. Heads or flow need to be calibrated.
- Interpretive purpose
  - to understand how a system works, organize field data. Not necessarily calibrated.
- Generic purpose
  - to present and analyse dynamics of groundwater systems
  - to evaluate hydraulic parameters and flow boundaries
  - to evaluate recharge, discharge and aquifer storage processes

Numerical Groundwater Model - Components

- Groundwater flow equations
  - Mass balance

    $Q_{in} - Q_{out} = \Delta Storage$
  - Darcy's law

$$q = \frac{Q}{A} = -K\frac{dh}{dl}$$

- Boundary conditions
- Initial conditions

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-W=S_s\frac{\partial h}{\partial t},$$

where

K_{xx}, K_{yy}, and K_{zz} are values of hydraulic conductivity in the x, y, and z directions along Cartesian coordinate axes, which are assumed to align with principal directions of hydraulic conductivity (LT^{-1}),

h is hydraulic head (L),

W is a volumetric flux per unit volume and represents sinks and/or sources (T^{-1}),

S_s is the specific storage of the porous material (L^{-1}), and

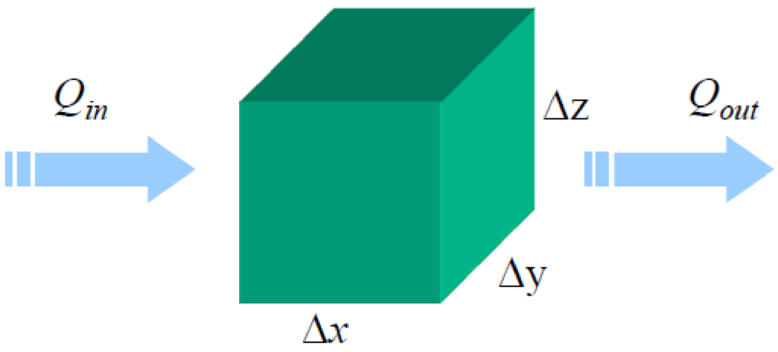
t is time (T).

Groundwater Flow Equation

$$\text{INFLOW}: \quad Q_{in} = q_1(\Delta y \Delta z)\Delta t$$

$$\text{OUTFLOW}: \quad Q_{out} = q_2(\Delta y \Delta z)\Delta t$$

$$\Delta\text{STORAGE} = S(\Delta x \Delta y)\Delta h = S_s \Delta z(\Delta x \Delta y)\Delta h$$



$$\boxed{\text{INFLOW - OUTFLOW} = \Delta\text{STORAGE}}$$

$$q_1 \Delta y \Delta z \Delta t - q_2 \Delta y \Delta z \Delta t = S_s \Delta z(\Delta x \Delta y)\Delta h$$

$$\frac{q_1 - q_2}{\Delta x} = S_s \frac{\Delta h}{\Delta t}$$

$$-\frac{\Delta q}{\Delta x} = S \frac{\Delta h}{\Delta t} \qquad [\Delta q = q_2 - q_1]$$

where q_1 and q_2 are specific discharges at left and right faces, respectively, and S_s is specific storage

https://hydro.geo.ua.edu/GEO406_506/Lecture7.pdf

Groundwater Flow Equation

$$-\frac{\Delta q}{\Delta x} = S\frac{\Delta h}{\Delta t} \qquad [\Delta q = q_2 - q_1]$$

$$\text{Becasue}: \lim_{\Delta x \to 0} \frac{\Delta q}{\Delta x} = \frac{dq}{dx}$$

The size of control volume approaches infinitesimal

$$\text{we obtain}: -\frac{dq}{dx} = S_s \frac{dh}{dt}$$

$$\text{Applying Darcy's Law}: q = -K\frac{dh}{dx}$$

$$\text{we have}: -\frac{d}{dx}\left(-K\frac{dh}{dx}\right) = S_s\frac{dh}{dt}$$

$$\text{or} \qquad \frac{d}{dx}\left(K\frac{dh}{dx}\right) = S_s\frac{dh}{dt}$$

$$\text{If } K \text{ is uniform}: K\frac{d^2h}{dx^2} = S_s\frac{dh}{dt}$$

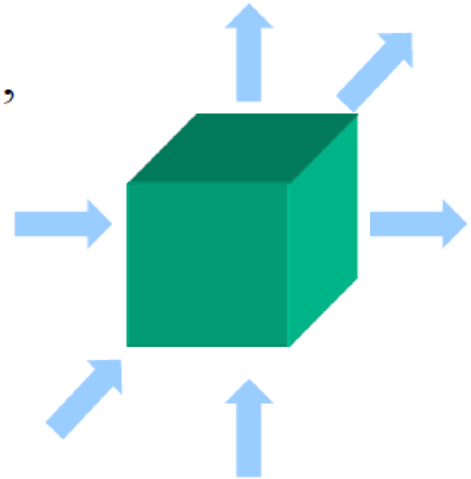
Groundwater Flow Equation

In a multidimensional system,

replace ordinary derivatives with partial dervatives,

leading to

$$K\frac{\partial^2 h}{\partial x^2}+K\frac{\partial^2 h}{\partial y^2}+K\frac{\partial^2 h}{\partial z^2}=S_s\frac{\partial h}{\partial t}$$



More generally, assuming hydraulic conductivity K

is heterogeneous and anisotrpic, and with sinks/sources :

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)+q_s=S_s\frac{\partial h}{\partial t}$$

Groundwater Flow Equation

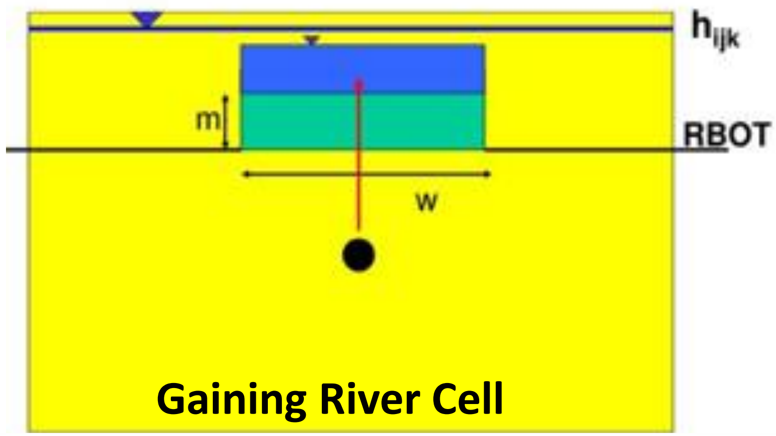
- What need to be solved?
  - Partial differential equations
- How to solve?
  - Finite difference method
- Input data
  - Aquifer properties (K_x, K_y, K_z, S_s)
  - Sources and sinks (q_s)
  - Boundary conditions & initial conditions
- Solution
  - Hydraulic head

Boundary Conditions (BC)

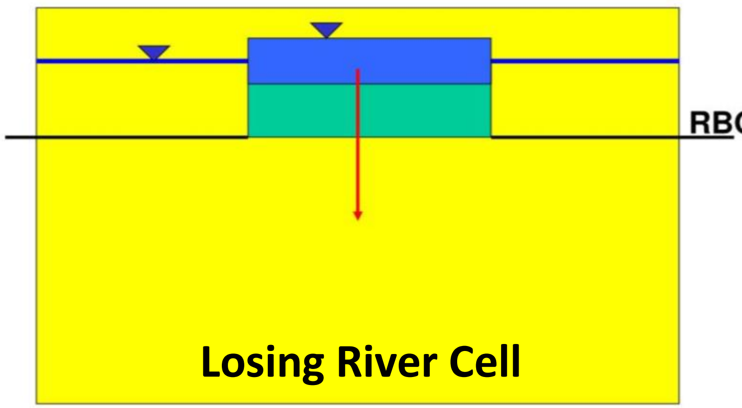
- Represent locations in the model where water flows into or out of the model domain. There are three types of boundary conditions:
  - Dirichlet condition
    - specified heads
    - e.g. constant head boundary
  - Neumann condition
    - specified fluxes
    - e.g. no flow boundary, well, recharge
  - Mixed condition
    - head dependant fluxes
    - e.g. river, drain, general head boundary, evapotranspiration

Examples of BC

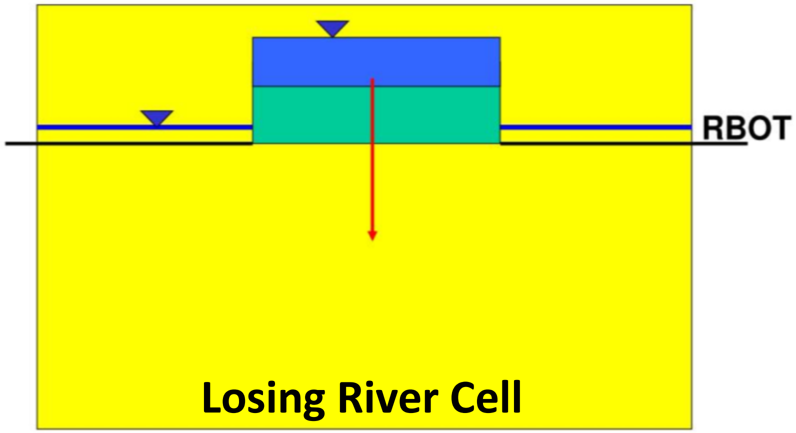
$Q = C\,(h_R - h_{ijk})$



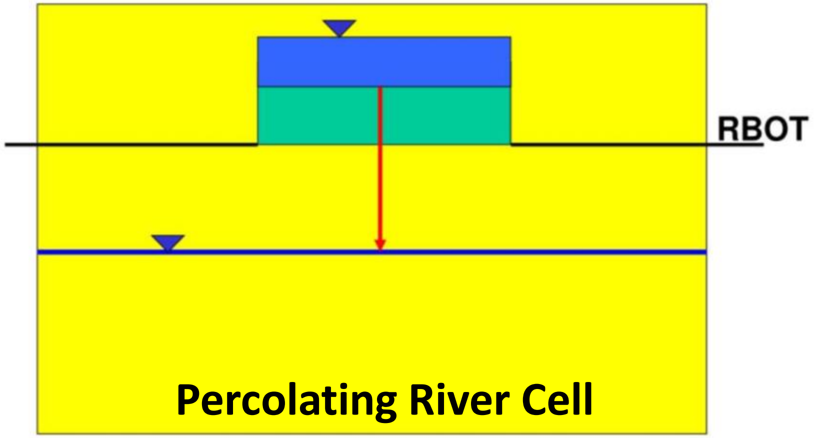
$Q = C\,(h_R - h_{ijk})$



$Q = C\,(h_R - h_{ijk})$



$Q = C\,(h_R - \text{RBOT})$

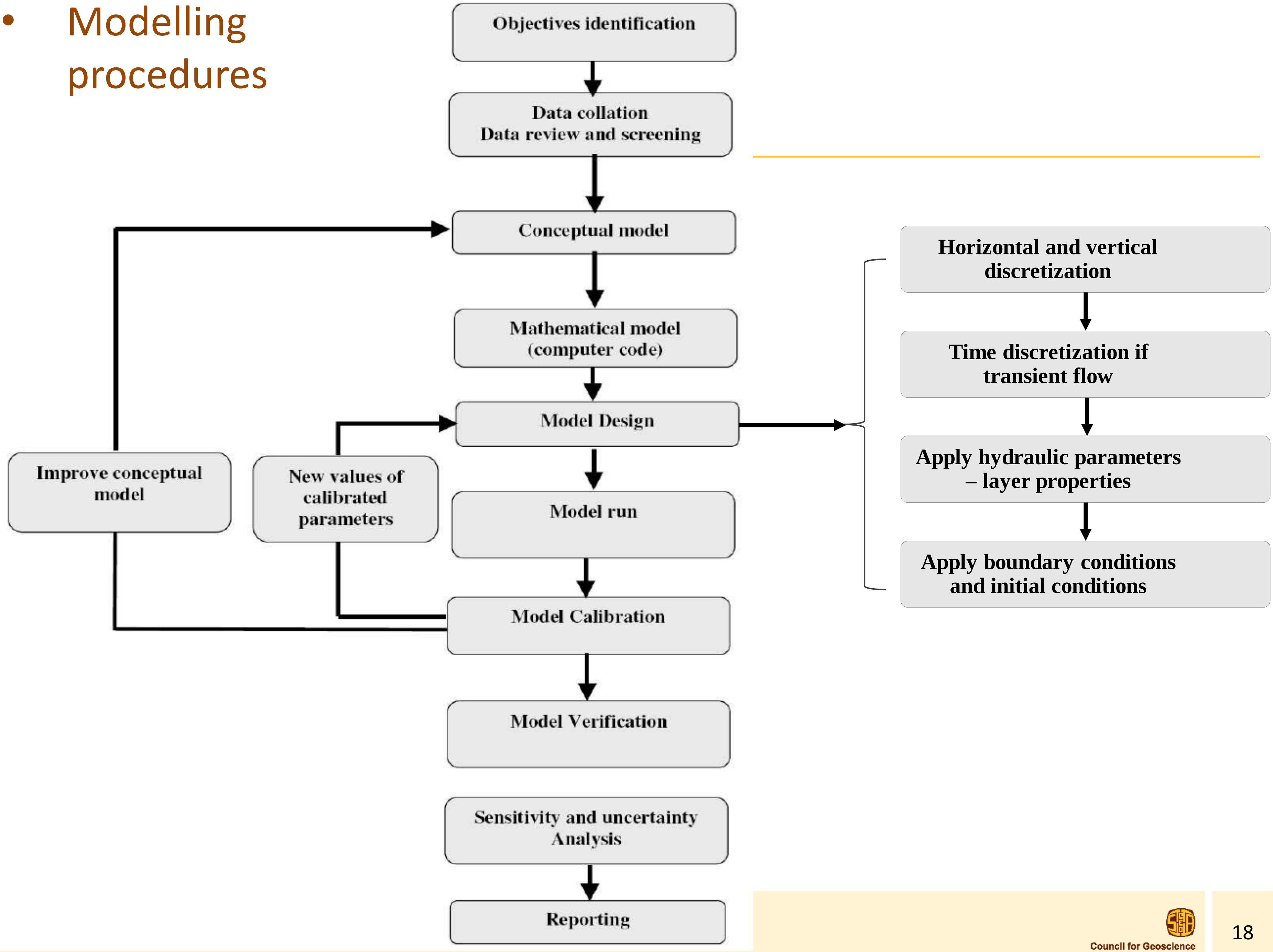


https://www.slideserve.com/keran/types-of-boundary-conditions-powerpoint-ppt-presentation

Initial Condition (IC)

- Initial conditions:
  - The state of system variables (hydraulic head) at the start of simulation

- Modelling procedures



MODFLOW

- USGS modular finite-difference flow model
- Solve the groundwater flow equations
- Free, open source, well documented
- From MODFLOW 88 to MODFLOW 6 with variants
- Many UIs, free or commercial:
  - ModelMuse, PMWIN, GMS, Visual MODFLOW, Groundwater Vista, Flopy…
- Many related USGS programs:
  - MODPATH, MT3D-USGS, PEST++, ZoneBudget and etc.

Processes and Packages of MODFLOW 2005

- Processes: parts of the code that solve a fundamental equation or set of related equations and that consist of sets of the underlying packages. In MODFLOW 2005:
  - GWF process (the core process, GW flow equation)
  - OBS process (y=y'+e)
  - SWR process
- Packages: Independent, modular-programming components to simulate specific aspects of a groundwater flow system. Under GWF process, there are:
  - General: BAS, DIS, ZONE, PVAL…
  - GW flow: BCF, LPF, HUF, HFB…
  - Boundary condition: CHD, RCH, WEL, RIV, DRN, GHB…
  - Solver: PCG. Newton solver for MF-NWT.
  - Output: OC

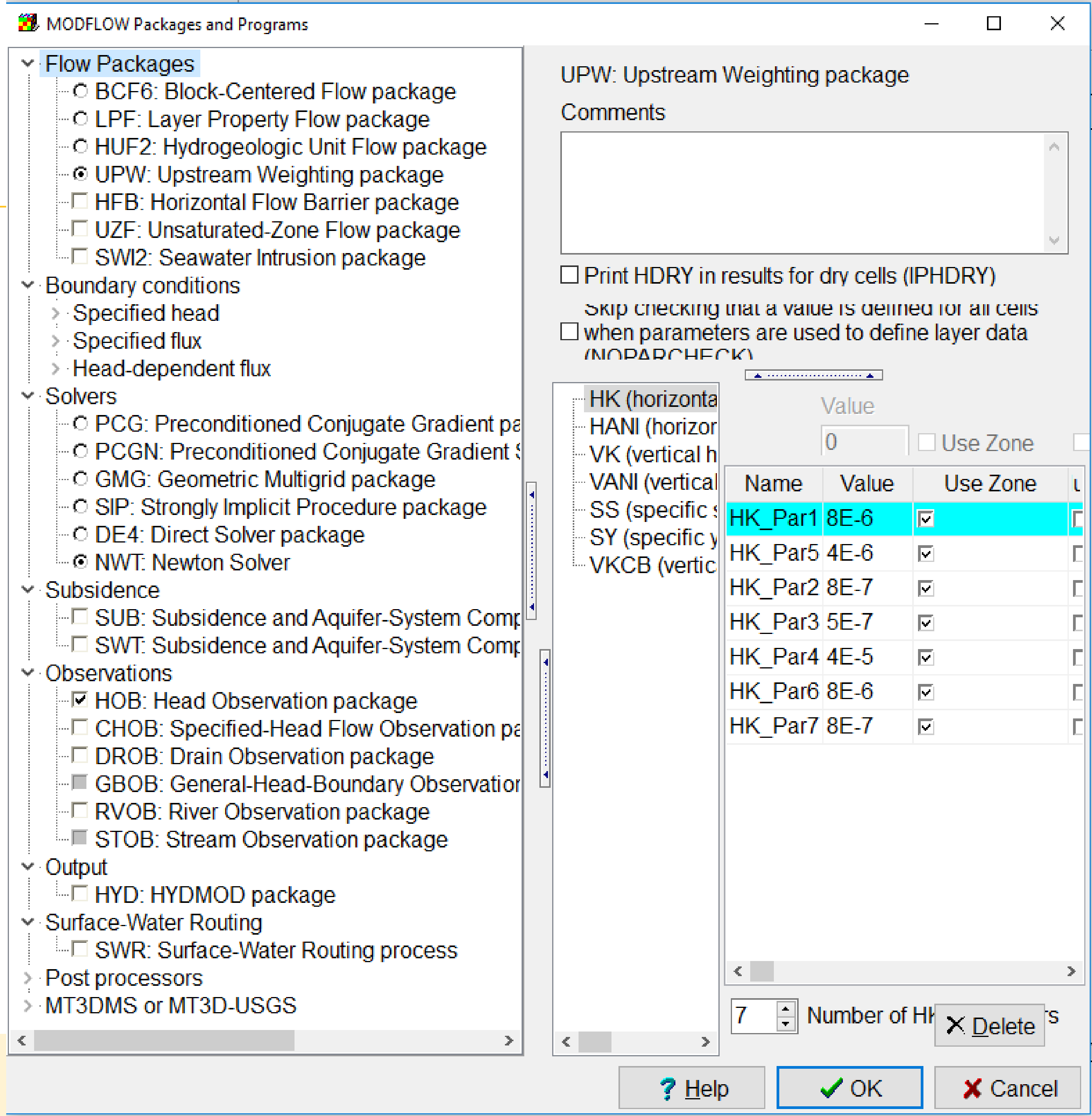
Documentation of MODFLOW-2005 Processes and Packages

The list below provides quick access to the key documentation for MODFLOW processes and packages. *Online Help* links point to the most up-to-date input instructions and related details for the process or package in the Online MODFLOW User's Guide. *Original Report* links point to the official USGS report describing the theory and input instructions at the time the package or process was first released.

- **BAS (Basic Package):** BAS Online Help | *Original Report*: Harbaugh, 2005
- **BCF (Block-Centered Flow Package):** BCF Online Help | *Original Report*: Harbaugh, 2005
- **CHD (Time-Variant Specified-Head Option):** CHD Online Help | *Original Report*: Harbaugh, 2005
- **DE4 (Direct Solver):** DE4 Online Help | *Original Report*: Harbaugh, 2005
- **DIS (Discretization File):** DIS Online Help | Original Report: Harbaugh, 2005
- **DRN (Drain Package):** DRN Online Help | *Original Report*: Harbaugh, 2005
- **DRT (Drains with Return Flow Package):** DRT Online Help | *Original Report*: Banta, 2000
- **ETS (Evapotranspiration with a Segmented Function Package):** ETS Online Help | *Original Report*: Banta, 2000
- **EVT (Evapotranspiration Package):** EVT Online Help | *Original Report*: Harbaugh, 2005
- **FHB (Flow and Head Boundary Package):** FHB Online Help | *Original Report*: Leake and Lilly, 1997
- **GAGE (Gage Package):** GAGE Online Help| *Original Reports*: Prudic and others, 2004; Niswonger and Prudic, 2005; and Merritt and Konikow, 2000
- **GHB (General Head Boundary Package):** GHB Online Help | *Original Report*: Harbaugh, 2005
- **GMG (Geometric MultiGrid Solver Package):** GMG Online Help | *Original Report*: Wilson and Naff, 2004
- **HFB (Horizontal Flow Barrier Package):** HFB Online Help | *Original Report*: Harbaugh, 2005
- **HUF (Hydrogeologic-Unit Flow Package):** HUF Online Help | *Original Reports*: Anderman and Hill, 2000; Anderman and others, 2002; and Anderman and Hill, 2003
- **HYD (Hydrograph capability):** HYD Online Help | *Original Report*: Hanson and Leake, 1999
- **IBS (Interbed Storage Package):** IBS Online Help | *Original Report*: Leake and Prudic, 1991
- **LAK (Lake Package):** LAK Online Help | *Original Report*: Merritt and Konikow, 2000
- **LMT6 (Link to the MT3DMS contaminant-transport model):** LMT6 Online Help | *Original Report*: Zheng and others, 2001
- **LPF (Layer-Property Flow Package):** LPF Online Help | *Original Report*: Harbaugh, 2005
- **MNW1 (Version 1 of Multi-Node Well Package):** MNW1 Online Help | *Original Report*: Halford and Hanson, 2002
- **MNW2 (Version 2 of the Multi-Node Well Package):** MNW2 Online Help | *Original Report*: Konikow and others, 2009
- **MNWI (Multi-Node Well Information Package):** MNWI Online Help | Original Report: Konikow and others, 2009
- **MULT (Multiplier File):** MULT Online Help | Original Report: Harbaugh, 2005
- **OBS (Observation Process):** OBS Online Help | *Original Report*: Hill and others, 2000
- **OC (Output Control Option):** OC Online Help | Original Report: Harbaugh, 2005
- **PCG (Preconditioned-Conjugate Gradient Package):** PCG Online Help | *Original Report*: Harbaugh, 2005
- **PCGN (Preconditioned Conjugate Gradient solver with improved nonlinear control):** PCGN Online Help | *Original Report*: Naff and Banta, 2008
- **PVAL (Parameter Value File):** PVAL Online Help | Original Report: Harbaugh, 2005
- **RCH (Recharge Package):** RCH Online Help | *Original Report*: Harbaugh, 2005
- **RES (Reservoir Package):** RES Online Help | *Original Report*: Fenske and others, 1996
- **RIV (River Package):** RIV Online Help | *Original Report*: Harbaugh, 2005
- **SFR (Streamflow-Routing Package):** SFR Online Help | *Original Report*: Prudic and others, 2004; and Niswonger and Prudic, 2005
- **SIP (Strongly Implicit Procedure Package):** SIP Online Help | *Original Report*: Harbaugh, 2005
- **STR (Stream Package):** STR Online Help | *Original Report*: Prudic, 1989
- **SUB (Subsidence Package):** SUB Online Help | *Original Report*: Hoffman and others, 2003
- **SWI2 (Seawater Intrusion Package):** SWI2 Online Help | *Original Reports*: Bakker and others, 2013; and SWI2 Example Problems [66MB ZIP]
- **SWR (Surface-Water Routing Process):** SWR Online Help | *Original Report* Hughes and others, 2012
- **SWT (Subsidence and Aquifer-System Compaction Package for Water-Table Aquifers):** SWT Online Help | *Original Report*: Leake and Galloway, 2007
- **UZF (Unsaturated Zone Package):** UZF Online Help | *Original Report*: Niswonger and others, 2006
- **WEL (Well Package):** WEL Online Help | *Original Report*: Harbaugh, 2005
- **ZONE (Zone File):** ZONE Online Help | Original Report: Harbaugh, 2005

https://www.usgs.gov/software/modflow-2005-usgs-three-dimensional-finite-difference-ground-water-model

MODFLOW packages in ModelMuse



Common GWF Packages (MF2005)

- Packages used to define the basic information
  - Basic package (BAS6)
  - Discretization package (DIS)
- Package that defines model layers and properties
  - Layer-Property Flow Package (LPF)
- Packages used to add/remove water at a specified rate:
  - Well (WEL)
  - Recharge (RCH)
- Package used to add/remove water based on head
  - General Head Boundary (GHB)
  - River (RIV)
  - Drain (DRN)
  - Evapotranspiration (EVT)

Prepare Model Input – MF2005

- Name file: specify the names of the input and output files, each file with a unit number and identifies the packages that will be used in the model.

```
# Name File for MODFLOW created on 3/2/2020 by ModelMuse Version 4.1.0.0
LIST               11 Grahamstown.lst REPLACE
DATA(BINARY)        9 Grahamstown.cbc REPLACE
DIS                12 Grahamstown.dis OLD
BAS6               13 Grahamstown.bas OLD
OC                 39 Grahamstown.oc OLD
DATA(BINARY)       37 Grahamstown.bhd REPLACE
DATA               38 Grahamstown.fdn REPLACE
LPF                14 Grahamstown.lpf OLD
CHD                17 Grahamstown.chd OLD
RIV                21 Grahamstown.riv OLD
DRN                22 Grahamstown.drn OLD
RCH                24 Grahamstown.rch OLD
ZONE               15 Grahamstown.zon OLD
MULT               16 Grahamstown.mlt OLD
HOB                41 Grahamstown.ob_hob OLD
DATA               42 Grahamstown.hob_out REPLACE
PVAL               52 Grahamstown.pval OLD
```

Prepare Model Input – MF2005

- DIS file: specify certain data used in all models. These include:
  - the number of rows, columns and layers
  - the cell sizes
  - the presence of Quasi-3D confining beds
  - the time discretization

• Input Instruction of DIS file

Input Instructions

Discretization information is read from the file that is specified by "DIS" as the file type.

FOR EACH SIMULATION	
Data Set 0	[#Text] Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times. ⊞ Text
Data Set 1	NLAY NROW NCOL NPER ITMUNI LENUNI ⊞ Explanation of variables
Data Set 2	⊞ LAYCBD(NLAY)
Data Set 3	DELR(NCOL) - U1DREL ⊞ DELR
Data Set 4	DELC(NROW) - U1DREL ⊞ DELC
Data Set 5	Top(NCOL,NROW) - U2DREL ⊞ Top
Data Set 6	BOTM(NCOL,NROW) - U2DREL Item 6 is repeated for each model layer and Quasi-3D confining bed in the grid. These layer variables are read in sequence going down from the top of the system. Thus, the number of BOTM arrays must be NLAY plus the number of Quasi-3D confining beds. ⊞ BOTM
FOR EACH STRESS PERIOD	
Data Set 7	PERLEN NSTP TSMULT Ss/tr [***STARTTIME*** StartingYear] ⊞ Explanation of variables

https://water.usgs.gov/ogw/modflow/MODFLOW-2005-Guide/index.html?dis.htm

Model output – MF2005

- LST file shows the basic output items, including the following:
  - Hydraulic heads
  - Drawdown
  - Flow rates
  - Water Balance
  - Optional info at specified times
  - Iteration information

Model output – MF2005

```
# Name File for MODFLOW created on 3/2/2020 by ModelMuse Version 4.1.0.0
LIST             11 Grahamstown.lst REPLACE
DATA(BINARY)      9 Grahamstown.cbc REPLACE
DIS              12 Grahamstown.dis OLD
BAS6             13 Grahamstown.bas OLD
OC               39 Grahamstown.oc OLD
DATA(BINARY)     37 Grahamstown.bhd REPLACE
DATA             38 Grahamstown.fdn REPLACE
LPF              14 Grahamstown.lpf OLD
CHD              17 Grahamstown.chd OLD
RIV              21 Grahamstown.riv OLD
DRN              22 Grahamstown.drn OLD
RCH              24 Grahamstown.rch OLD
ZONE             15 Grahamstown.zon OLD
MULT             16 Grahamstown.mlt OLD
HOB              41 Grahamstown.ob_hob OLD
DATA             42 Grahamstown.hob_out REPLACE
PVAL             52 Grahamstown.pval OLD
```

Introduction to FloPy

What is FloPy?

The FloPy package consists of a set of Python scripts to run MODFLOW, MT3D, SEAWAT and other MODFLOW-related groundwater programs. FloPy enables you to run all these programs with Python scripts. The FloPy project started in 2009 and has grown to a fairly complete set of scripts with a growing user base. FloPy3 was released in December 2014 with a few great enhancements that make FloPy3 backwards incompatible.

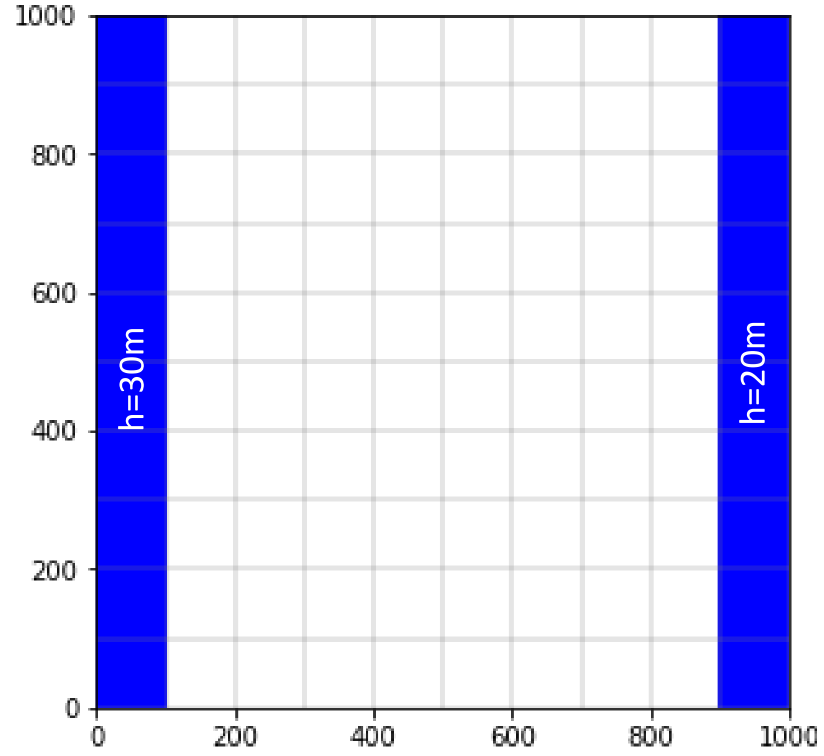
https://modflowpy.github.io/flopydoc/introduction.html

Resource for FloPy

- FloPy websites:
  - https://modflowpy.github.io/flopydoc/code.html#base-classes
  - https://github.com/modflowpy/flopy/tree/develop/examples/Notebooks
- Free blogs and tutorials from Hatari Labs:
  - https://www.hatarilabs.com/ih-en
- Course from Hatari Labs
  - https://elearning.hatarilabs.com/

Tutorial on FloPy

- Unconfined steady state flow model
  - 1000m×1000m
  - One layer, constant layer top (50m) and bottom (0m)
  - 10 rows, 10 columns
  - Constant head along first and last column
  - h=30 along 1st column and h=20 along 10th column.
- Confined steady state flow model



Unconfined steady state flow model domain