

# GRTD README

February 1, 2018

## 1 Introduction

This file describes software that supports the data and analysis in Starn and Belitz (in review) submitted to Water Resources Research (2017WR021531). This readme file describes the order of processing, required input, dependencies, and output from Jupyter Notebooks (JN) for the creation and processing of groundwater residence time distributions (GRTD) from groundwater flow models created using MODFLOW. Software and data supporting this work is available through the Science Base catalog of the U.S. Geological Survey at <https://doi.org/10.5066/F7FQ9VTD>.

### 1.1 Disclaimer

This software is preliminary or provisional and is subject to revision. It is being provided to meet the need for timely best science. The software has not received final approval by the U.S. Geological Survey (USGS). No warranty, expressed or implied, is made by the USGS or the U.S. Government as to the functionality of the software and related material nor shall the fact of release constitute any such warranty. The software is provided on the condition that neither the USGS nor the U.S. Government shall be held liable for any damages resulting from the authorized or unauthorized use of the software.

### 1.2 Dependencies

#### 1.2.1 Provided in /Data

- **P** -- shapefile of head calibration points
- **W** -- shapefile of watershed boundaries used to create the General Models
- **S** -- shapefile of sample data
- **T** -- Excel workbook containing tracer curves (TracerLPM)

#### 1.2.2 Provided in /Models

- **R** -- raster images of land surface (ned), model top (top), and model active area (ibound)
- **F** -- a MODFLOW model readable by FloPy; may include head and budget output files for some JN
- **K** -- par.csv file containing MODFLOW parameter information (created by General Model JN4)

### 1.2.3 Created in these JNs

- **M** -- MODPATH endpoint file
- **A** -- tau.txt file containing mean age and recharge information

## 2 GRTD JNs

Some JN are meant to be run on individual models and others are meant to process a number of models at once in batch mode. In either case, the model(s) to be processed are those that have .nam files in a directory in the homes directory list. Results from JN are in model directories (Individual) or fig\_dir (Batch). The assignment of directory names in homes and fig\_dir is made in each JN. Curly braces {} in file names below mean that the file is created in individual model directories and the braces are to be replaced with the model name.

- MODFLOW model output is required and can be created by executing the runMF.ipynb.
- The number and letter at the beginning of each JN name indicates the suggested order of processing; however, JN can be run in any order if the required input is present.
- These JN were used to generate figures in Starn and Belitz (in review). The figure number is listed in the description section.

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### 2.1 01a Calculate flux-weighted whole aquifer--Particles.ipynb

*Individual*

#### 2.1.1 Input

- **F**

#### 2.1.2 Output

- **M, A**

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### 2.2 01b Calculate flux-weighted whole aquifer--RTDs.ipynb

*Individual*

#### 2.2.1 Input

- **F, M, A**

#### 2.2.2 Output

- fit\_dict\_res\_all\_layers.pickle
- plots

### 2.2.3 Description

- `fit_dict_res_all_layers.pickle` contains all the information about particle travel times and the RTDs that fit them.
  - Plots show fits to individual models for all distributions including mixtures
  - Figure 6 shows plot for model number 4.
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## 2.3 02 General Model model summary.ipynb

*Batch*

### 2.3.1 Input

- F, A, K

### 2.3.2 Output

- `master_modflow_table.csv`
- `tau_summary.csv`

### 2.3.3 Description

- `master_modflow_table.csv` contains a summary of explanatory features in multiple models
  - `tau_summary.csv` contains a concatenation of individual `tau.txt` files
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## 2.4 03 Age grids and sections.ipynb

*Individual*

### 2.4.1 Input

- F, M

### 2.4.2 Output

- plots

### 2.4.3 Description

- Plots show maps and cross sections of age and head
  - Figure 3 shows plots of age for model number 4
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## 2.5 04 Compile multi-model head residuals.ipynb

*Batch*

### 2.5.1 Input

- $P, W, F$

### 2.5.2 Output

- `head_resid_df.csv`
- `plots`

### 2.5.3 Description

- `head_resid_df.csv` contains head residual information for multiple models
  - Figure 2 shows boxplots of residuals by model
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## 2.6 05 Plot boxplots of multi-model distribution fits.ipynb

*Batch*

### 2.6.1 Input

- `fit_dict_res_all_layers.pickle`

### 2.6.2 Output

- `rtd_error_all_layers_summary.csv`
- `plots`

### 2.6.3 Description

- `rtd_error_all_layers_summary.csv` contains the RMSE errors for all fitted distributions for multiple models
  - Figure 4 shows boxplots of RMSE errors for multiple models
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## 2.7 06 Plot multi-model RTDs.ipynb

*Batch*

### 2.7.1 Input

- $A, W$
- `fit_dict_res_all_layers.pickle`

### 2.7.2 Output

- `weib_and_exp_fit.csv`
- `plots`

### 2.7.3 Description

- `weib_and_exp_fit.csv` contains parameters and errors on Weibull and exponential fits
  - Figure 5 shows XY plots of RTD from multiple models.
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## 2.8 07a Calculate flux-weighted whole aquifer--Process Wells.ipynb

*Batch*

### 2.8.1 Input

- $F, S, R, W$

### 2.8.2 Output

- `node_df.csv`
- `well_gdf.shp`
- `sample_gdf.shp`
- `plots`

### 2.8.3 Description

- `sample_gdf.shp` contains point locations and sampling data
  - `well_gdf.shp` contains point locations and well construction details
  - `node_df.csv` contains well information for each model layer the well penetrates
  - `well_diagrams` is a directory that contains plots of well construction
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## 2.9 07b Calculate flux-weighted whole aquifer--Well RTDS.ipynb

*Batch*

### 2.9.1 Input

- $F, M$
- `node_df.csv`
- `well_gdf.shp`
- `sample_gdf.shp`

### 2.9.2 Output

- `fit_dict_wells_{}.pickle`

### 2.9.3 Description

- `fit_dict_wells_{}.pickle` contains the distribution parameters at well cells
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## 2.10 08 Plot BTCs and sample.ipynb

*Batch or individual*

### 2.10.1 Input

- T
- fit\_dict\_wells\_{}.pickle

### 2.10.2 Output

- sample\_dict\_wells.csv (batch)
- plots (individual)

### 2.10.3 Description

- sample\_dict\_wells.csv is created in individual model directories and contains sample information, simulated equivalent concentrations, and the optimal porosity that produced them
  - Figure 8 shows an XY plot of  $^3H$  breakthrough in two wells in model number 4
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## 2.11 09 Plot Observed and Simulated Tracers with porosity adjusted.ipynb

*Batch*

### 2.11.1 Input

- sample\_dict\_wells.csv

### 2.11.2 Output

- master\_sample\_fit.csv
- trit\_fit\_df.csv
- plot

### 2.11.3 Description

- master\_sample\_fit.csv contains a concatenation of sample\_dict\_wells.csv from all individual models
  - trit\_fit\_df.csv contains the results of the Kendall Tau statistical test
  - Figure 7 shows XY plot of  $^3H$  residuals
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## 2.12 10 Create and plot RTD metamodel.ipynb

*Batch*

### 2.12.1 Input

- **W**
- `master_modflow_table.csv`
- `weib_and_exp_fit.csv`

### 2.12.2 Output

- plots

### 2.12.3 Description

- Figure 9a shows XY plot showing results of LASSO tuning
  - Figure 9b shows XY plot showing fitted parameters versus independent variables (labels)
  - Figure 9c shows bar chart showing importance of variables
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## 2.13 11 Create and plot RTD poly metamodel.ipynb

same as above but with quadratic expansion of the explanatory features

Figure 10a-c shows results