RDAVT

version 1.1.4 manual

Software release (https://code.usgs.gov/water/espd/hgb/rdavt)

Web application (https://rconnect.usgs.gov/RDAVT/)

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This app was developed to support the interpretation of datasets acquired using the Mobile-Immobile Porosity Exchange Tool (Mi-PET) that was designed and prototyped as part of Environmental Security Technology Certification Program (ESTCP) project ER201732. However, it can be applied to any dataset where tracer tests are monitored with electrical geophysical methods during the injection of an electrical tracer. Example previous applications of geoelectrical inference of dual domain mass transfer where DVAT might be applied to quickly interpret datasets include in laboratory column experiments (Swanson et al., 2015), in stream beds for understanding redox dynamics (Briggs et al., 2018) , in the field to better understand uranium transport (Briggs et al., 2013), in the field to understand hyporheic flow systems (Singha et al., 2008) and deeper in the Earth for understanding managed aquifer recharge (Singha et al., 2008).

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Purpose

RDAVT is an R Shiny-based app used to estimate immobile porosity (θ_{im}), mobile porosity (θ_m), and the mass transfer rate coefficient (α) in dual-domain porosity media using the method of geoelectrical inference (Briggs et al., 2014). These properties can be difficult to assess by traditional methods but can play an important role in the success of remediation efforts, as contaminant rebound may occur following cleanup from solute stored in the immobile porosity domain (back diffusion). This app allows for interactive fitting of the fluid versus bulk conductivity hysteresis curve from electrical tracer experiments using the semi-analytic graphical approach of Briggs et al. (2014) to provide near real-time estimates of θ_{im}, θ_m, and α based on user inputs. Such an approach can not only be used to provide estimates of these key parameters, but also to gauge uncertainty by observing how changes to inputs (within reasonable expected ranges) affects output estimates of θ_{im}, θ_m, and α. These parameter estimates can then be used as input to groundwater flow modeling software such as MODFLOW (Langevin et al., 2017).

This app was developed to support the interpretation of datasets acquired using the Mobile-Immobile Porosity Exchange Tool (Mi-PET) that was designed and prototyped as part of Environmental Security Technology Certification Program (ESTCP) project ER201732. However, it can be applied to any dataset where tracer tests are monitored with electrical geophysical methods during the injection of an electrical tracer. Example previous applications of geoelectrical inference of dual domain mass transfer where DVAT might be applied to quickly interpret datasets include in laboratory column experiments (Swanson et al., 2015), in stream beds for understanding redox dynamics (Briggs et al., 2018) , in the field to better understand uranium transport (Briggs et al., 2013), in the field to understand hyporheic flow systems (Singha et al., 2008) and deeper in the Earth for understanding managed aquifer recharge (Singha et al., 2008).

Installation

RDAVT is available as a web-based app. To use the software, one simply needs internet access and to follow this link https://rconnect.usgs.gov/RDAVT/. The web application should run from most phones and tablets, but it is recommended to use a web browser from a desktop PC for visibility.

The source R code is available in the public U.S. Geological Survey (USGS) software release packaged with this manual (https://code.usgs.gov/water/espd/hgb/rdavt, (Terry & Day-Lewis, 2023). The software release contains a tutorial video and example input files. Use of the code will require the user to install R and required libraries as described in the code documentation. It is also recommended the user install an integrated development environment such as Rstudio. R/Rstudio are available for free across several computer platforms (MacOS, Windows, Linux). In this document, any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

Needed data

- Bulk electrical conductivity and fluid electrical conductivity over time during injection and flush of an electrical tracer. Missing values are not allowed.
- Total porosity and a cementation exponent must be known (or assumed).

The specifications of the tracer will depend on the groundwater specific conductance encountered at the site. In some cases, the ‘tracer’ might be a natural change in specific conductance, e.g., salinity changes associated with tidal forcing, or salinity changes associated with groundwater discharging into streambed sediments. In the case of direct injection of a tracer, a specific conductance contrast of two orders of magnitude or more with the native groundwater is recommended. The more common scenario is injection of an electrically more conductive tracer, although injection of relative resistive tracers is also feasible, and more appropriate in certain situations, e.g., investigations in saline coastal aquifers or highly contaminated aquifers. Assuming an electrically conductive tracer, a simple ionic solution such as sodium bromide is preferred. The major ion chemistry is not important and can be adjusted to best represent the groundwater chemistry of the field site.

The mass transfer rate coefficient (α) determined from the geoelectrical tracer test is specific to the ionic tracer utilized in the test. This coefficient is related to the molecular diffusion coefficient of the solute and a characteristic length scale (λ),

$$\alpha = \frac{D}{\lambda^2}. \qquad (1)$$

Exchange rate coefficients for different solutes are directly related to one another via,

$$\alpha_2 = \alpha_1 \frac{D_2}{D_1}, \qquad (2)$$

where subscripts 2 and 1 represent two different solutes. Thus, if α is determined for one solute using a tracer test, then the equivalent α for a solute of interest (e.g., a contaminant) can be determined knowing the diffusion coefficients of the two solutes.

Introduction

Soils and rock may have variable porosity at different scales that can be critically important, for example, at contaminated sites where contaminant rebound following cleanup is observed. This effect can sometimes be explained by back-diffusion, wherein contaminant stored in a low permeability rock/soil matrix porosity (immobile or less-mobile porosity domain) diffuses back into fractures or more permeable materials (mobile porosity domain). The concept of dual domain porosity media is shown in Figure 1.

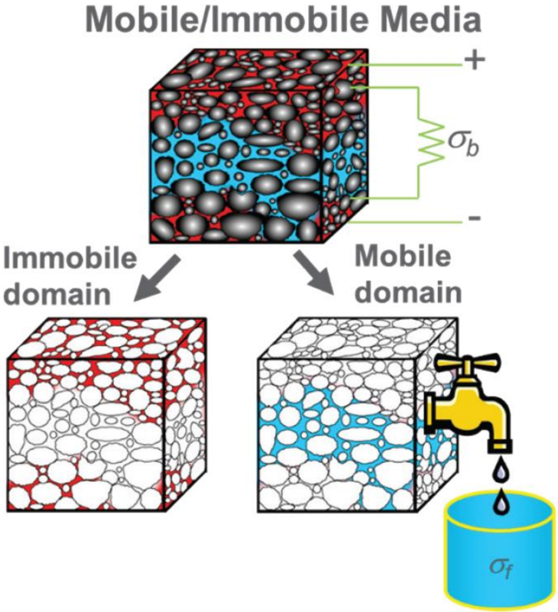


Figure 1 – conceptual diagram of dual domain porosity media. Measured fluid electrical conductivity is sensitive to the mobile domain, while measured bulk electrical conductivity (as from geophysics) is sensitive to all porosity domains (mobile and immobile).

Various studies have demonstrated the use of electrical tracer experiments to characterize dual-domain porosity media. In these experiments, the injection and flush of an electrical tracer is monitored through time with both geophysics (that measures bulk electrical conductivity, sensitive to both mobile and immobile domains) and fluid sampling (that measures fluid electrical conductivity, sensitive to the mobile domain only). A schematic of such an experiment is shown in Figure 2. In cases where dual-domain porosity exists, a characteristic hysteretic curve is revealed when fluid versus bulk conductivity is plotted for both injection and flush phases of the experiment. The shape of this curve is an indicator of dual-domain porosity parameters - larger vertical sections of the hysteresis curve indicate a larger immobile domain, while the lack of any vertical sections suggests no significant immobile porosity. An example hysteresis curve is shown in Figure 3. The “hinge points” (corners) of this curve indicate four key moments in a tracer injection/flush experiment: the starting bulk conductivity before electrical tracer injection ($\sigma_{b,0}$), the bulk conductivity after the mobile domain is saturated with tracer ($\sigma_{b,1}$), the bulk conductivity after the immobile domain is entirely saturated with tracer ($\sigma_{b,2}$), and the bulk conductivity after the mobile domain has been flushed of tracer ($\sigma_{b,3}$). Further information is provided in the “Implementation” section of this document.

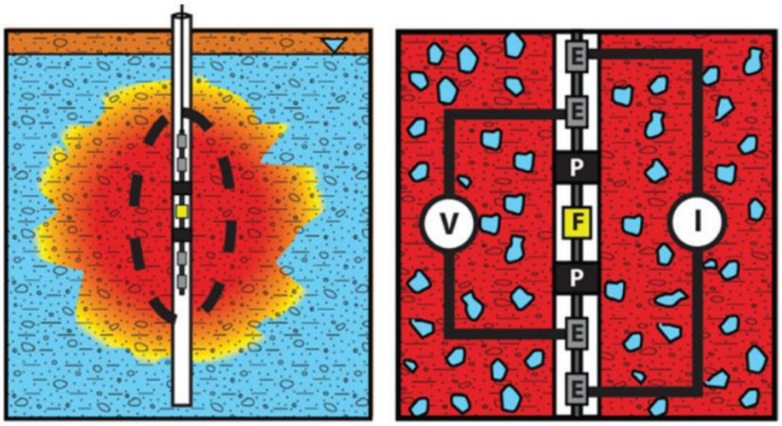


Figure 2 – conceptual diagram of a field borehole electrical tracer experiment. Solute injection/extraction and measurement of fluid electrical conductivity takes place (F). Bulk electrical conductivity is measured at electrodes (E). Packers (P) separate the electrodes from the fluid injection/measurement point.

Details

Briggs et al. (2014) provide a complete description of how 1D advective-dispersion transport partial differential equations describing dual-domain mass transfer can be coupled with a bi-continuum extension of the classical Archie model (Singha et al., 2008). For the (Briggs et al., 2014) semi-quantitative, graphical approach to estimate immobile porosity (θ_{im}), mobile porosity (θ_m), and the mass transfer rate coefficient (α), RDAVT solves the following ordinary differential equation,

$$\frac{\partial \sigma_b}{\partial t} = \theta^{q-1} \left\{ \theta_m f'(t) + \alpha \left[f(t) - \left(\frac{\sigma_b / \theta^{q-1} - \theta_m f'(t)}{\theta_{im}} \right) \right] \right\} f'(t) \qquad (3)$$

where,

σ_b, bulk electrical conductivity [Siemens/L]

$\sigma_m = \sigma_f$, electrical conductivity of the mobile domain = fluid electrical conductivity

$f(t)$, a differentiable function approximating σ_m through time ($\frac{\partial \sigma_m}{\partial t}$) as it approaches equilibrium

$f'(t)$, derivative of $f(t)$

t, time [T]

θ_m, mobile porosity [-]

θ_{im}, less mobile porosity [-]

$\beta = \frac{\theta_{im}}{\theta_m}$, distribution coefficient, ratio of immobile to mobile porosity [-]

$\theta = \theta_m + \theta_{im}$, total porosity [-]

q, cementation exponent [-]

α, mass transfer rate coefficient [1/T]

β is the ratio of immobile to mobile porosity, and is computed (in this approach) by fitting of hinge points to the hysteresis curve (Figure 3) which provide four bulk electrical conductivity values: the starting bulk conductivity before electrical tracer injection ($\sigma_{b,0}$), the bulk conductivity after the mobile domain is saturated with tracer ($\sigma_{b,1}$), the bulk conductivity after the immobile domain is saturated with tracer ($\sigma_{b,2}$), and the bulk conductivity after the mobile domain has been flushed of tracer ($\sigma_{b,3}$). Either the "rising limb" corresponding to the injection phase of the experiment can be used to estimate beta (as shown in Figure 3), or the "falling limb" from the flush phase of the experiment. An estimate of beta from the rising limb is computed as $\beta = (\sigma_{b,2} - \sigma_{b,1})/(\sigma_{b,1} - \sigma_{b,0})$, while for the falling limb beta is computed as $\beta = (\sigma_{b,3} - \sigma_{b,0})/(\sigma_{b,2} - \sigma_{b,3})$.

Implementation

Step 1: Provide total porosity and the Archie cementation exponent, both of which must be known (or assumed) for analysis to proceed. Laboratory electrical resistivity experiments of cores can be performed to ascertain these values, or literature values may be used. The Archie cementation exponent is essentially a measure of the connectivity of the pore space and varies over a relatively small range (Glover, 2009). Most porous sediments, including unconsolidated sediments and sandstones, have cementation exponents between 1.5 and 2.5, whereas values higher than 2.5 (and as high as 5) are found for carbonates and mudstones where the pore space is less well connected (Glover, 2009).

Step 2: Upload tables of time and paired bulk-fluid electrical conductivity data from both injection and flush phases of an electrical tracer experiment. Each of these files is a three-column, space separated ascii file with no header with time, fluid EC, and bulk EC as columns. See Step 2a.

Step 3: Hinge point fitting of hysteresis curve for immobile/mobile porosity (beta) estimation. The graphical fitting of this curve, combined with the user-provided estimate of total porosity, provides outputs of immobile and mobile porosity. See Figure 3. (Briggs et al., 2014) provide a detailed, illustrated explanation of how hinge points of the hysteresis curve are used to calculate beta. In this step, the user clicks and drags the four hinge points to fit to the corners of the hysteresis curve.

Step 4: Choice of data range for alpha estimation (injection or flush). The user must interactively choose the range of injection or flush data that are used to estimate $f(t)$ and $f'(t)$ based on σ_f data. This is done by clicking and dragging lines on the plots of the datasets to select the range of data that will be used. It is generally recommended to include as much data as possible while still obtaining a good model fit as described in Step 5.

Step 5: From here RDAVT will solve for $\frac{\partial \sigma_b}{\partial t}$ and can therefore provide estimates of σ_b through time which can be compared to actual data. Similarly, the estimate of $f(t)$ as an approximation of $\frac{\partial \sigma_m}{\partial t}$ can be compared to actual σ_f data. "Fits" of these models are evaluated through the squared Kendall rank correlation coefficient (R^2). The user is advised to visually examine the σ_f and σ_b model fit curves to assess whether the models are reasonable (i.e., do the model fit curves approximately match the data?) and not to assume that higher reported model fit values equate to better models.

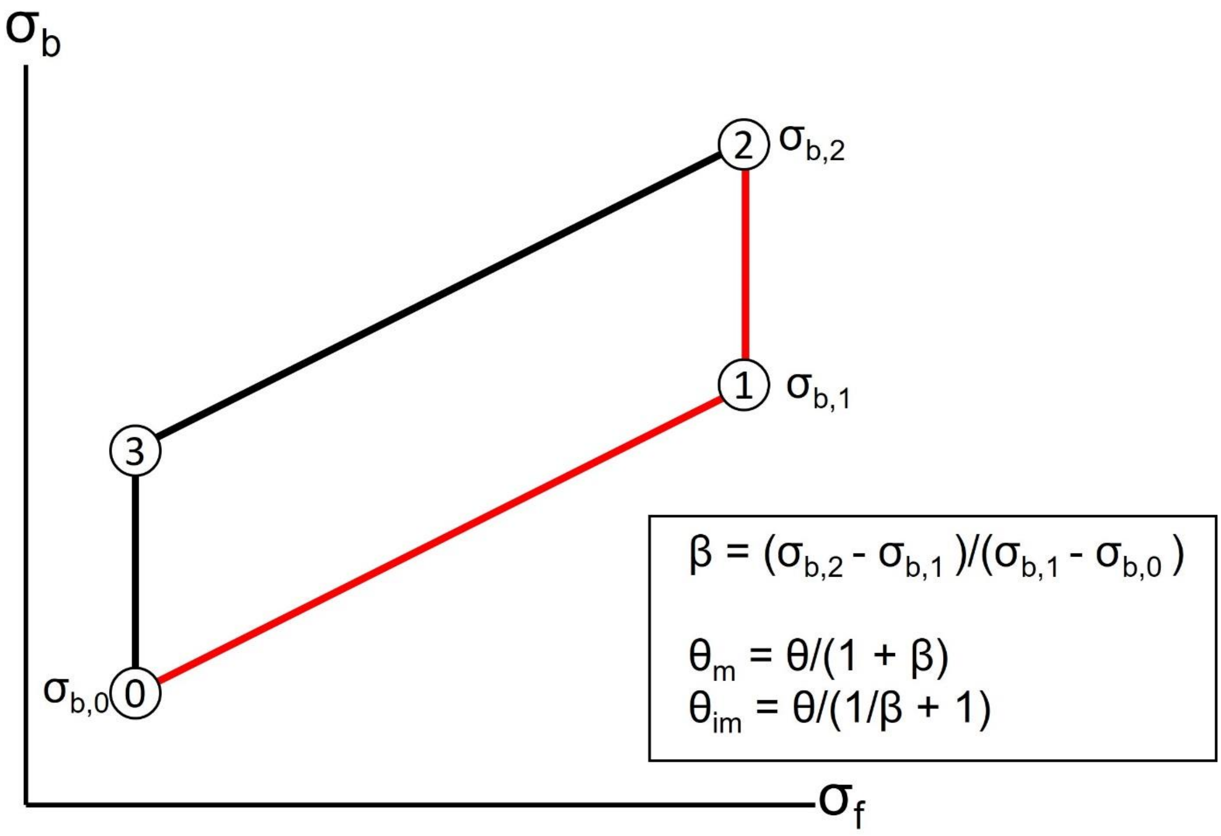


Figure 3 – Computation of mobile and immobile porosity from fitting of hinge points on the hysteresis curve.

Recommended approach

After inputting needed parameters and data (Steps 1-2), it is recommended the user explore a sensitivity analysis of output immobile porosity (θ_{im}), mobile porosity (θ_m), and the mass transfer rate coefficient (α) to reasonable changes in the graphical inputs. For example, if both flush and injection phase data appear free of problems, it is advised to test both options for alpha estimation. It is also advised to experiment with the portion of the injection or flush curve that is used for alpha estimation.

It is also recommended to experiment with using both “rising limb” and “falling limb” for beta estimation, and interactively adjust the hinge points to observe the effects on output parameters – see steps 3 and 5 below.

At any point during the analysis, the user can “save” the current RDAVT state to file by pressing the “save DAVT state” button. The saved output is a text file that contains all parameters and inputs used by RDAVT. Saved state files can be later loaded back into RDAVT by pressing the “load DAVT state” to restore a previously saved state.

Example of recommended approach with test data set

Initial DAVT screen: adjust browser scaling if inputs/outputs seem jumbled


MI-PET Data Analysis and Visualization Tool (DAVT)

α estimation: flush

β estimation: rising limb

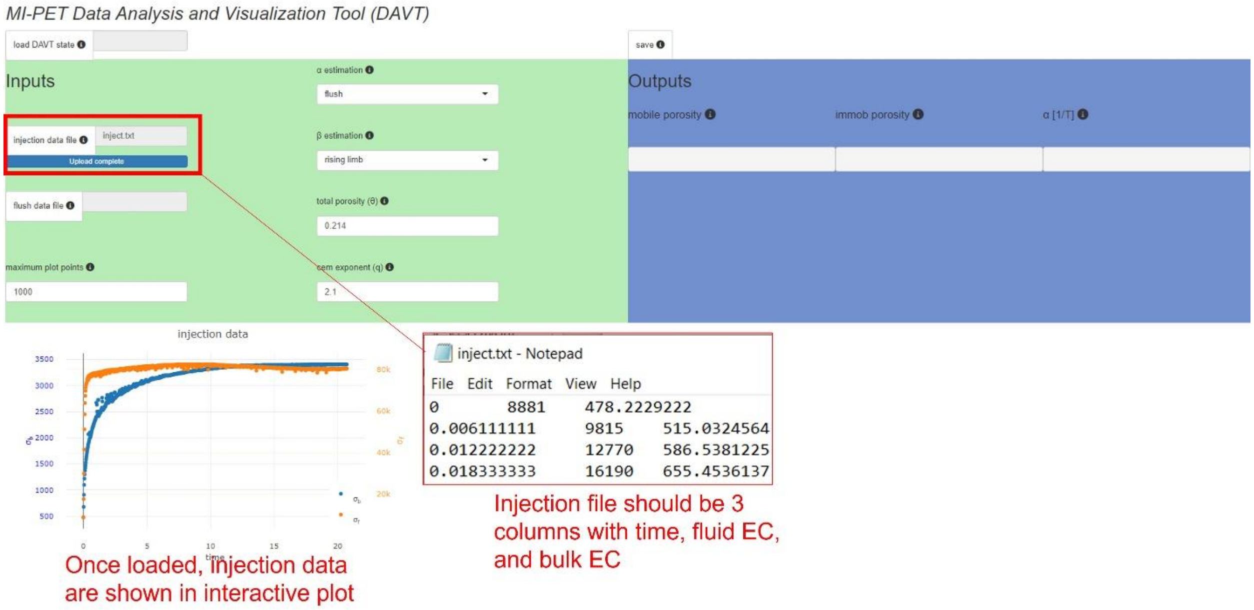
total porosity (θ): 0.214

cem exponent (q): 2.1

maximum plot points: 1000

User should update total porosity and cementation exponents

Step 1: enter porosity and cementation exponent



MI-PET Data Analysis and Visualization Tool (DAVT)

Inputs

injection data file: inject.txt

Upload complete

maximum plot points: 1000

α estimation: flush

β estimation: rising limb

total porosity (θ): 0.214

cem exponent (q): 2.1

Outputs

inject.txt - Notepad

```
0	8881	478.2229222
0.006111111	9815	515.0324564
0.012222222	12770	586.5381225
0.018333333	16190	655.4536137
```

Injection file should be 3 columns with time, fluid EC, and bulk EC

Once loaded, injection data are shown in interactive plot

Step 2a: load solute injection phase data

Once both injection and flush data are loaded, outputs are interactively updated based on user adjustments

MI-PET Data Analysis and Visualization Tool (DAVT)

Inputs

injection data file: inject.txt

Upload complete

flush data file: flush.txt

Upload complete

maximum plot points: 10000

α estimation: flush

β estimation: rising limb

total porosity (θ): 0.214

cem exponent (q): 2.1

Outputs

mobile porosity: 0

immob porosity: 0.214

α [1/T]: 0.822

Step 2b: load solute flush phase data

MI-PET Data Analysis and Visualization Tool (DAVT)

load DAVT state

save

Inputs

injection data file: inject.txt (Upload complete)

flush data file: flush.txt (Upload complete)

maximum plot points: 10000

α estimation: flush

β estimation: rising limb

total porosity (θ): 0.214

cem exponent (q): 2.1

Outputs

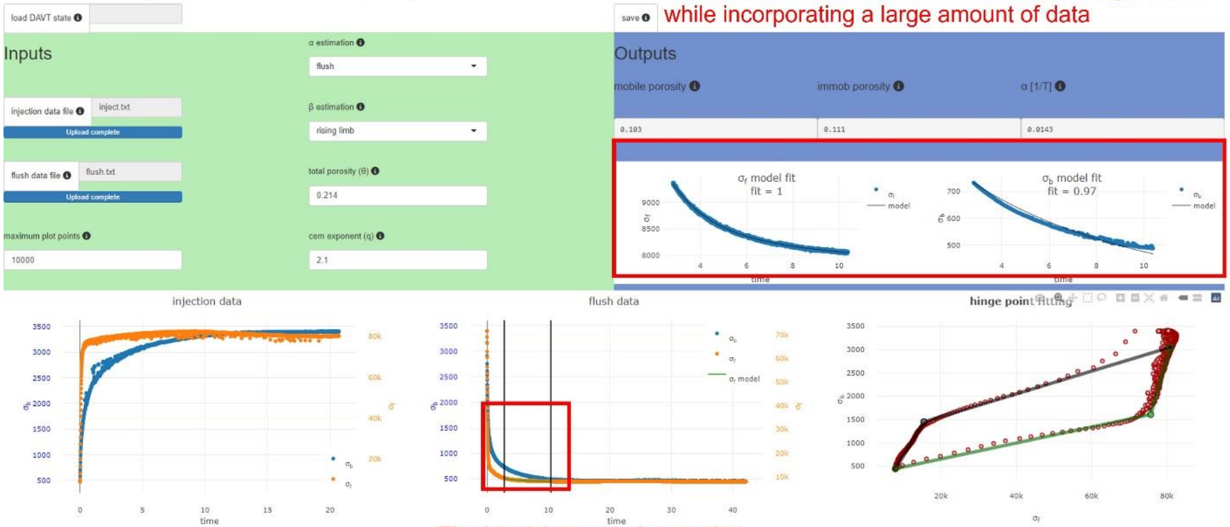
mobile porosity: 0.103

immob porosity: 0.111

α [1/T]: 0.108

To refine estimates of mobile/immobile porosity, adjust hingepoints of the hysteresis curve; note only the "rising limb" or "falling limb" of this curve is used, depending on user input

Step 3: fit hinge points (corners) of hysteresis curve. This is performed by clicking and dragging the black circles in the plot. It is generally recommended to fit the linear sections of the plot (as in the figure) as opposed to the actual corners.



Adjustment of the time region will show updated fluid and bulk EC model fits. One should aim for good fits while incorporating a large amount of data

MI-PET Data Analysis and Visualization Tool (DAVT)

load DAVT state

save

Inputs

injection data file: inject.txt (Upload complete)

flush data file: flush.txt (Upload complete)

maximum plot points: 10000

α estimation: flush

β estimation: rising limb

total porosity (θ): 0.214

cem exponent (q): 2.1

Outputs

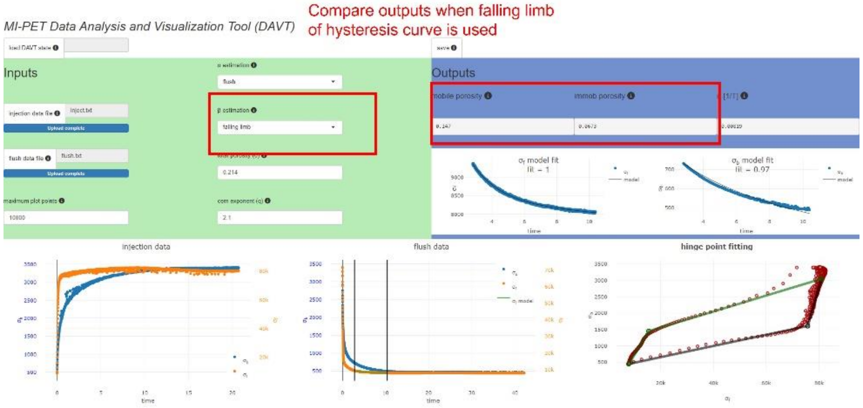
mobile porosity: 0.103

immob porosity: 0.111

α [1/T]: 0.0143

The black bars can be used to select the time region for fitting models to fluid EC and bulk EC data.

Step 4: Adjust time range for fluid and bulk EC model fits. Note that for the selected data, good fits are achieved for both fluid electrical conductivity and bulk electrical conductivity models, with fit values close to one and model fits that closely resemble the data. The time range should be selected in a balance of including as much data as possible while still achieving good fits.



Compare outputs when falling limb of hysteresis curve is used

MI-PET Data Analysis and Visualization Tool (DAVT)

Inputs

injection data file: inject.txt

flush data file: flush.txt

maximum plot points: 10000

α estimation: flush

β estimation: falling limb

total porosity (ϕ): 0.214

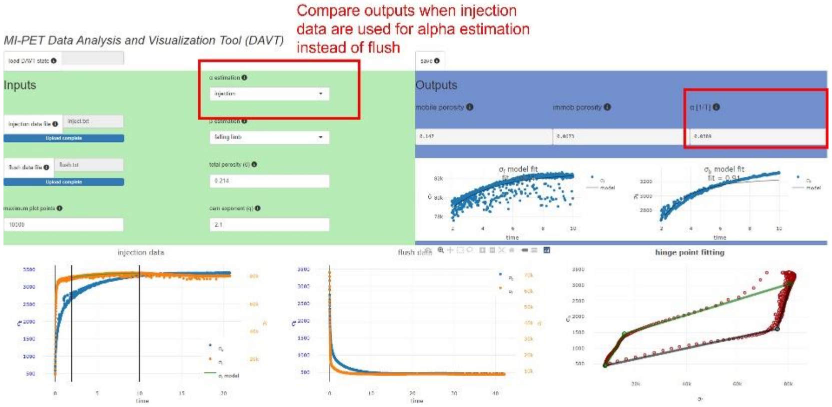
cem exponent (q): 2.1

Outputs

mobile porosity: 0.147

immob porosity: 0.0673

α [1/T]: 0.00819



Compare outputs when injection data are used for alpha estimation instead of flush

MI-PET Data Analysis and Visualization Tool (DAVT)

Inputs

injection data file: inject.txt

flush data file: flush.txt

maximum plot points: 10000

α estimation: injection

β estimation: falling limb

total porosity (ϕ): 0.214

cem exponent (q): 2.1

Outputs

mobile porosity: 0.147

immob porosity: 0.0673

α [1/T]: 0.0189

Step 5: Compare outputs using different combinations of flush/injection data & rising/falling limb

Concluding remarks

This software tool is intended to facilitate estimation of immobile porosity (θ_{im}), mobile porosity (θ_m), and the mass transfer rate coefficient (α) in dual-domain porosity media from electrical tracer experimental data. Required data include bulk electrical conductivity and fluid electrical conductivity over time during injection and flush of an electrical tracer, as well as estimates of petrophysical properties including total porosity and the cementation exponent. Values for these properties may need to be determined from separate experimentation.

The semi-analytic model fitting used by this software assumes that an Archie-type relation between measured bulk electrical conductivity and fluid conductivity and petrophysical properties is valid. Further, two extreme porosity domains (mobile and immobile) are assumed, though it is possible that there could be intermediate porosity domains that influence data.

The various user choices available in the software will affect output – the placement of the hysteresis curve hinge points, the time range of injection or flush data used, whether the rising or falling limb of the hysteresis curve is used, and of course estimates of porosity and the cementation exponent. That is why it is recommended for the user to perform basic sensitivity analysis of how their various choices affect the output values (θ_{im},θ_m,α); thereby providing some estimate of the uncertainty and reliability of the estimates produced from this tool. The interactive nature of RDAVT allows such an analysis to be quickly performed.

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