

Sphere Centers and Conductivity Data. The directory “sphere_locations” contains information on the 203 low-conductivity spheres used in the experiment. The file “sphere_centers_conductivity.csv” contains a plain-ASCII text file in comma separated value (CSV) format which indicates the location, hydraulic conductivity, and porosity for each of the. The data are stored in the following order (by column). The data set contains 2 header lines as follows:

```
%% Sphere Number   Sphere ID      x      y      z      K      Porosity
%% (n/a)          (n/a)         (cm)   (cm)   (cm)   (cm/min) (n/a)
(+ 203 lines of data)
```

Here, “Sphere Number” is an index (1-203) used only to reference the data set; “Sphere ID” is a unique ID number for each of the 203 spheres (note that Sphere Number and Sphere ID are not the same!); x, y, and z are the coordinate values for locating the center of the spheres, K is the hydraulic conductivity. The second line contains the units for the data (if applicable). Note that there are no spheres with ID numbers 35, 106, 107, 108, 127, 129, 130, 132, 136, 146, 153, 157, 160, 168, 183, 192, 217, and 219. Spheres with these ID numbers were not used in the experimental system.

The file “sphere_map.csv” is a CSV formatted file that contains the identification of each sphere (by ID number) used to create the flowcell. These data are arranged as information for sphere centers, organized in y-z planes (i.e, the centers are located on a grid; there are 10 such grids locating the y-z position for a specified plane perpendicular to the x-axis). To help better understand these data, the file “flow_cell_geometry.pdf” contains an image illustrating how the flow cell was sectioned into 10 planes (located at x = 2.5, 7.5, 12.5, 17.5, 22.5, 27.5, 32.5, 37.5, 42.5, and 47.5 cm). The file “sphere_map.csv” can be used with the file “sphere_centers_conductivity.csv” to determine the hydraulic conductivity of each sphere in the flow cell. NOTE: In the paper associated with this work, an averaged value of the hydraulic conductivity for the low-conductivity spheres was used for the spheres rather than each measured value.

Breakthrough Curve Data. The breakthrough curve data for both fluorescein and for lithium are presented in the file “breakthrough_conc.csv”. This file is a CSV-formatted file containing three header lines. The three header lines include the following information

```
%% number_spheres      203
%% average_Q          5.59 ml/min
%% Time (hr)   Fluorescein Concentration (ppm)   C/Co   Time (hr)   Li+
              (C/Co)
```

Where the headers are self-explanatory and correspond to the 5 columns of data. After the three header lines are 435 lines of data corresponding to the time-concentration data set. NOTE. There are many fewer data for lithium (86 times) than for fluorescein (435 times).

Mesh Data. The mesh data in this repository appears in two formats. The first is exported as a NASTRAN file, one of the formats natively exported from COMSOL. The NASTRAN file (.nas) is an ASCII formatted file that can be read by many open-source mesh tools including the tool GMSH (<http://gmsh.info/>) which is available for most operating systems. The NASTRAN format itself is well-documented in many sources; the Wikipedia entry (<https://en.wikipedia.org/wiki/Nastran>) is one stable resource that contains a substantial description of the format. The original NASA source code was available (as of 1 January 2018) on GitHub (<https://github.com/nasa/NASTRAN-93>). This also provides documentation that can be used to interpret the NASTRAN format.

The second file format is the “.msh” format, which is also an ASCII-formatted file, and it represents the proprietary output format for the open-source mesh-handling software GMSH (<http://gmsh.info/>).

COMSOL Models. In the subdirectory “comsol_models” both native COMSOL model formatted (“.mph”) and MATLAB format (“.m”) files are provided for (1) the fully-resolved flow cell (3D), (2) the simplified flowcell (3D), and (3) the averaged model (1D). The files are stored in COMSOL 5.3a format. They will be readable with version 5.3a or later, but they are not reverse compatible with earlier versions of COMSOL. The “.m” formatted files can be run in MATLAB if the appropriate COMSOL libraries are loaded.