Groundwater

Technology Spotlight/ David Lipson, Technology Editor

Fitting the Transport and Attachment of Dense Biocolloids in One-Dimensional Porous Media: ColloidFit

Vasileios E. Katzourakis[1] and Constantinos V. Chrysikopoulos[2]

The ColloidFit is autonomous, modular, multipurpose curve fitting software for colloid and biocolloid (e.g. viruses and bacteria) fate and transport phenomena in porous media, which is accompanied by an intuitive and easy to use graphical user interface. The initial version of ColloidFit was developed by Sim and Chrysikopoulos

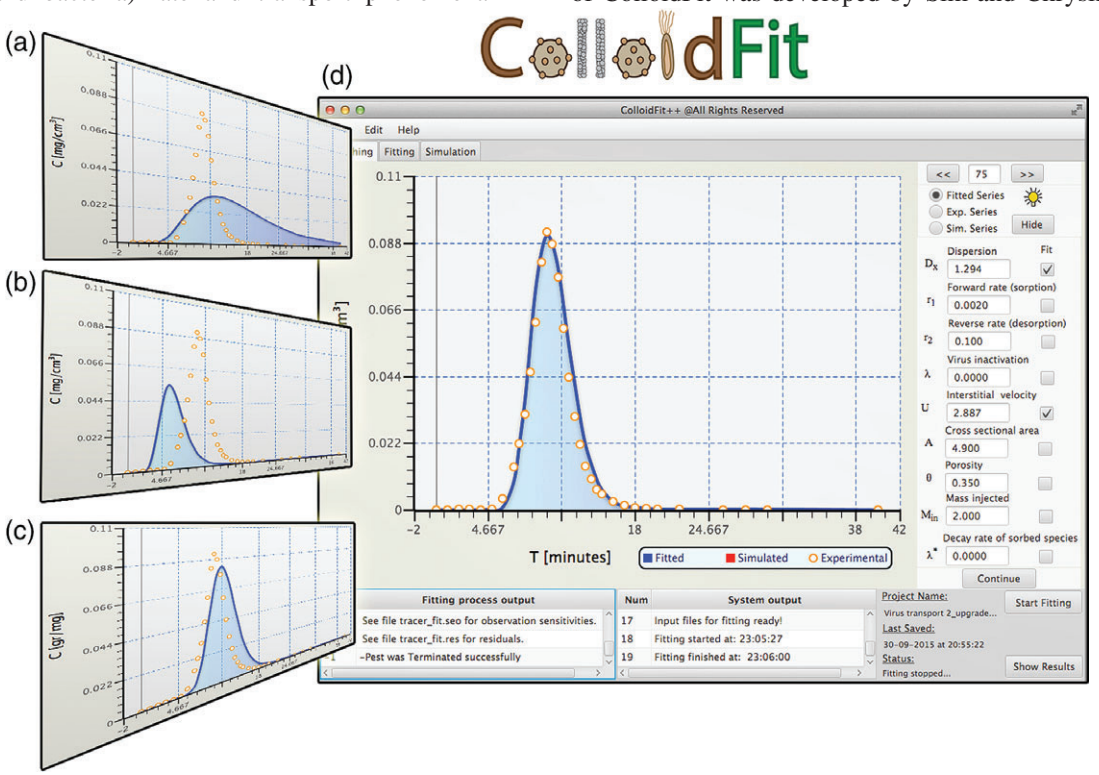

Figure 1. The "Graphing" tab during: (a)–(c) early stages of the fitting process, and (d) when the fitting procedure is successfully completed.

[1]Environmental Engineering Laboratory, Civil Engineering Department, Fokionos Street, University of Patras, Patras 26500, Greece

[2]Corresponding author: School of Environmental Engineering, Technical University of Crete, Building K1, Chania 73100, Greece; cvc@enveng.tuc.gr

Received December 2016, accepted December 2016.

doi: 10.1111/gwat.12501

(1995). Because then it was improved several times, now it can simulate: (1) the migration of suspended colloid or biocolloid particles in one-dimensional water saturated, homogeneous porous media with uniform flow, accounting for equilibrium or nonequilibrium attachment onto the solid matrix, as well as gravitational effects; and (2) the attachment of colloids and biocolloids onto solids under batch conditions (Keller et al.

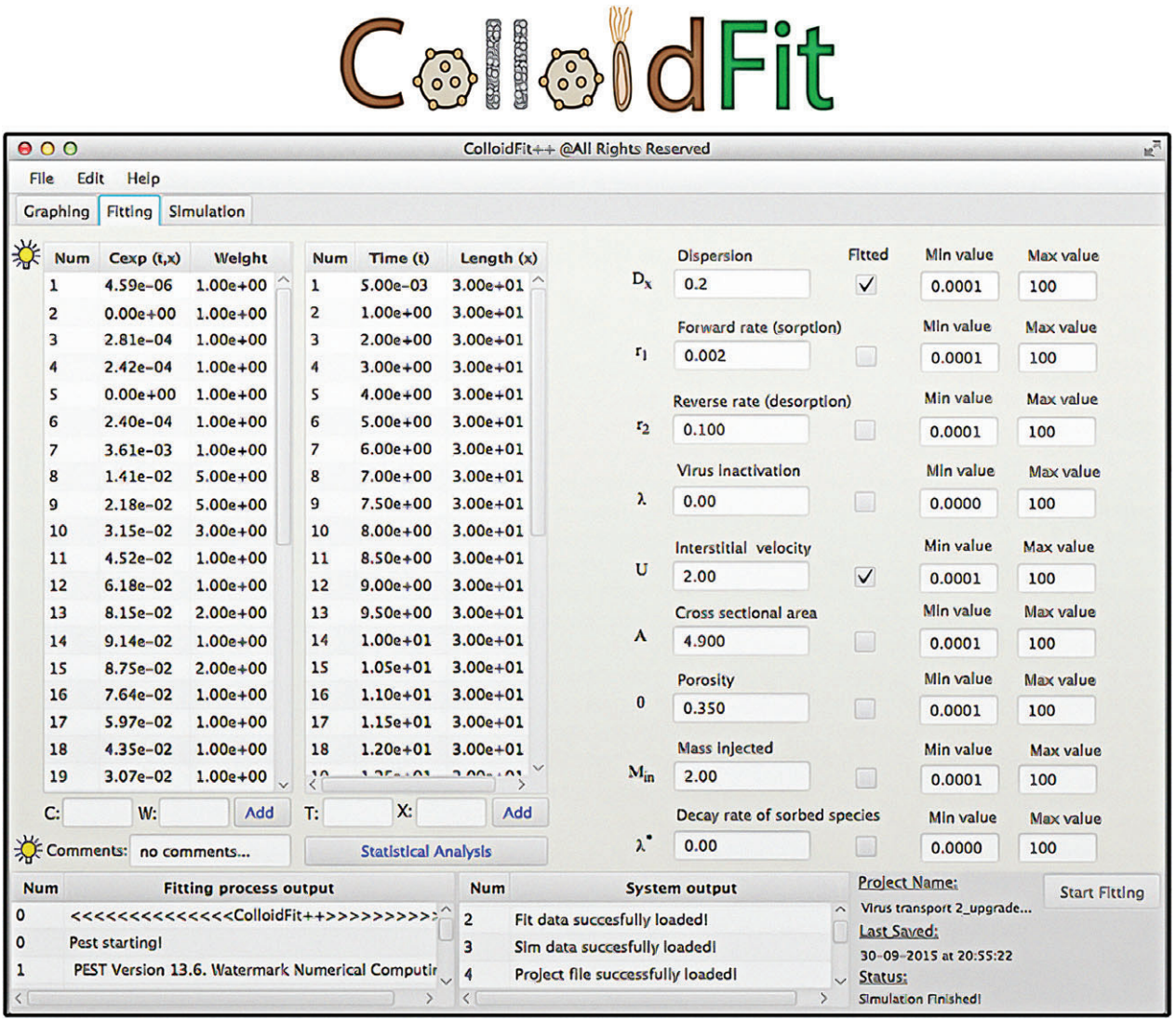

Figure 2. The user interface of the "Fitting" tab.

2004; Anders and Chrysikopoulos 2005; Syngouna and Chrysikopoulos 2011; Chrysikopoulos and Syngouna 2014; Chrysikopoulos and Katzourakis 2015).

The colloid and biocolloid transport models can be used with either instantaneous or broad pulse source loadings. Colloid particles may be either suspended in the aqueous phase or attached reversibly and/or irreversibly onto the solid matrix (Katzourakis and Chrysikopoulos 2014). Biocolloid particles (e.g. viruses and bacteria) may be either suspended in the aqueous phase or attached reversibly onto the solid matrix (Sim and Chrysikopoulos 1995; Thomas and Chrysikopoulos 2007). Biocolloids suspended in the aqueous phase and attached onto the solid matrix are assumed to undergo inactivation with different rates. All of the transport models used in ColloidFit can handle dense particles (Chrysikopoulos and Syngouna 2014; Katzourakis and Chrysikopoulos 2015) by accounting for gravity forces with interactive options on graphic user interface. Furthermore, for batch attachment data, ColloidFit incorporates some of the frequently used equilibrium (linear, Freundlich, and Langmuir) and nonequilibrium (linear reversible, nonlinear reversible, kinetic product, bilinear, and mass transfer) attachment model equations.

ColloidFit uses the parameter fitting capabilities of "PEST" (Welter et al. 2015) to adjust the model parameters in order to minimize the discrepancies between model-generated data and the corresponding measurements. ColloidFit is capable of estimating unknown model parameters together with their 95% confidence intervals. The concentration histories are graphed and displayed simultaneously, allowing the user to observe the fitting progress.

The user interface of ColloidFit mainly consists of three tabs: Graphing, Fitting, and Simulation. The "Graphing" tab (Figure 1) presents the graph area with the experimental data, fitted curve, and simulated curve. The orange circles represent the experimental concentration data that need to be fitted, the blue curve represents the fitted concentration curve, and the red curve (not shown) represents the simulated concentration curve produced with model parameters defined by the

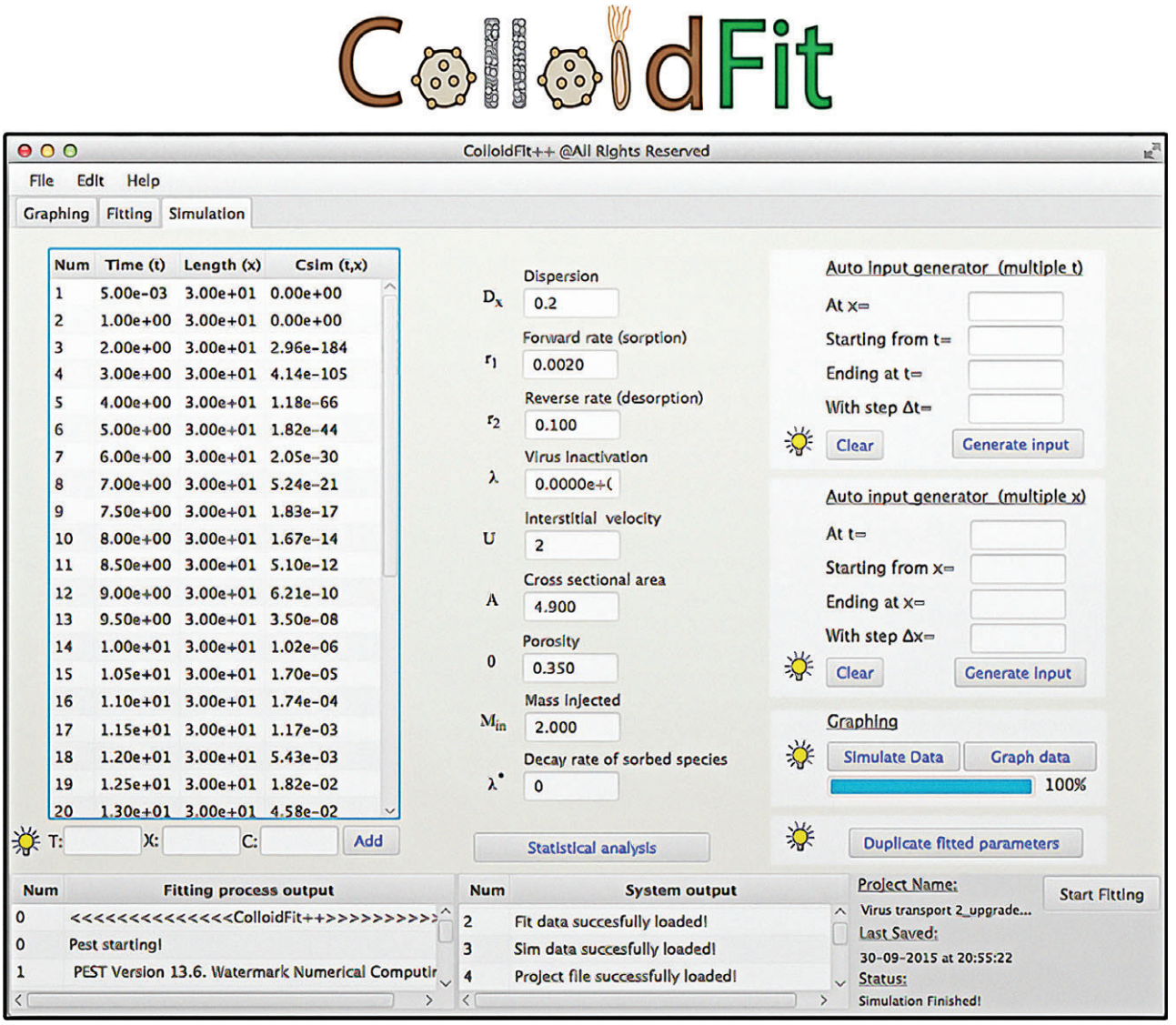

Figure 3. The user interface of the "Simulation" tab.

user. As soon as the fitting button is pressed, the "Graphing" tab becomes active and the experimental data are graphically illustrated. Furthermore, the progress report for the parameter fitting process from PEST is displayed on the bottom left corner (Figure 1d). As time passes, the consecutive model simulations improve and progressively match better the experimental data. At the same time the parameters used to produce the current model simulations are listed on the right side of the current display (Figure 1d).

The "Fitting" tab (Figure 2) contains the necessary boxes that allow the user to input all the experimental data, collection times, and longitudinal coordinates, but also to define the desired fitting options. The available parameters for each simulation model may have status either Fixed or Fitted. The fixed parameters are hold constant, whereas the parameters to be fitted start from a specified initial guess and progressively are updated and improved. For each parameter, minimum and maximum possible parameter values must be provided. These values act as boundaries in the fitting process. Finally, available in the "Fitting" tab is the "Statistical Analysis" button, which when clicked various statistics are calculated.

The "Simulation" tab (Figure 3) allows the user to perform additional single transport simulations at preselected specific points in time and space, independently of any fitting process. The user may either manually fill the "Time (t)" and "Length (x)" columns by typing in the appropriate values, or generate input data automatically over the temporal and the spatial domains. The simulation results can be graphed and displayed in the "Graphing" tab (Figure 1).

ColloidFit contains several options that allow the user to define numerous general or specific model options making the fitting process as easy as possible. The complete software with the accompanying manual can be found and obtained free of charge at http://tuceel.tuc.gr/. The requirements of computer hardware and operation system (OS) are listed in Table 1.

Table 1
The Minimum Computer Hardware and OS Requirements for the ColloidFit

Processor	Minimum Intel Core i3 or similar Recommended Intel Core i7 or similar
RAM	More memory allows even larger graphs, but runs the risk of inducing larger Garbage Collection operations. Minimum 2 GB Recommended 16–32 GB or more
Hard Disk Space	Minimum 10 GB SATA Recommended 100 GB SSD w/ SATA
OS	Windows • Windows 10 • Windows 8.x (Desktop) • Windows 7 SP1 • Windows Vista SP2 • Windows Server 2008 R2 SP1 (64-bit) • Windows Server 2012 and 2012 R2 (64-bit) Mac OS X • Intel-based Mac running Mac OS X 10.8.3+, 10.9+ • Administrator privileges for installation
Video	1280 × 800, 256 colors (recommended: 1920 × 1080, true color 32-bit)

References

Anders, R., and C.V. Chrysikopoulos. 2005. Virus fate and transport during artificial recharge with recycled water. *Water Resources Research* 41, no. 10: W10415. DOI:10.1029/2004WR003419.

Chrysikopoulos, C.V., and V.E. Katzourakis. 2015. Colloid particle size-dependent dispersivity. *Water Resources Research* 51: 4668–4683. DOI:10.1002/2014WR016094.

Chrysikopoulos, C.V., and V.I. Syngouna. 2014. Effect of gravity on colloid transport through water-saturated columns packed with glass beads: Modeling and experiments. *Environmental Science & Technology* 48: 6805–6813. DOI:10.1021/es501295n.

Katzourakis, V.E., and C.V. Chrysikopoulos. 2015. Modeling dense-colloid and virus cotransport in three-dimensional porous media. *Journal of Contaminant Hydrology* 181: 102–113. DOI:10.1016/j.jconhyd.2015.05.010.

Katzourakis, V.E., and C.V. Chrysikopoulos. 2014. Mathematical modeling of colloid and virus cotransport in porous media: application to experimental data. *Advances in Water Resources* 68: 62–73. DOI:10.1016/j.advwatres.2014.03.001.

Keller, A.A., S. Sirivithayapakorn, and C.V. Chrysikopoulos. 2004. Early breakthrough of colloids and bacteriophage MS2 in a water-saturated sand column. *Water Resources Research* 40, no. 8: W08304. DOI:1029/2003WR002676.

Sim, Y., and C.V. Chrysikopoulos. 1995. Analytical models for one-dimensional virus transport in saturated porous media. *Water Resources Research* 31: 1429–1437. (Correction, 1996. *Water Resources Research* 32: 1473).

Syngouna, V.I., and C.V. Chrysikopoulos. 2011. Transport of biocolloids in water saturated columns packed with sand: Effect of grain size and pore water velocity. *Journal of Contaminant Hydrology* 126: 301–314. DOI:10.1016/j.jconhyd.2011.09.007.

Thomas, J.M., and C.V. Chrysikopoulos. 2007. Experimental investigation of acoustically enhanced colloid transport in water-saturated packed columns. *Journal of Colloid and Interface Science* 308: 200–207. DOI:10.1016/j.jcis.2006.12.062.

Welter, D.E., J.T. White, R.J. Hunt, and J.E. Doherty. 2015. Approaches in highly parameterized inversion: PEST++ Version 3, a Parameter ESTimation and uncertainty analysis software suite optimized for large environmental models. U.S. Geological Survey Techniques and Methods, book 7, section C12, 54 pp.