One-Dimensional Transport with Inflow and Storage (OTIS)

Summer Intern Project/Model at
Stroud Water Research Center

Xiaojuan (Cathy) Yu

If we knew what we were doing, it wouldn't be called Research.

– A. Einstein

Outline

- Introducing OTIS
- Mathematical model in OTIS
- Applications of OTIS at Stroud

What is OTIS?

- **OTIS** (One-Dimensional Transport with Inflow and Storage) is a mathematical simulation model used in conjunction with field-scale data **to quantify hydrologic processes** (advection, dispersion, and transient storage) affecting solute transport and certain chemical reactions (sorption and first-order decay).
- **trial-and-error approach**;
- The goal of the solute transport modeling is to **estimate parameters**;
- **OTIS-P**, a modified version of OTIS, employs parameter-estimation techniques such as Nonlinear Least Squares (NLS).
- **OTIS/OTIS-P** is available on USGS (US Geological Survey) website

Where did OTIS come from?

- OTIS is based on a transient storage model presented by Bencala and Walters (1983).

- Robert Runkel wrote the FORTRAN code that solves the model equations

Research Hydrologist
- Robert Runkel

Some Technical terms in OTIS

- **Advection**: the downstream transport of solute mass at a mean velocity
- **Dispersion**: the spreading, or longitudinal mixing, of solute mass due to shear stress, turbulence, and molecular diffusion
- **Transient storage**: the temporary detainment of solutes in sediments, small eddies, and stagnant pockets of water that are stationary relative to the faster moving waters near the center of the channel

Transient Storage

The pockets of water and porous areas of the streambed are the two areas contributing to transient storage.

Transient Storage Mechanisms

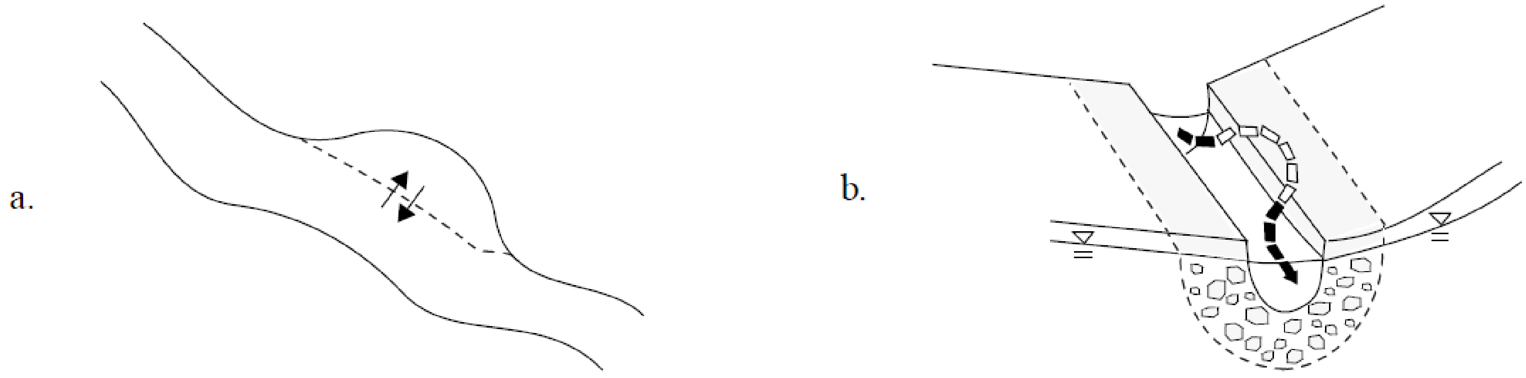


Figure 1. Transient storage mechanisms. Transient storage occurs (a) when solutes enter small pockets of slow-moving water and (b) when solutes leave the main channel and enter the porous media that makes up the bed and banks of the channel. Arrows denote solute movement between the main channel and the transient storage zone (adapted from Runkel and Bencala, 1995).

Why OTIS?

- Estimating nutrient uptake in streams – Denis Newbold
- Studying particle dynamics – transport ,deposition and suspension – Denis Newbold
- Estimating the exchange of water between stream and sediments
- Assessing the fate of contaminants that are released into surface waters

Conceptual Model: Main Channel and Storage Zone

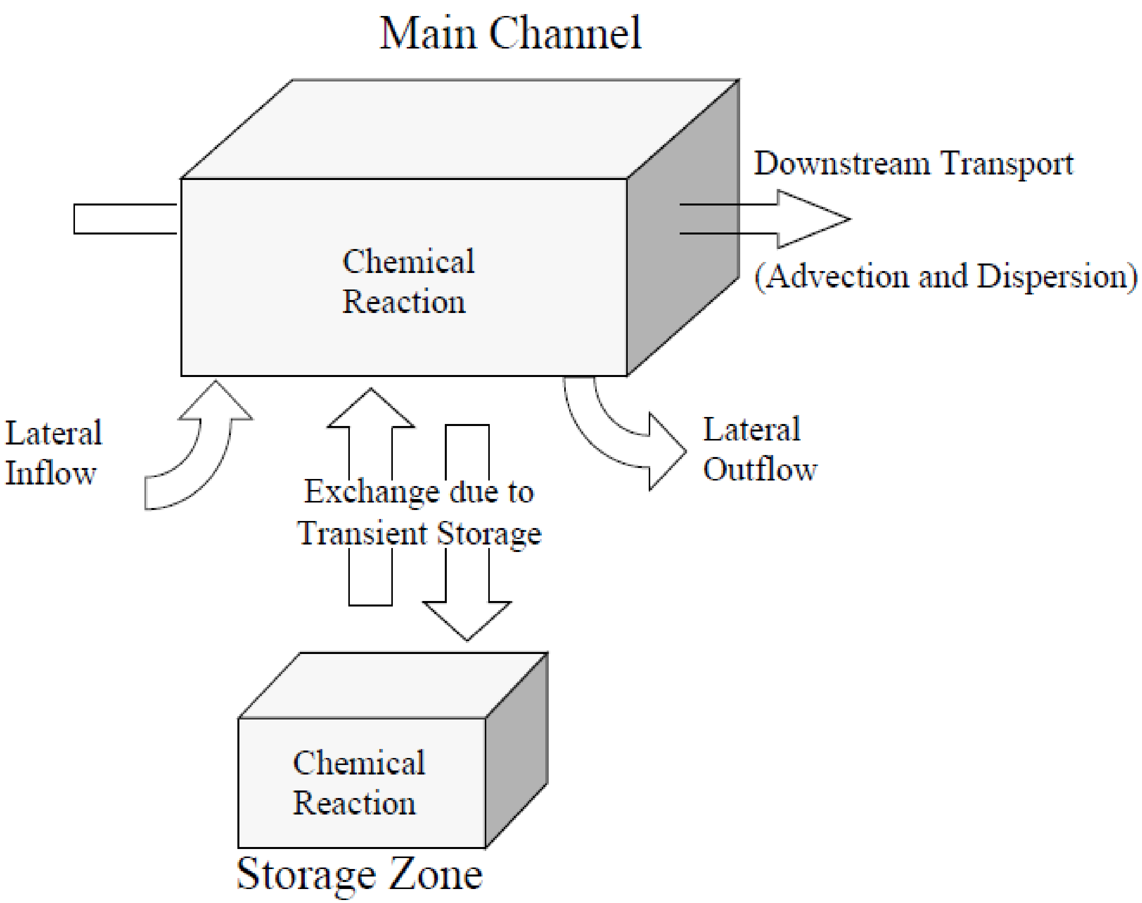


Figure 2. Conceptual model that includes the main channel and the storage zone.

Governing Differential Equations in OTIS

Assumptions

The primary Assumption

* Solute concentration varies only in the longitudinal direction.

Model assumptions

* The physical processes that affect solute concentrations include advection, dispersion, lateral inflow, lateral outflow, and transient storage.

* Advection, dispersion, lateral inflow, and lateral outflow do not occur in the storage zone.

Conceptual Model: Main Channel and Storage Zone

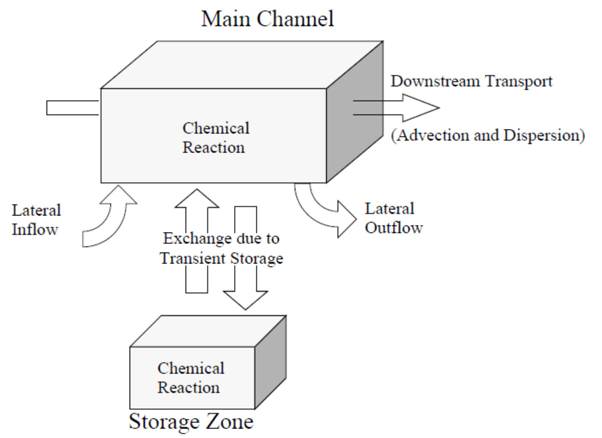


Figure 2. Conceptual model that includes the main channel and the storage zone.

Governing Differential Equations – the Conservative Case

In the Main Channel:

$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) + \frac{q_{LIN}}{A}(C_L - C) + \alpha(C_s - C) \qquad (1)$$

In the storage-zone:

$$\frac{dC_s}{dt} = \alpha\frac{A}{A_s}(C - C_s) \qquad (2)$$

Where

A - main channel cross-sectional area $[L^2]$

A_s - storage zone cross-sectional area $[L^2]$

C – main channel solute concentration $[\mathrm{M}/L^3]$

C_L - lateral inflow solute concentration $[\mathrm{M}/L^3]$

C_s - storage zone solute concentration $[\mathrm{M}/L^3]$

D – dispersion coefficient $[L^2/\mathrm{T}]$

Q – volumetric flow rate $[L^3/\mathrm{T}]$

q_{LIN} - lateral inflow rate$[L^3/\mathrm{T\text{-}L}]$

t – time [T]

x – distance [L]

α – storage zone exchange coefficient [/T]

Conceptual System - Reaches and Segments

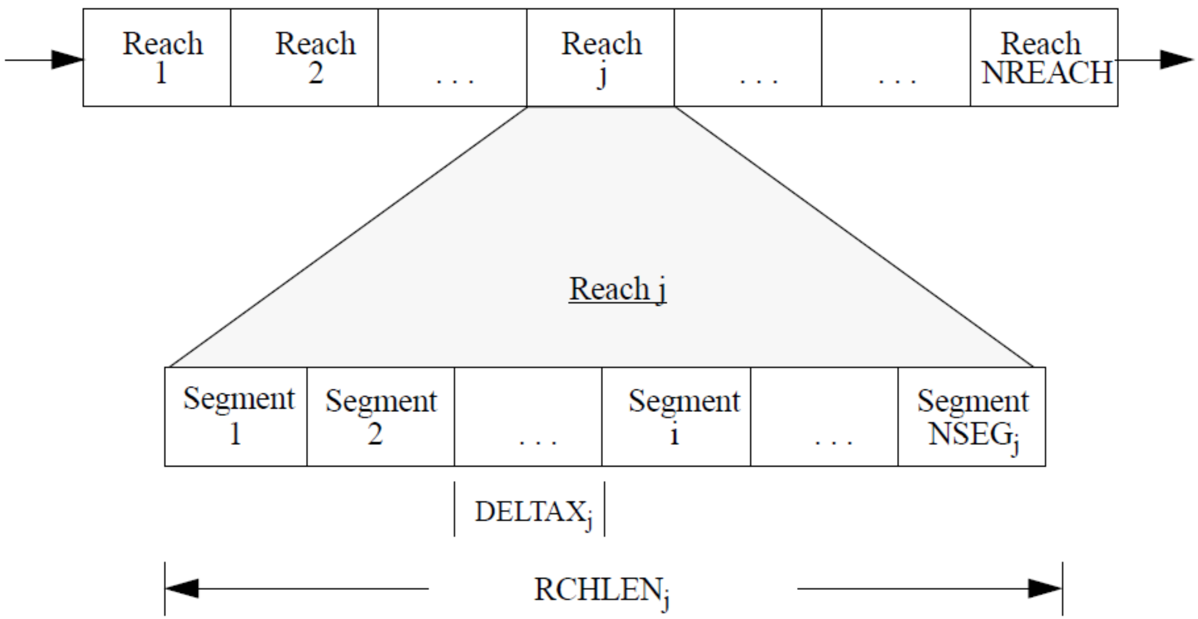


Figure 8. Conceptual system that includes one or more reaches. Each reach is subdivided into a number of computational elements or segments.

A reach is defined as a continuous distance along which model parameters remain constant.

- a single reach
- several reaches

Each reach is subdivided into a number of computational elements or **segments**.

Conceptual System

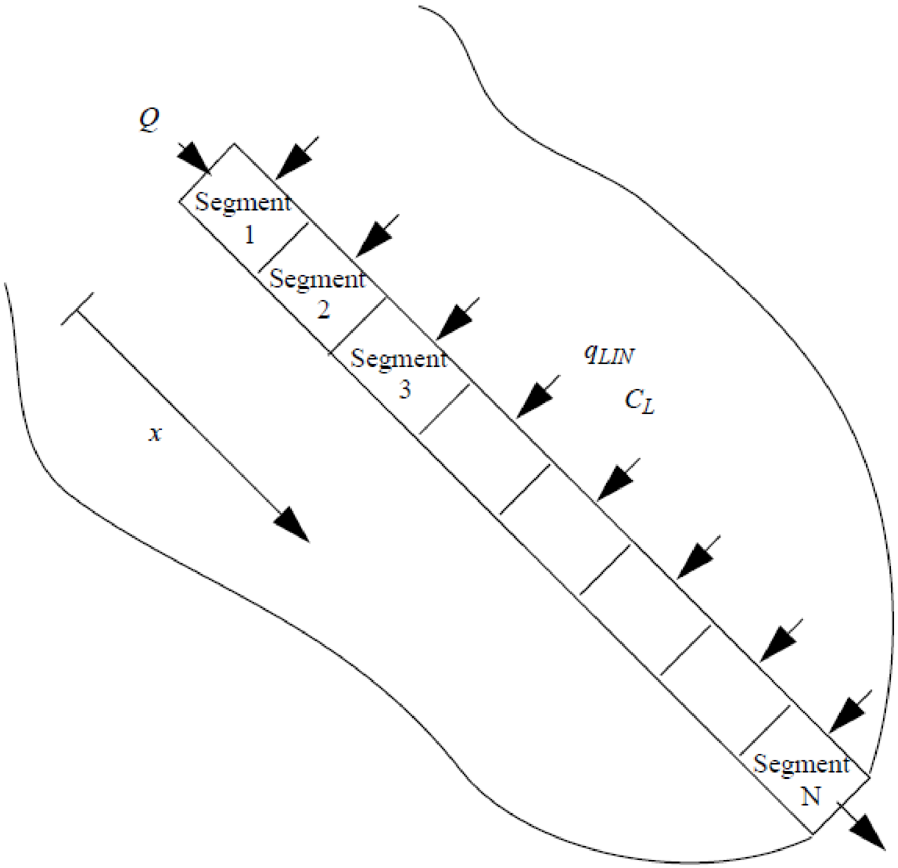


Figure 3. Conceptual system subdivided into a number of discrete segments (control volumes).

Segmentation Scheme

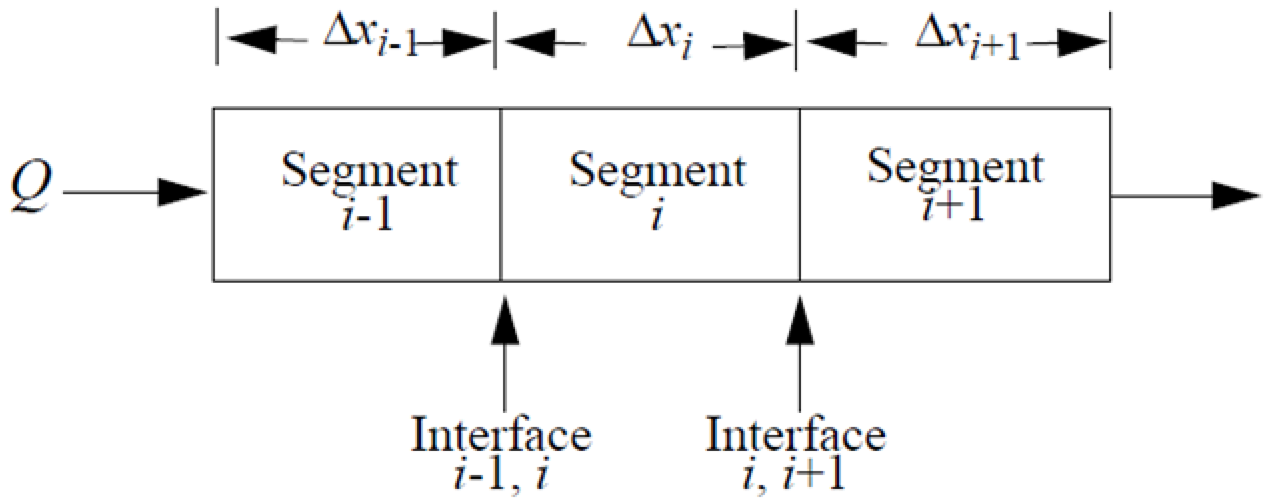


Figure 4. Segmentation scheme used to implement the numerical solution.

Boundary Conditions

Segment 1 - Upstream Boundary Condition

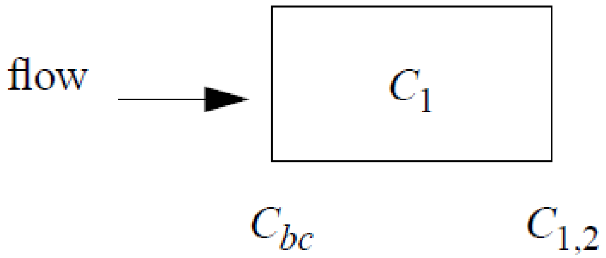


Figure 5. Upstream boundary condition defined in terms of a fixed concentration, c_{bc}.

Downstream condition(DSBOUND): a fix dispersive flux at $C_{1,2}$ is defined by $\left(D\,\frac{\partial C}{\partial x}\right)|_{1,2}$ = DSBOUND.

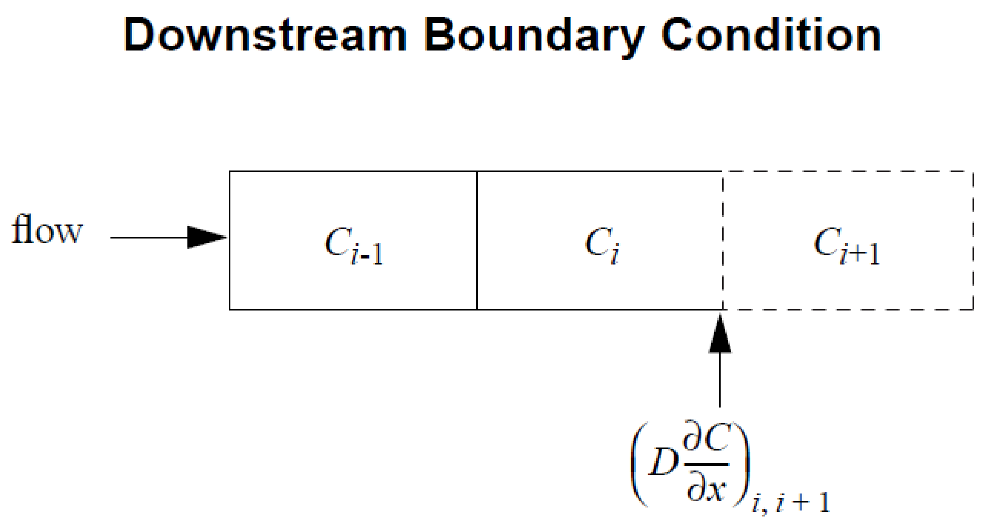


Figure 6. Downstream boundary condition defined in terms of a fixed dispersive flux.

Numerical Solutions

After applying the finite-difference approximations, Eqn(1) becomes:

$$\frac{dC}{dt} = L(C) + \frac{q_{LIN}}{A_i}(C_L - C_i) + \boldsymbol{\alpha}(C_s - C_i) \qquad (3)$$

Where

$$L(C) = -\left(\frac{Q}{A}\right)_i \left(\frac{C_{i+1} - C_{i-1}}{2\Delta x}\right) + \frac{1}{A_i}\left\{\frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{2\Delta x^2}\right\}$$

Here, i subscripts the segments, and Δx is the length of each segment.

Crank-Nicolson Method

The time derivate dC/dt, is estimated using a forward difference approximation:

$$\frac{dC}{dt} = \frac{C_i^{j+1} - C_i^j}{\Delta t} \qquad (4)$$

Δt – the integration time step [T]
j – denotes the value of a parameter or variable at the current time
j+1 – denotes the value of a parameter or variable at the advanced time

Eqn(3) and (4) were developed into (5) for all the segments in the modeled system,

$$E_i C_{i-1}^{j+1} + F_i C_i^{j+1} + G_i C_{i+1}^{j+1} = R_i \quad (5)$$

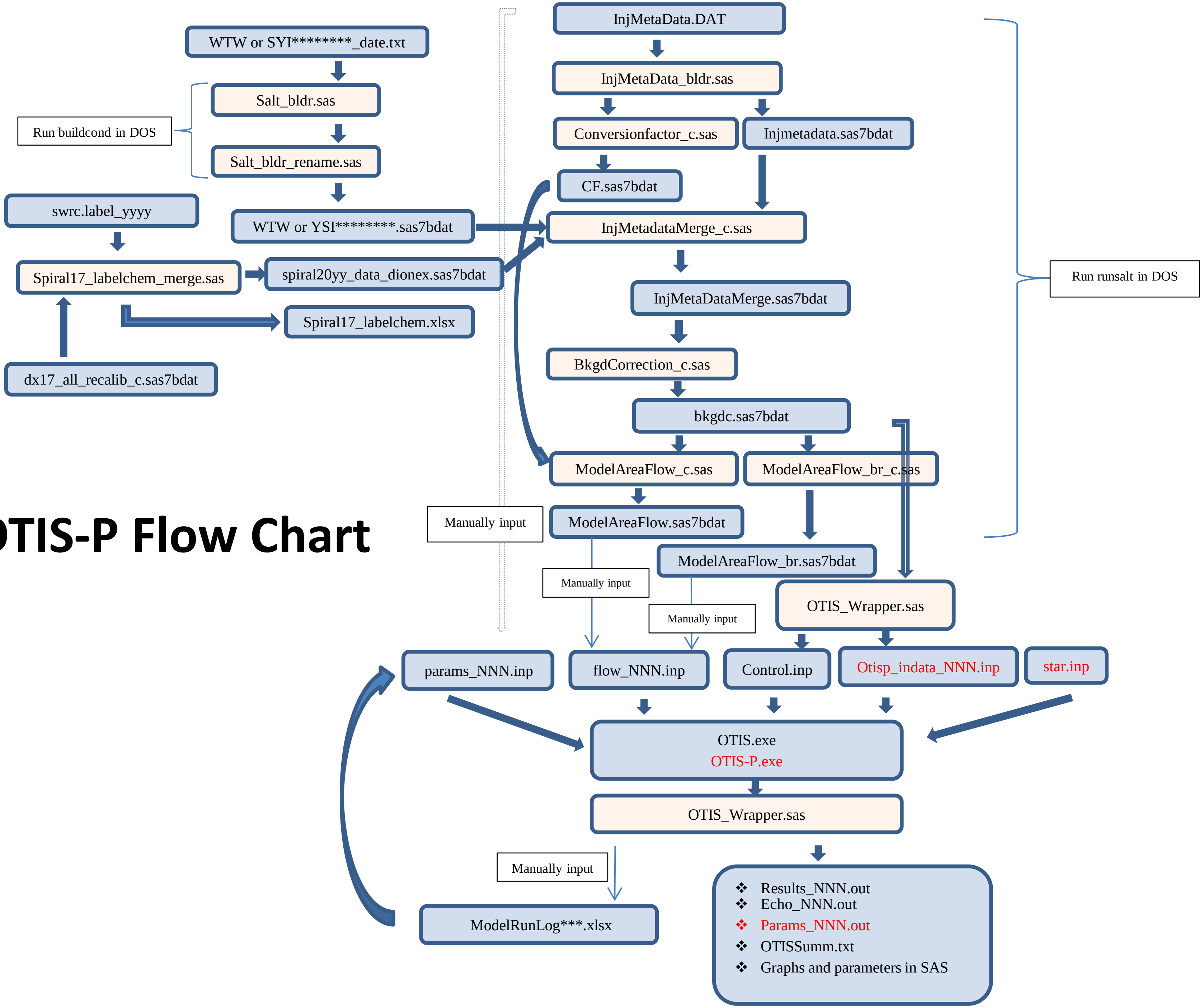
$$\begin{bmatrix} F_1 & G_1 & & & \\ E_2 & F_2 & G_2 & & \\ & E_3 & F_3 & G_3 & \\ & & E_4 & F_4 & G_4 \\ & & & E_5 & F_5 \end{bmatrix} \begin{bmatrix} C_1^{j+1} \\ C_2^{j+1} \\ C_3^{j+1} \\ C_4^{j+1} \\ C_5^{j+1} \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \\ R_5 \end{bmatrix}$$

A hypothetical set of equations representing a five-segment system

Systems of equations above can be efficiently solved using the Thomas Algorithm.

Applications of OTIS

OTIS/OTIS-P Flow Chart



Our OTIS/OTIS-P model

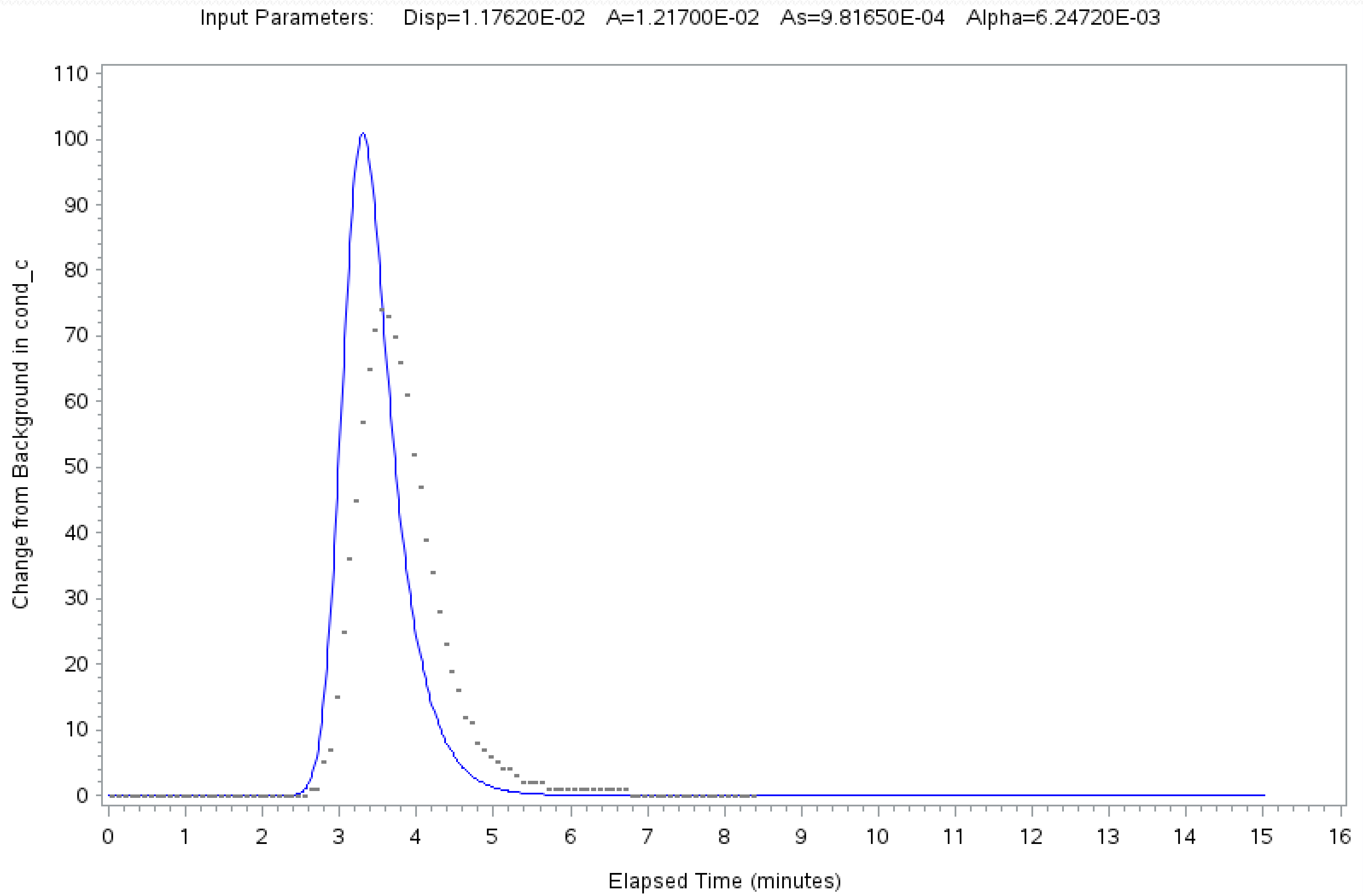
	Flumes	Stream
Solute (conservative)	Yes	Yes
Spatially uniform	Yes	No (assumed uniformity)
Temporally steady flow	Yes	No (assumed steady flow during experiment)
lateral inflow	No	Yes (assumed no inflow)
Lateral outflow	No	No

Application 1 The flume experiment

The Procedure of the Experiment on the flumes

Goal: find out if the flumes with more biofilm tend to have larger storage zone exchange coefficient.

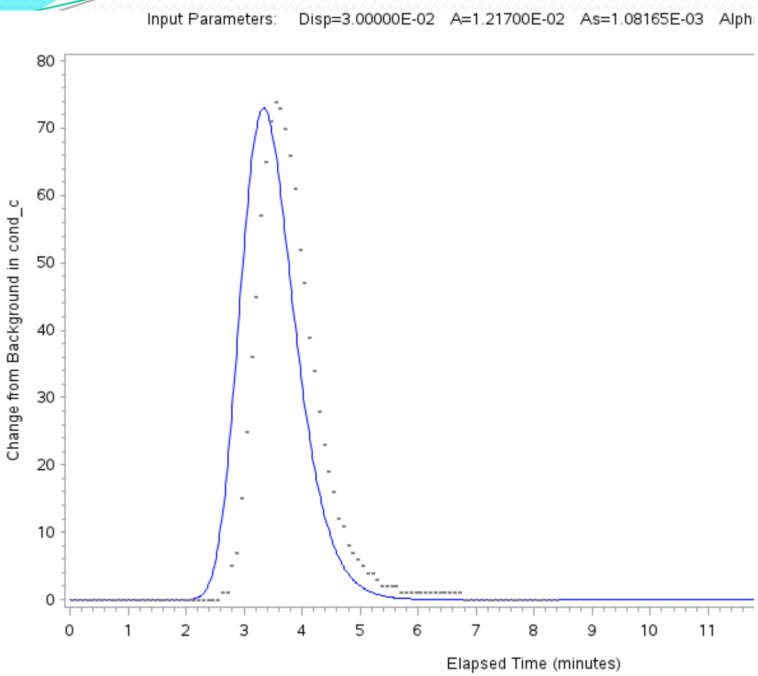
- Build a flume with some rocks on the bottom
- Pump water into the flume
- Measure the flow before the experiment
- Put a conductivity logger under the water at the end of the flume
- Release the water mixed with salt from the beginning end of the flume
- The conductivity logger will record conductivity at the end of flume
- Analyze the data downloaded from the logger with OTIS (and SAS) to find the parameters, Dispersion, main channel cross-sectional area , storage zone cross-sectional area , storage zone exchange coefficient

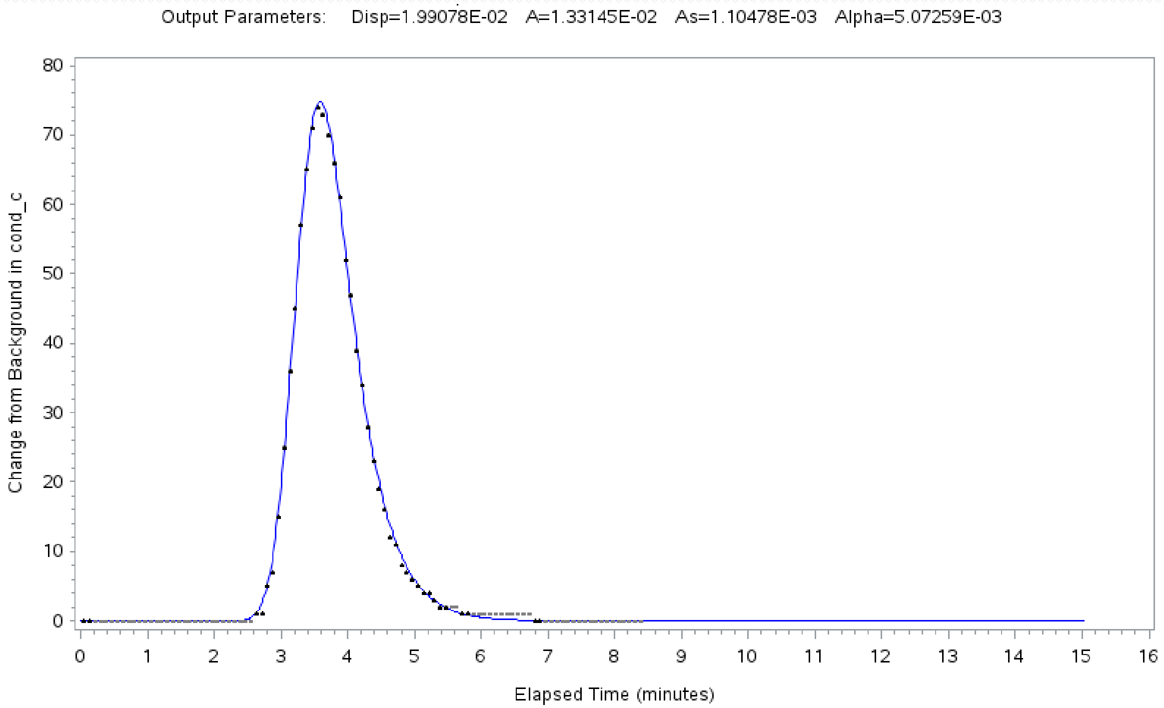


OTIS graphical result for one of the flume experiments

Results after Changing Parameters

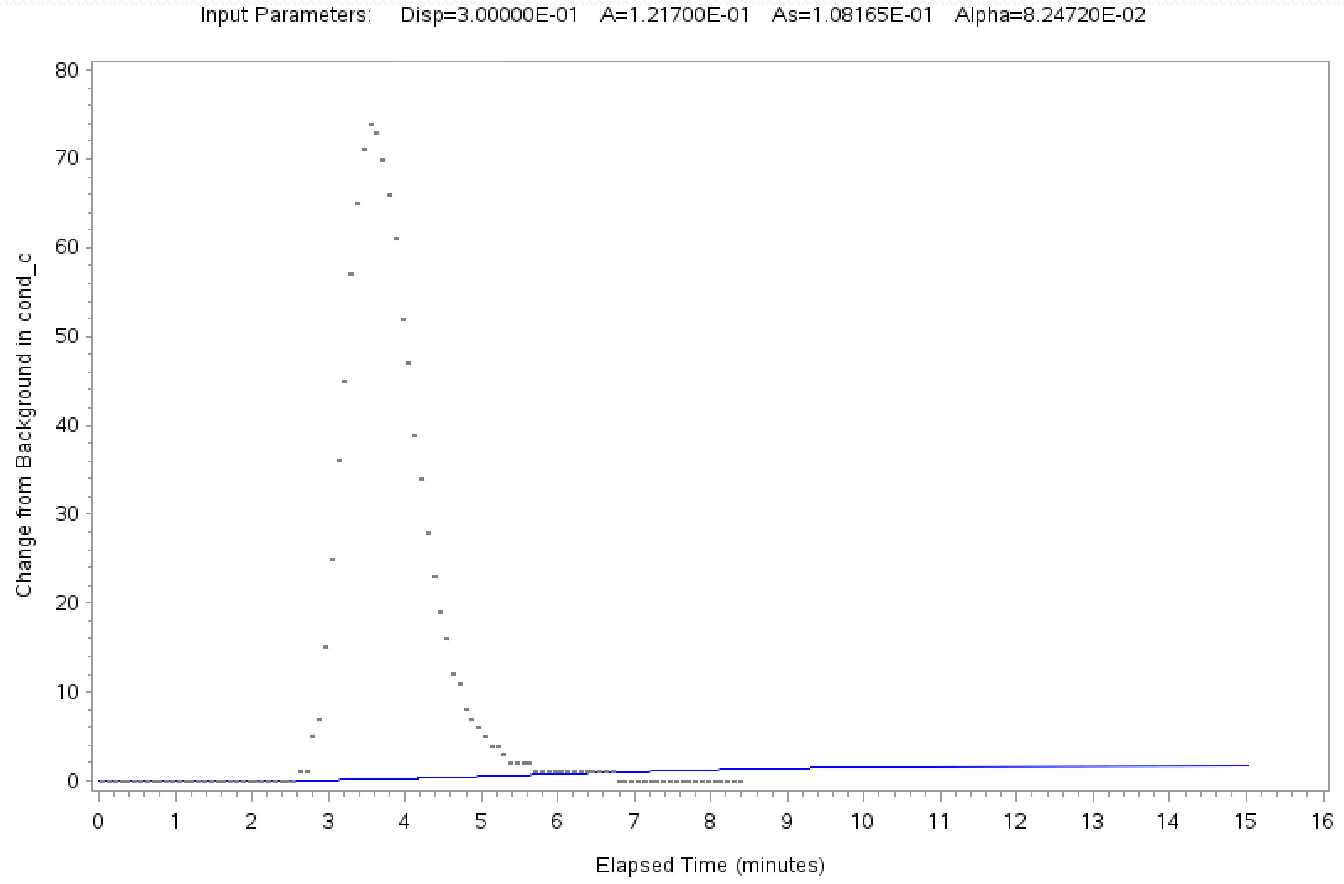
	Increase	Decrease
Disp	Lower max and wider	
A	Shift right and slightly wider	
As	Lower max and extend tail	
Alpha	Lower max and steepen tail	





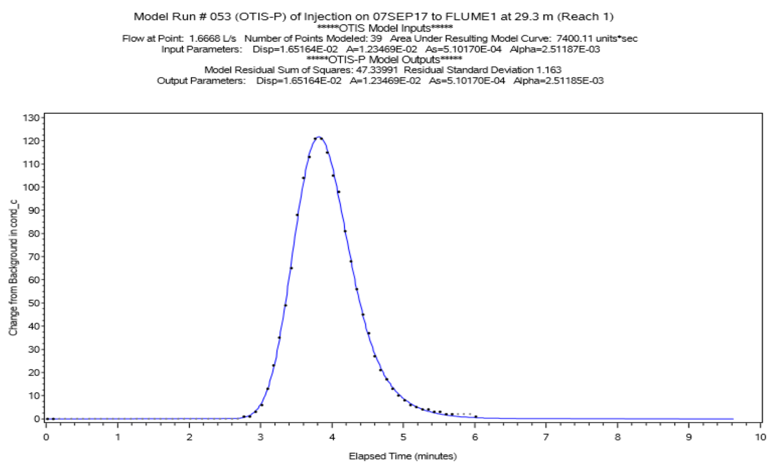
	Left Graph -OTIS	Right Graph-OTIS-P
Dispersion	3.0000E-02	1.99078E-02
Area	1.21700E-02	1.33145E-02
Area2	1.08165E-03	1.10478E-03
Alpha	8.24720E-03	5.07259E-03

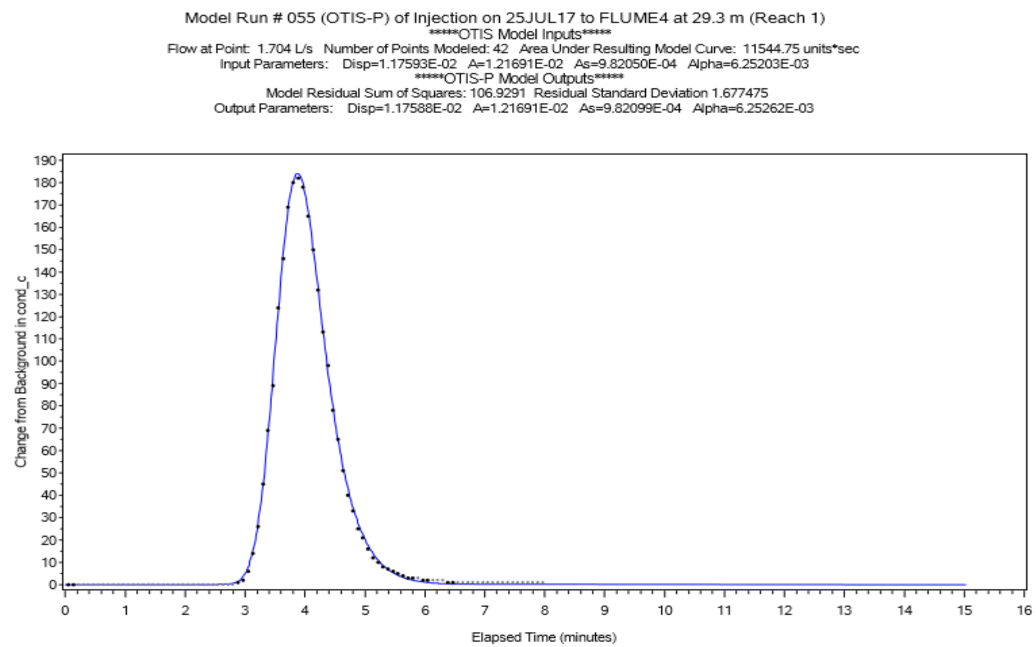
An Example of failed modeling in OTIS-P



OTIS-P does not work when the input parameters are too different from the true values.

Flume 1 (no biofilm) VS Flume 4 (with biofilm)





	Left Graph –Flume1	Right Graph- Flume4
Dispersion	1.65E-02	1.18E-02
A	1.23E-02	1.22E-02
As	5.10E-04	9.82E-04
Alpha	2.51E-03	6.25E-03

Conclusion

The biofilm made the storage zone exchange coefficient and storage zone cross-sectional area larger.

Application 2 - experiments on the Stream

Purpose: **we want to find out how trees and branches that fell into the stream affect transient storage in White Clay Creek**

In Sep. and Oct. 2017, we

- Selected a reach about 200 meters long and marked five stations within the reach;
- Set up the conductivity loggers at the injection site located upstream from the injection site (for background), and at stations 1 and 5.
- Set up barrels and equipment at the injection site and metered NaCl and NaBr to the stream using a pump;
- The pump worked for 17 hours and the loggers recorded for more than 24 hours.
- The data in the loggers were downloaded to computer and analyzed for the four parameters, Disp, Area, Area 2 and Alpha with OTIS/OTIS-P.

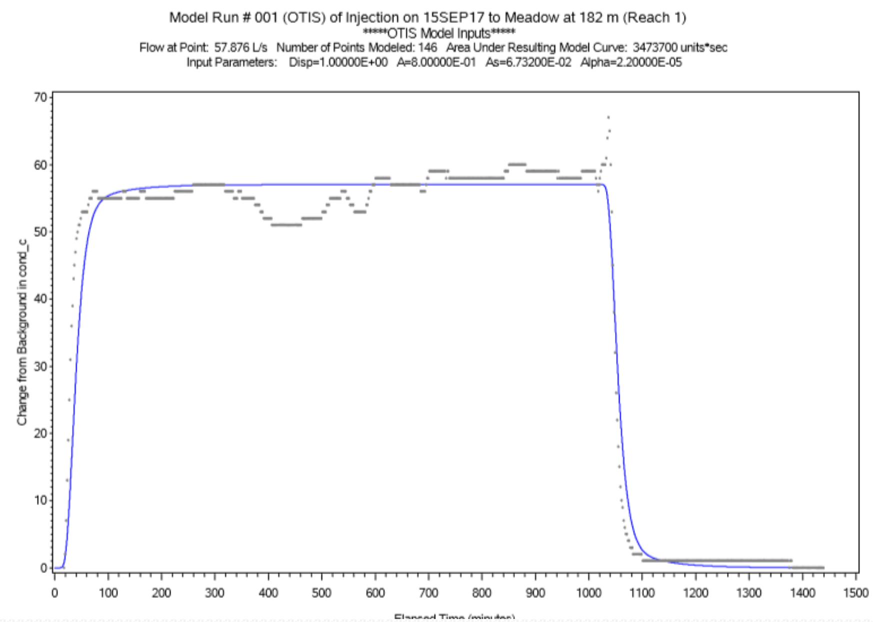
Then we will place woody debris into the stream on the site(s)in White Clay Creek.

Next year, run the experiment again to see the change of the four parameters.

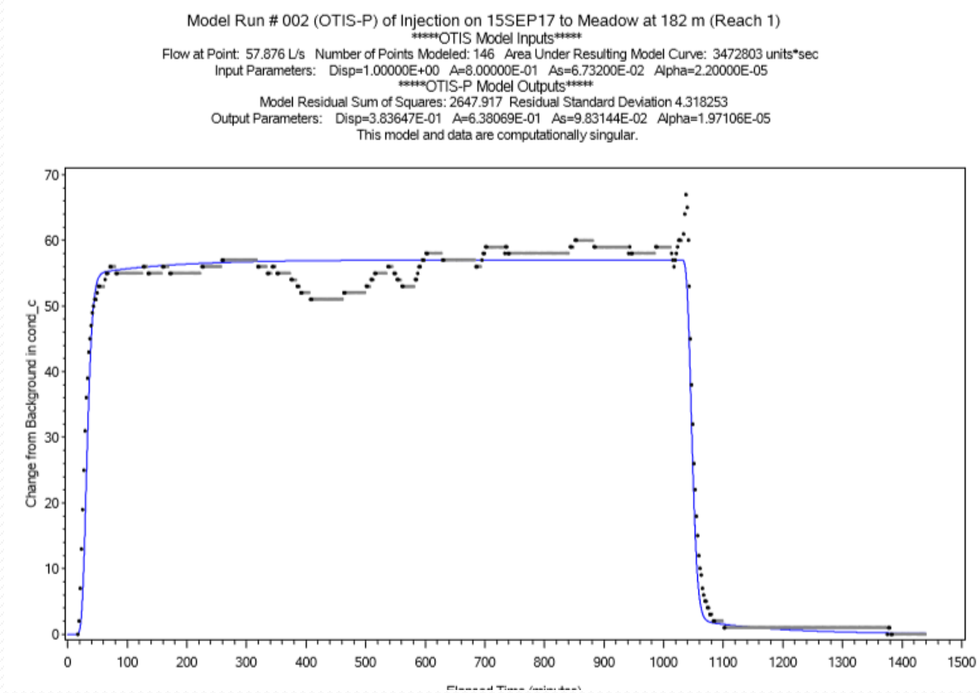
NaCl and NaBr are metered into the stream

Conductivity Meter

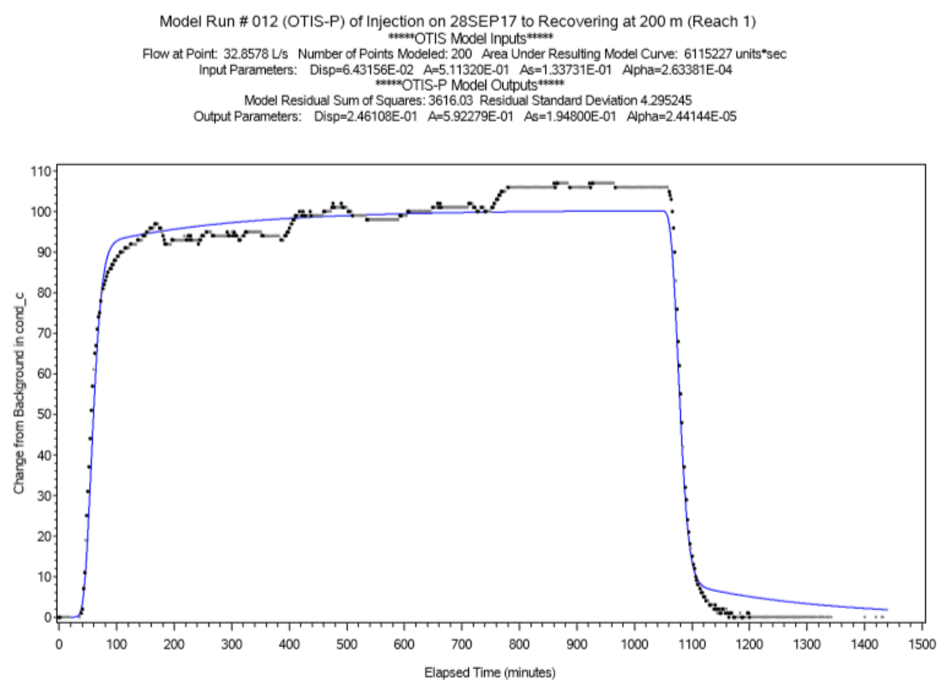
OTIS/OTIS-P Results for Meadow Reach

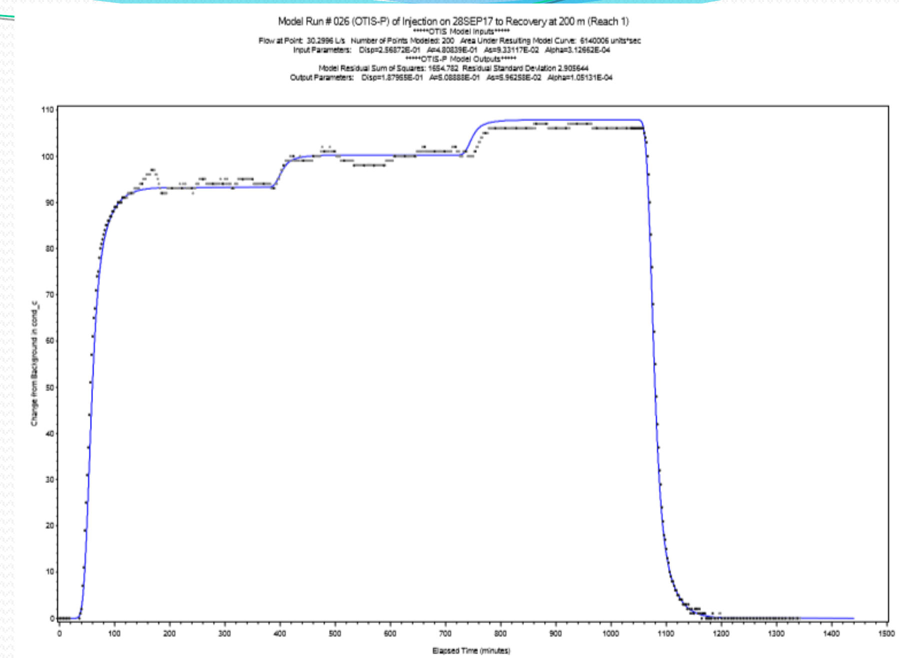


OTIS



OTIS-P






```
#USTIME        USBC (for i=1,NSOLUTE)
#             |              |
####################################
0.0           0.00000
0.0002778     3.297
17.0002778    0.00000
```

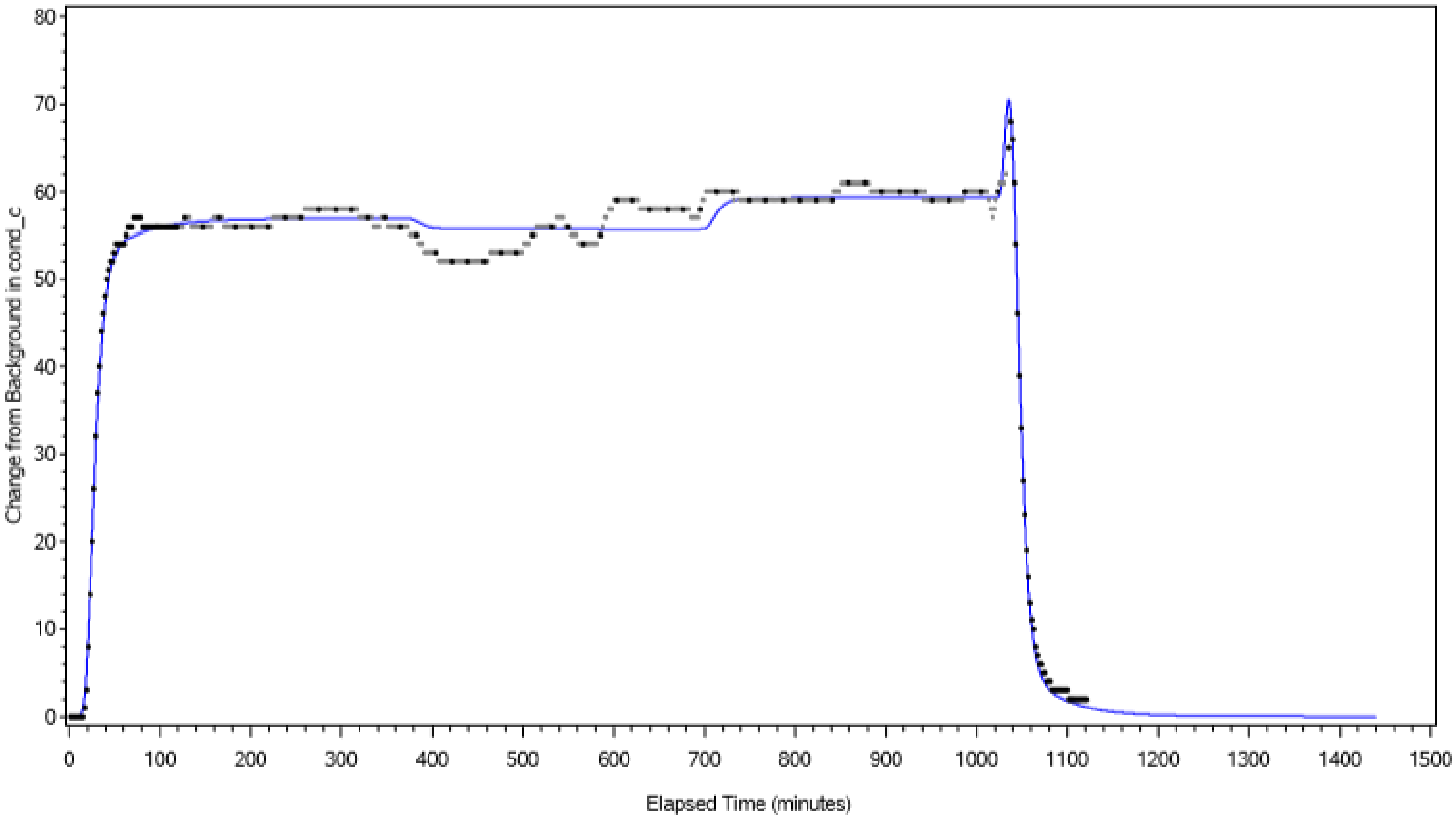
Flux input in param file; flux is considered to be uniform.

```
#USTIME        USBC (for i=1,NSOLUTE)
#             |              |
####################################
0.0000        0.0000
0.0002778     2.824988999
5.7502778     3.037069939
11.5002778    3.267479736
17.0002778    0.0000
```

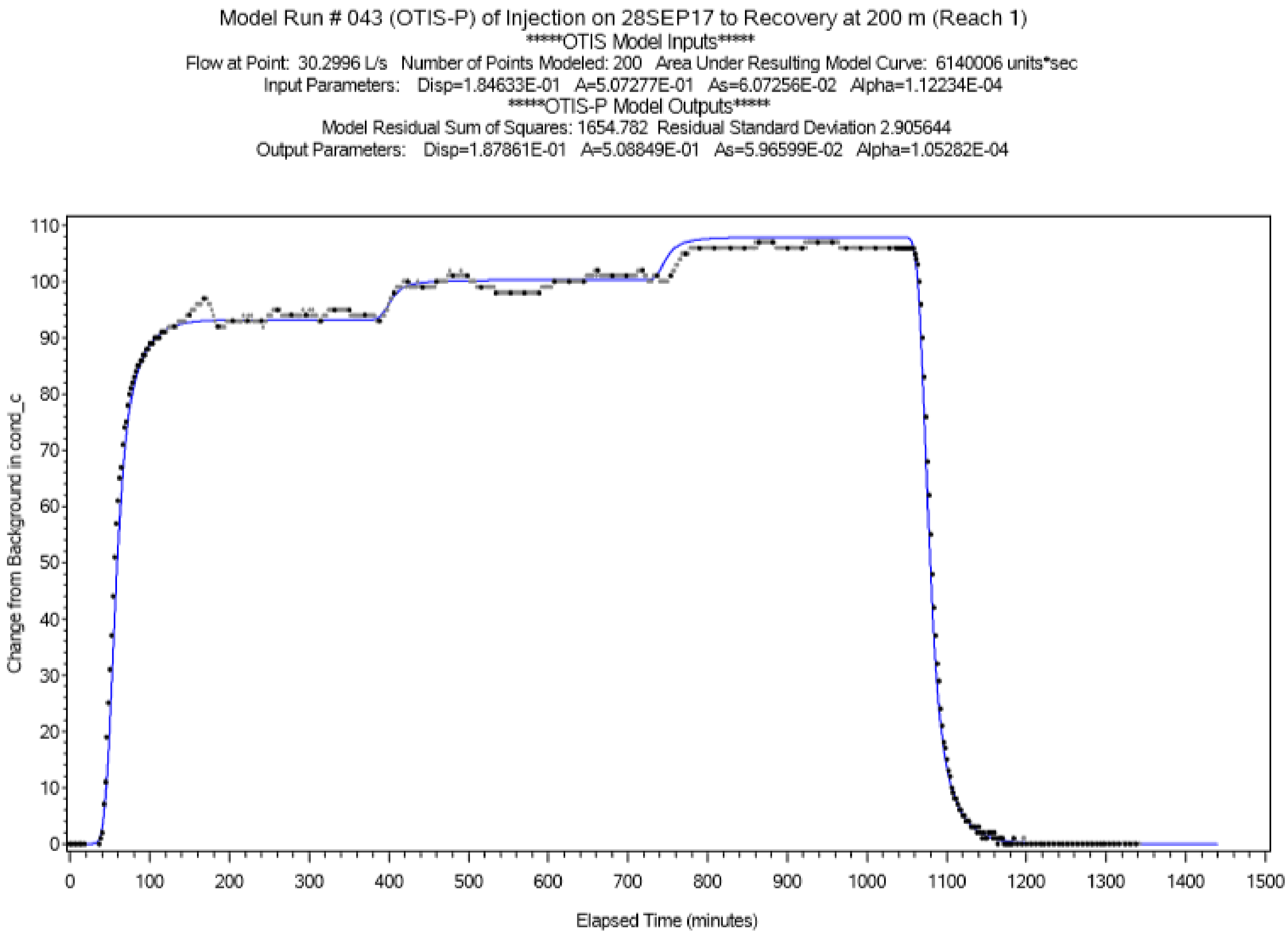
Flux input in param file; flux is different for each barrel.

Best OTIS-P Result for Meadow Reach

Model Run # 046 (OTIS-P) of Injection on 15SEP17 to Meadow at 182 m (Reach 1)
*****OTIS Model Inputs*****
Flow at Point: 48.3003 L/s   Number of Points Modeled: 154   Area Under Resulting Model Curve: 3522806 units*sec
Input Parameters: Disp=8.98923E-01   A=4.63564E-01   As=5.70044E-02   Alpha=5.04602E-05
*****OTIS-P Model Outputs*****
Model Residual Sum of Squares: 272.0178 Residual Standard Deviation 1.346645
Output Parameters: Disp=8.98901E-01   A=4.63562E-01   As=5.70022E-02   Alpha=5.04702E-05

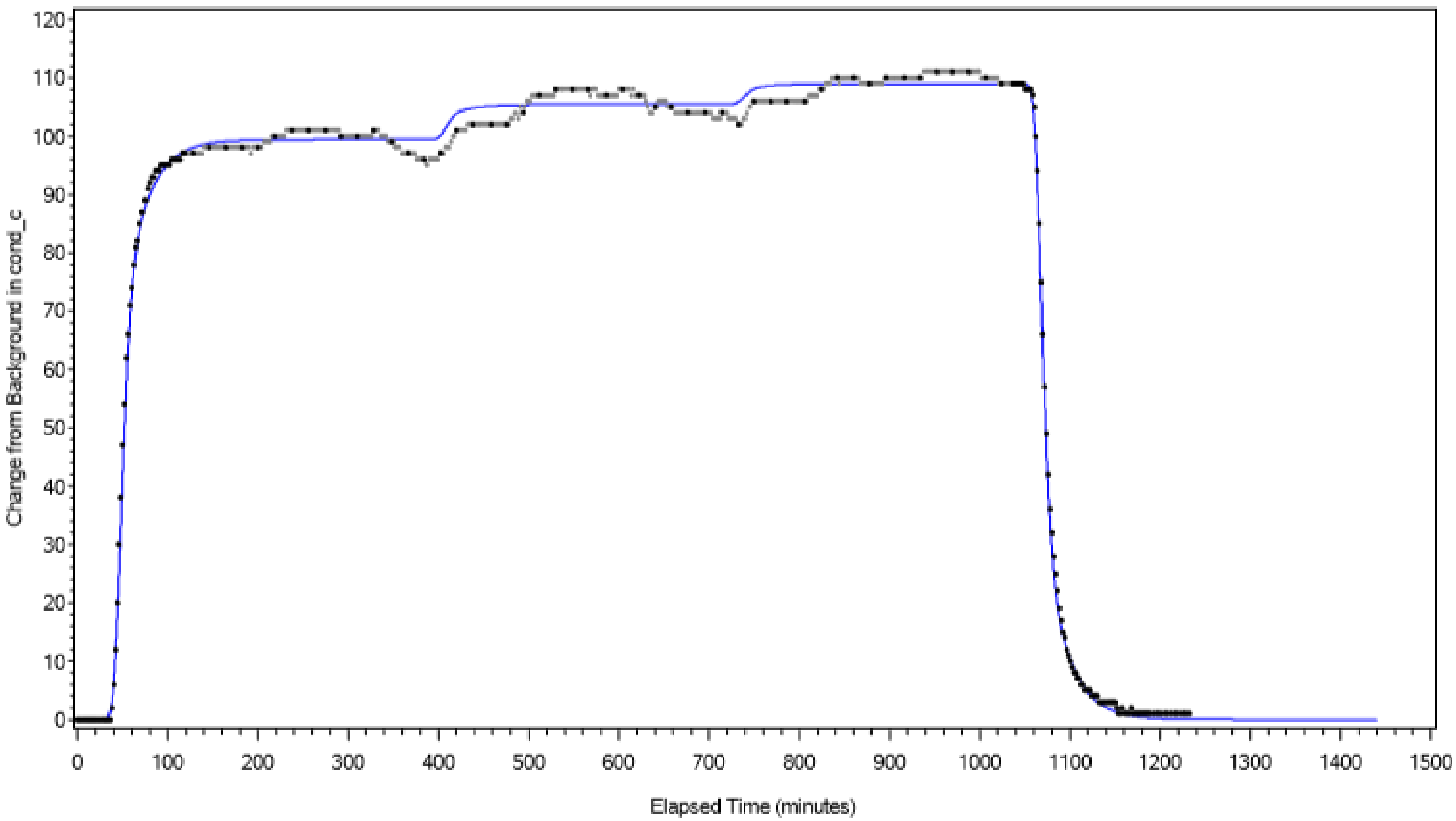


Best OTIS-P Result for Recovery Reach



Best OTIS-P Result for Forested Reach

Model Run # 044 (OTIS-P) of Injection on 05OCT17 to Forested at 184 m (Reach 1)
*****OTIS Model Inputs*****
Flow at Point: 29.3908 L/s Number of Points Modeled: 200 Area Under Resulting Model Curve: 6392341 units*sec
Input Parameters: Disp=7.21479E-02 A=4.54398E-01 As=8.79725E-02 Alpha=2.49500E-04
*****OTIS-P Model Outputs*****
Model Residual Sum of Squares: 532.9894 Residual Standard Deviation 1.64904
Output Parameters: Disp=1.22457E-01 A=4.79372E-01 As=6.96837E-02 Alpha=1.16022E-04



Summary

	Meadow	Recovery	Forested
Dispersion (m^2/s)	0.899	0.188	0.122
Main Channel Cross-sectional Area (m^2)	0.464	0.509	0.479
Storage Zone Cross-sectional Area (m^2)	0.0570	0.0597	0.0697
Storage Zone Exchange Coefficient Alpha (s^{-1})	5.05E-05	1.05E-04	1.16E-04

Summary

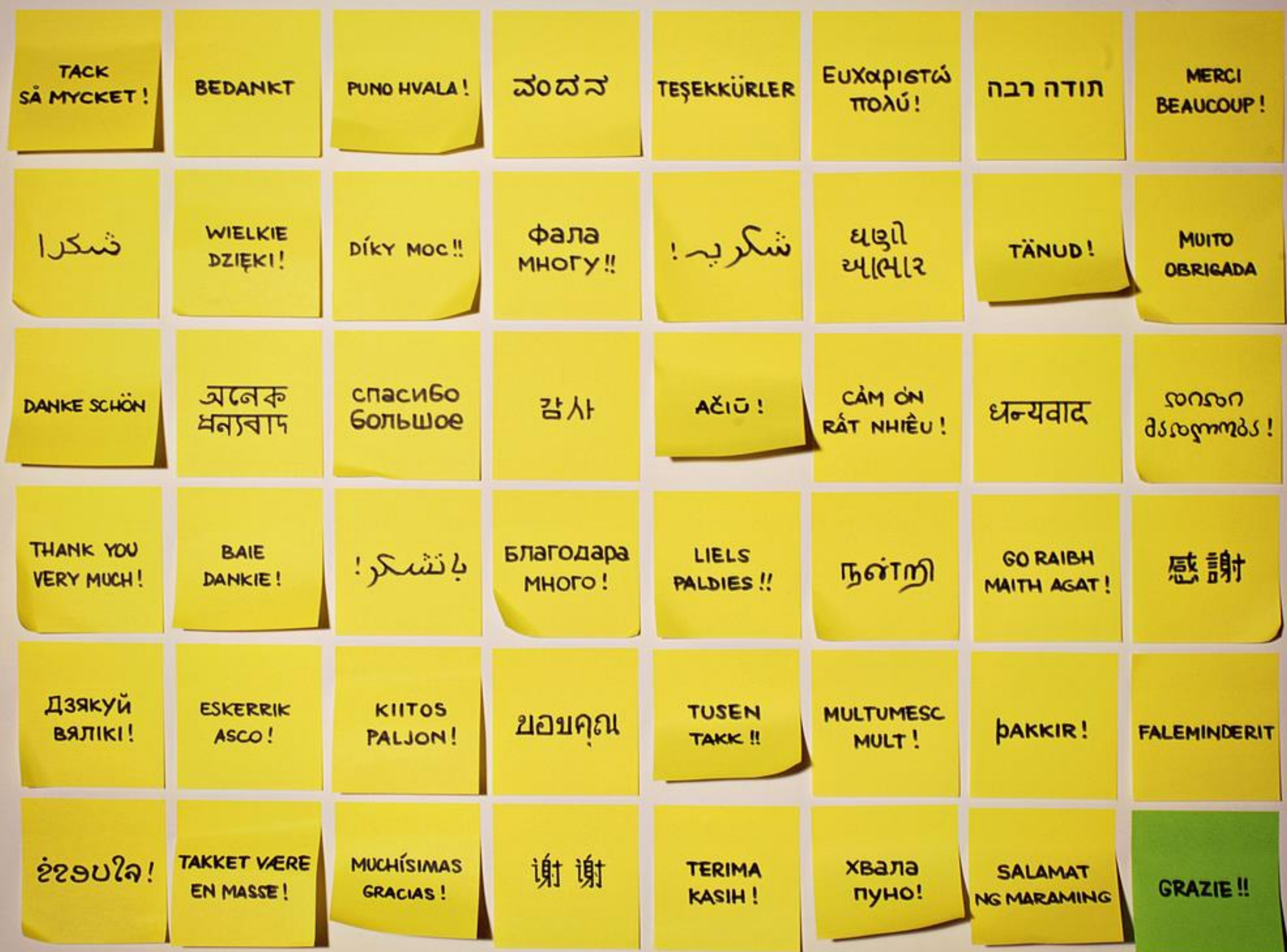
Reach	As/A	1/alpha [second]	(As/A)*(1/alpha) [second]
Meadow	1.23E-01	1.98E+04	2.43E+03
Recovery	1.17E-01	9.52E+03	1.12E+03
Forested	1.46E-01	8.62E+03	1.25E+03

As/A: this ratio shows how big the transients storage zones were
1/alpha: average time in seconds it takes for water to enter transient storage
(**As/A**)*(**1/alpha**): the time in seconds water stays in transient storage before returning to the water column.

Conclusion

- The size of the transient storage zone was similar among reaches.
- The transient storage exchange coefficient in the forested reach was higher than the other two reaches.

Any Questions?


TACK SÅ MYCKET!
BEDANKT
PUNO HVALA!
ವಂದನ
TEŞEKKÜRLER
Ευχαριστώ πολύ!
תודה רבה
MERCI BEAUCOUP!
شكرا
WIELKIE DZIĘKI!
DÍKY MOC!!
фала многу!!
شکریہ!
ઘણો આભાર
TÄNUD!
MUITO OBRIGADA
DANKE SCHÖN
অনেক ধন্যবাদ
спасибо большое
감사
AČIŪ!
CẢM ƠN RẤT NHIỀU!
धन्यवाद
დიდი მადლობა!
THANK YOU VERY MUCH!
BAIE DANKIE!
باتشکر!
Благодара много!
LIELS PALDIES!!
நன்றி
GO RAIBH MAITH AGAT!
感謝
Дзякуй вялікі!
ESKERRIK ASCO!
KIITOS PALJON!
ขอบคุณ
TUSEN TAKK!!
MULTUMESC MULT!
ÞAKKIR!
FALEMINDERIT
TAKKET VÆRE EN MASSE!
MUCHÍSIMAS GRACIAS!
谢谢
TERIMA KASIH!
хвала пуно!
SALAMAT NG MARAMING
GRAZIE!!

Citations

Robert Runkel, USGS, www.usgs.gov/staffprofiles/robert-runkel?qtstaff_profile_science_products=3#qt-staff_profile_science_products.

Runkel, Rob. "OTIS." *USGS Water Resources*, USGS, water.usgs.gov/software/OTIS/.