Simulation/Validation of Pollutant Transport in Rivers Using COMSOL

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Figure 1. Advancing Dye Plume Simulating Chemical Plume in a River

Introduction

Our atmosphere, land, and water are being continuously besieged by pollutants caused by such events as heavy metals leaching from mine tailing ponds, chemical spills from railroad and truck tanker accidents, and petroleum pipeline failures, to name just a few. These environmental insults are usually point generated but quickly become expanded to 2 and 3-dimensional problems, depending upon the flow regimes of the receiving surface and subsurface water bodies.

Dye tracer studies have been used to develop an understanding of water feature based pollutant transport. Because they require significant time and preparation to conduct, these studies are not practical for rapid response to an event that has already happened, and much too expensive to do on a wide scale for emergency planning exercises.

Dye tracer study information can be generated by simulation to add reality to emergency response and management planning related to chemical spills into flowing water bodies. Rapid estimation of a moving plume of a pollutant can be developed for real-time events if the stream geometry is readily available prior to a real event.

The COMSOL Multiphysics platform provides the tools to relatively quickly and inexpensively provide this type of environmental engineering information.

The simulation presented here is based upon a river reach of 25.5 miles and is validated using actual field measurements of a dye tracer. The Washington Department of Ecology (WaDOE) conducted a Rhodamine dye tracer study on the Pilchuck River in Snohomish County, from river mile 25.5, downstream to river mile 0.0, during the month of August 2016. The gradient of the river is a consistent .3 percent, with few, if any, sections of rapids or significant water surface turbulence.

For this example, river velocity and dye concentration information gained from the WaDOE study serve as the basis for the simulation validation. The WaDOE uses the results of dye tracer studies for the modeling and development of water quality management plans for streams and rivers.

Theory

The Fluid Flow Interface, coupled with the Transport of Diluted Species Interface, can be used to estimate the extent and movement of pollutants introduced into flowing water bodies.

The Laminar Flow Interface can be used as a tool to determine an approximation of the overall water surface velocity field of a stream segment of interest. By definition, consideration of water surface flow that is confined to the surface layer of the water body can most often be treated as laminar flow.

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution, over time and distance, of chemical species concentration transported by diffusion and convection.

Governing Equations / Simulation / Methods / Use of Simulation Apps

The COMSOL approach to river pollution transport relies upon the Navier-Stokes equation in the Laminar Flow Interface in the stationary state and the Mass Transport equation in the Transport of Diluted Species Interface in a time dependent mode. The equations used are of the form:

Navier-Stokes

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$$

Mass Transport

$$\frac{\partial c_i}{\partial t} + \nabla\cdot(-D\nabla c_i) + \mathbf{u}\cdot\nabla c_i = R_i$$

Where:

- ρ = density
- t = time
- ∇ = differential (gradient) operator
- c = concentration of the species i
- D = diffusion coefficient
- R = reaction rate expression for species i
- u = velocity vector
- I = identity matrix
- p = pressure
- μ = dynamic viscosity
- T = matrix transpose operator.

The simulation geometry, Figure 2, is created through the digitization of both stream banks from available aerial photographs from geographic information systems (GIS), government agency natural resource mapping, or other similar products commonly available For this simulation, stream geometry is obtained through the process of digitization of left and right streambank limits from the National Resource Conservation Service (NRCS) aerial photographs available on its website. The digital files are then converted into a .dxf format, using one of many COMSOL compatible computer aided drafting software packages, for direct import into COMSOL's GUI. The date of the aerial photography for the aerial mapping provides a basis for relating stream geometry to discharge information provided by various water resources management entities.

The resulting geometry is comprised of one domain, 2,393 boundary segments, a surface area of 8,844,000 square feet and variable widths that range from approximately 70 to 100 feet.

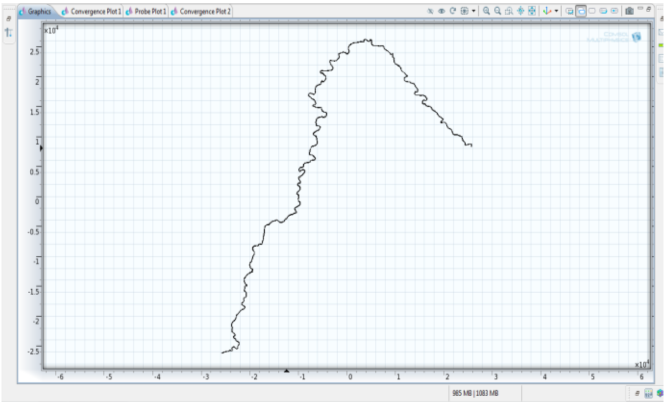

Figure 2. Model Geometry - Pilchuck River Dye Study Reach – 25.5 Miles

Parameters used in the simulation include the estimated water velocity at the head end of the study reach and the diffusion coefficient for Rhodamine dye. The numerical values for these two items are input directly into the boundary conditions steps.

Input for this simulation includes the two-dimensional river geometry walls defined as "No slip" conditions.

The inflow velocity for the Laminar Flow interface at the head end of the study reach is initially estimated at .22 meters per second based upon available hydrologic model data of the river provided by the WaDOE. This estimate is more readily available than actual flow measurements determined in the field. The inflow velocity is adjusted to .24 meters per second so that the simulated peak is more closely aligned with the actual measured concentration peak at Robe Menzel Road, .28 days from the introduction of the dye, approximately 4 miles downstream.

The inlet condition is entered as a simple average estimate of the stream velocity at that point, while the outlet condition is entered as pressure equal to zero.

Similarly, "No flux" wall conditions are established for the river banks to fulfill the Transport of Diluted Species Interface. The concentration of the flux of the dye amount introduced into the stream at the head end of the study which is estimated and entered.

The WaDOE reports that 375 milliliters were introduced into the river, or 435 grams. When converted to mass using a density of 1.16g/ml for Rhodamine WT, this equates to approximately .48 moles when using a molecular weight of 567g/mole for the dye. The flux rate estimated from these measurements is .12 moles per square meter per second for the four seconds required to empty the dye bottles across the river section. The diffusion coefficient for Rhodamine dye is approximately 4e-6 centimeters squared per second. The water temperature in this area is on the order of 60 degrees F.

A Physics based mesh, Figure 3, is used, with a pre-defined mesh size of Coarse. Boundary layers are automatically created on each river bank by COMSOL's automatic meshing procedure. The boundary layers are modified to include just one layer on all bank segments. A width factor of 5 is used.

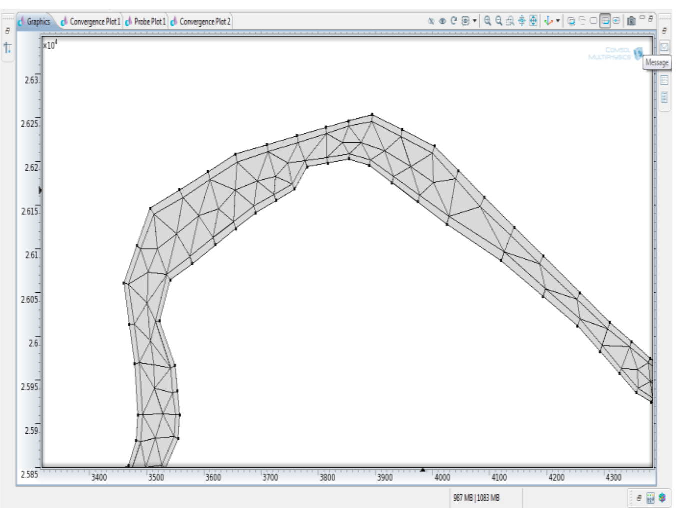

Figure 3. Model Mesh Detail – Pilchuck River Dye Study

The COMSOL predefined solver settings in the time-dependent mode are reflective of the settings used in the *Process Control Using a PID Controller* model available in the COMSOL application library.

The time range starts at time zero and ranges to the time to traverse the river length as estimated by the average velocity of the inlet conditions. For this example time steps of 900 seconds are initially used for expediency, but any step size can be entered depending upon the need for time precision. Time stepping of 1 second is used for the first 5 seconds during the period when the dye is introduced into the river. The study runs to convergence in approximately two to three hours.

Simulation Results / Conclusions

Figures 4 and 5 present the velocity field surface and the concentration field surface.

Figure 7 presents a probe plot of the dye concentration at Robe Menzel Road.

For validation purposes, Figure 7 presents an example of a portion of the results of the dye study conducted by the WaDOE. The graph depicts the measured dye concentration in the river at Robe Menzel Road, approximately 4 miles downstream from where the dye was introduced into the river.

The measured concentration of Rhodamine dye in the river at this location is 7 parts per billion (ppb) at 6.75 hours after the dye is released upstream.

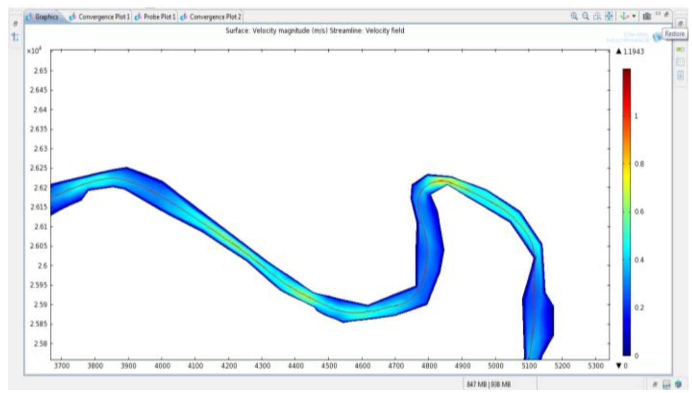

Figure 4. Partial Velocity Surface Plot

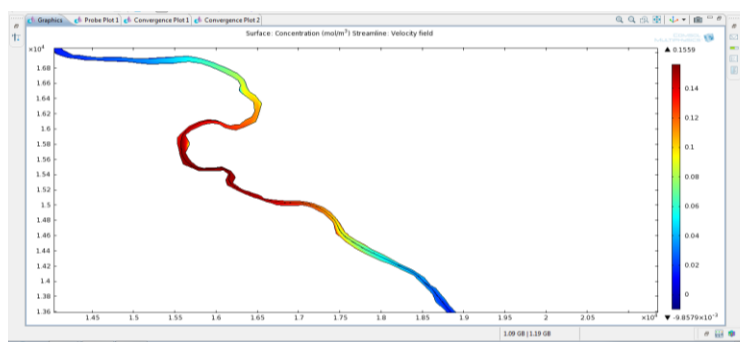

Figure 5. Partial Concentration Surface Plot

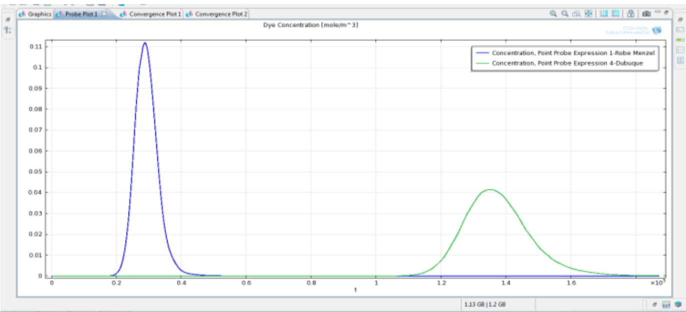

Figure 6. Solution - Probe Plot of Simulated Dye Concentration at Robe Menzel Road and at a Location Downstream

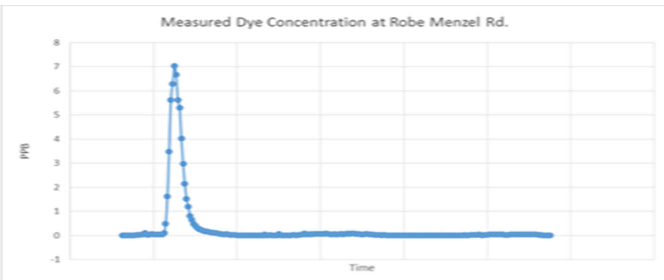

Figure 7. Measured Dye Concentration at Robe Menzel Road

Conclusions

COMSOL is able to simulate dye tracer studies in rivers and streams and, by extension, can be used as a quick response tool for estimating travel time and concentration degradation of pollutants and other chemicals in rivers and streams. This can be done with nothing more than stream bank geometry, readily available estimates of stream flow, and estimates of the mass of chemical introduced into the watercourse.

References

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Appendix

This paper is an excerpt from the book *Finite Element Solutions for Civil and Environmental Engineers using COMSOL Multiphysics*, Larry J. Matel, ISBN 978-1-7923-3260-9, 2020.