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About this Publication

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Executive Summary

Background

The U.S. Department of Defense has previously identified a need to predict and assess the consequences of chemical, biological, radiological, and nuclear (CBRN) releases. To help address this need, the Defense Threat Reduction Agency (DTRA) was assigned the responsibility of providing the DoD with core technical and operational support required to respond to CBRN release events. Subsequently, DTRA Reachback identified the Incident Command Tool for Protecting Drinking Water (ICWater) as one forecasting tool that can be used to predict the consequences of a chemical, biological, or radiological materials release within river or stream systems.

In 2012, DTRA tasked IDA to review ICWater version 3.2 and evaluate its utility as a tool for predicting waterborne transport and dispersion of hazardous materials. In a preliminary analysis, IDA reviewed the code's technical documentation and ran a few sample cases provided by DTRA Reachback. In this initial assessment we determined that, despite a few user-interface issues, ICWater operated as expected. These results are reported in detail in IDA Document D-4742, *Initial Assessment of Waterborne Hazardous Material Transport and Dispersion Prediction Tools for DoD Applications*.

Building upon the previous study, we have now completed a more in-depth evaluation of ICWater in which we compared model output to independent field data. The selected data came from a United States Geological Survey (USGS) dye study conducted in the Yellowstone River. We selected this study because it provided all the necessary information for setting up ICWater simulations and for comparing output and because the model developers have not used this region to calibrate their model.

Results of ICWater Evaluation using Yellowstone River Dye Studies

Early in this phase of IDA's waterborne model assessment, two bugs were discovered that prevented the code from working properly when simulating spills in the Yellowstone region. These bugs were resolved with a software patch provided by developers at Leidos. We presented the nature and resolution of these bugs to DTRA in a briefing in November 2013 and do not discuss them further here. However, the reader should note that all results presented in the remainder of this report were obtained using the patched version of ICWater 3.2. We ran three sets of simulations (see table below) to try to determine reasons for apparent discrepancies between the model results and field measurements. After running the ICWater model to simulate the Yellowstone River dye tracer studies, IDA reached the following key conclusions:

1. ICWater version 3.2 should not be used without installing the software patch provided by Leidos. Without this patch, ICWater should not be expected to operate correctly in the western United States.
2. The velocity-flow equation used in ICWater does not appear broadly applicable. The use of the current expression in the model likely contributes to notable discrepancies between model output and actual observations in the field.
3. Annual or seasonal variations in flow could also affect model predictions if default values in ICWater are used without verification.
4. Velocities calculated from flow measurements often fail to match observed or measured values. Mismatches between computed velocities and real-world velocities can result in simulated contaminant arrival times that are later than actual arrival times.
5. For the reasons cited above, it may be difficult to obtain ICWater predictions that accurately reflect the transport and dispersion of materials in many real-world rivers and streams.
6. Improving the model in the future will require a systematic approach for addressing differences between output and real-world observations. This might include using velocity measurements directly in the model rather than inferring it from flow data.
7. At present, the operational relevancy of ICWater might be limited.

The simulation results that led to the development of conclusions 2-7 are summarized in the table below. This table indicates where discrepancies occurred for each set of simulations. The header row indicates the simulation set, and the first column indicates the nature of the mismatch (i.e., the three areas in which predictions were off correspond to the arrival time, peak concentration, and duration). Yes or no signifies the predictions were correct or incorrect, respectively. The text after yes or no describes the nature of the error (e.g., No, delayed indicates that the model does not predict arrival times correctly and that the arrival of the model plume is later than the observed arrival).

Nature of Mismatch	**Case 1: Default or Base Case Simulations**	**Case 2: Simulations with Modified Velocity**	**Case 3: Simulations with Modified Velocity and Increased Dye Mass**
Correct arrival times?	No, delayed	Yes, notable improvement	Similar to case 2
Correct peak concentration?	No, overestimate	No, underestimate	Yes, but only for first measurement site

Correct plume duration?	No, too short	Yes, notable improvement	Similar to case 2

An important point arising from the above conclusions is that the model's assumed correlation between flow and velocity will strongly affect predicted contaminant arrival times and concentration values at arrival. Delayed arrival times or low concentration values could result in false negatives. In other words, model predictions may lead those responding to a spill to assume that a hazardous material will not arrive until a later time or that the concentration upon arrival will be too low to be of concern. ICWater's failure to accurately predict transport and dispersion in a real-world river indicates the possibility that local populations may be falsely warned of a threat, warned late, or not warned at all. A possible solution to this model limitation would be to collect velocity data directly. Doing so would help correct predictions of arrival times. However, the availability of velocity data is beyond the control of ICWater developers. Such data would need to be provided by the USGS (see Appendix C).

The ICWater developers were notified of IDA's findings in January 2014. At that time, they informed us that they were working on the next version of ICWater and that the changes in this version would address some of the limitations we found. As of this report, we have not evaluated a version of ICWater more recent than 3.2.

Next Steps for Validating Waterborne Hazardous Material Transport and Dispersion Models

Possible future areas for evaluating waterborne transport and dispersion models are discussed at the end of Chapter 4. Although additional features or aspects of ICWater can, and likely should, be evaluated, IDA's present findings suggest that emphasis should be placed on better understanding the physics and assumptions going into the model. This improved understanding is particularly important for determining velocity. Even though using measured velocity data directly seems to be the easiest way to achieve correct plume arrival times, ICWater cannot use these data unless they become widely available from the USGS. If measured velocity data are not available for use in the model calculations, taking steps to better understand the relationship between flow and velocity is important to improving the equations and/or modeling approach used in ICWater. Such improvements will hopefully yield more accurate time-concentration predictions in the future.

Similarly, it would be advisable to evaluate any newer versions of ICWater that may now exist. This would allow changes to the code to be tested and verified and any new or remaining limitations to be identified. Also useful would be the further identification of and, when possible, collection of data required for enhancing the model's operational relevancy (e.g., waterborne lethality data). Without such data, evaluating the implications of exposure to a waterborne hazardous material is not possible.

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Contents

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1. Introduction

A. Background and Project History

The release of chemical, biological, radiological, or nuclear (CBRN) materials into the environment can contaminate large areas, threaten food or water supplies, and potentially result in the death or sickness of large numbers of people, both military and civilian. Because of the significant threat posed by CBRN materials, the U.S. Department of Defense previously identified a need to predict and assess the consequences of CBRN releases [1, 2]. To help address this need, the Defense Threat Reduction Agency (DTRA) was assigned the responsibility of providing the DoD with core technical and operational support required to respond to chemical, biological, radiological, and nuclear release events.

In an earlier study [2], IDA provided DTRA an initial assessment of two waterborne transport and dispersion (T&D) modeling tools: the Incident Command Tool for Protecting Drinking Water (ICWater) and the System for the Hazard Assessment of Released Chemicals (SHARC). ICWater predicts the transport and dispersion of a toxic spill in a riverine environment; SHARC simulates the material transport and dispersion resulting from spills in littoral environments. IDA's initial assessment of these models focused on a review of the technical documentation and a series of preliminary analyses. These preliminary analyses were intended to demonstrate the reproducibility of model results by comparing output we obtained with example cases provided by DTRA Reachback and the developers of ICWater and SHARC.

The outcome of IDA's previous model assessment was that, besides a few minor user-interface issues, ICWater seemed to work as expected. On the other hand, SHARC was assessed as not yet ready for DoD applications or for rigorous validation. The conclusion that SHARC was unsuitable for general use was based on the code's lack of solid technical documentation, several apparent software bugs, and issues extracting outputs from the model. Details of IDA's earlier findings are provided in IDA Document D-4742 [2]. Because of the issues associated with the model, SHARC was not further evaluated during the present phase of IDA's waterborne T&D model evaluation.

For this study, IDA compared ICWater output to field data collected by the U.S. Geological Survey (USGS) during a series of dye tracer experiments in the Yellowstone River Basin [3]. During IDA's previous evaluations, ICWater was vetted using examples provided to the research team. By carrying out a comparative study using USGS field data, we could begin to independently assess the model's performance when applied to real-world conditions and to offer specific recommendations regarding ICWater's capability as a predictive tool. The following chapters discuss the current evaluation approach, study results, and implications of IDA's findings.

B. Study Summary and Motivation

To support DTRA Reachback's plans to model waterborne chemical transport and dispersion, IDA conducted a comparative study to evaluate the hazard prediction and assessment capabilities of ICWater. Our goal was to provide DTRA with follow-on information on the model's ability to simulate real-world conditions and to assess the implications for ICWater's operational relevancy. This report documents the second-year findings of IDA's assessment of ICWater.

As stated above, for this phase of the waterborne T&D model evaluation, we focused on comparing ICWater results to field data collected by the USGS [3]. Our main motivation in this analysis was to independently determine the extent to which ICWater is able to reproduce the transport and dispersion of a material released into a real-world river. During the previous phase the results from our initial analysis only verified that ICWater was able to reliably reproduce sample cases provided to IDA by the developer and DTRA Reachback. These sample cases modeled spills in rivers (e.g., the Potomac) that had been used previously by the developers to calibrate the model (e.g., [4]). Unlike the sample cases, the Yellowstone River has not been previously used to test ICWater and is located in a different hydrologic region than the rivers used in the earlier investigation.

Early in the study, IDA discovered two bugs in ICWater. The first issue was that ICWater maps would not open to the user-specified county and state (i.e., Yellowstone County in Montana). The second issue was that the user was unable to input flow and velocity data without crashing the code. IDA notified developers at Leidos[1] of the bugs in September 2013, and the issues were quickly resolved via a software patch provided in October.

After the installation of the software patch, these bugs are no longer an issue and are not further discussed in this report (the nature and resolution of these software bugs are documented in a briefing sent to DTRA in November 2013). The model results simulating the USGS Yellowstone river dye study are reported in Chapter 3. It is important to note that these results were obtained using the patched version of ICWater 3.2 (i.e., after the software bugs were resolved). The main finding from IDA's evaluation is that there will likely be some notable discrepancies between ICWater predictions and real-world observations.

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[1] In September 2013, the Science Applications International Corporation (SAIC) was split to create Leidos Holdings Inc. Leidos offers services to the national security, health, and energy sectors; SAIC remains focused on Government IT services. As a consequence of the split, ICWater developers are now part of Leidos.

The simulation results and conclusions reported in Chapter 3 were also presented to the developers at Leidos in January 2014. At that time, the developers told us that they were working on the next version of ICWater, which would incorporate changes to help address some of the limitations we identified. As of the writing of this report, ICWater 3.3 is available for assessment. However, we have yet to evaluate this latest version of ICWater.

C. Review of ICWater

This section provides a quick overview of the ICWater model. A more detailed description and additional references for the code can be found in Ref. 2. ICWater is a network-based, one-dimensional, semi-analytical transport and dispersion model[2] that incident commanders, water utility managers, and other emergency responders have used to make predictions regarding consequences of a toxic spill in a river or stream system. In general, the model was designed to assist with emergency management and response to chemical, biological, or radiological materials release within U.S. rivers. To obtain the necessary information on flow conditions, river networks, and public water supplies, ICWater interfaces with several online databases:

- The National Hydrography Database (NHDPlus)
- The U.S. Geological Survey real-time stream gauging network
- The EPA's Safe Drinking Water Information System (SDWIS).

The NHDPlus database supplies data on locations of connected river and stream networks in the contiguous United States and provides mean flow and velocity values for the reaches making up these networks. USGS river gauges return near-real-time stage data from stream-monitoring stations located throughout the United States (see Appendix C). Last, the SDWIS gives location and contact information for public water intakes and is used to identify populations that could be affected by a spill.

In addition to the values provided by the above databases, the user can supply information on the contaminant or agent that is released, the spill release location, spill size (i.e., concentration of released material), and flow rate (i.e., discharge) (Figures 1-1 and 1-2). We noted during our previous analysis that, although the user can specify flow by changing the value in the flow box in the Flow Factor GUI (Figure 1-2), he cannot specify velocity. Velocity is calculated internally using the velocity-flow equation hard-coded into ICWater. As discussed in Chapter 3, this feature causes a potential problem for reliably predicting transport and dispersion of waterborne materials in real-world rivers.

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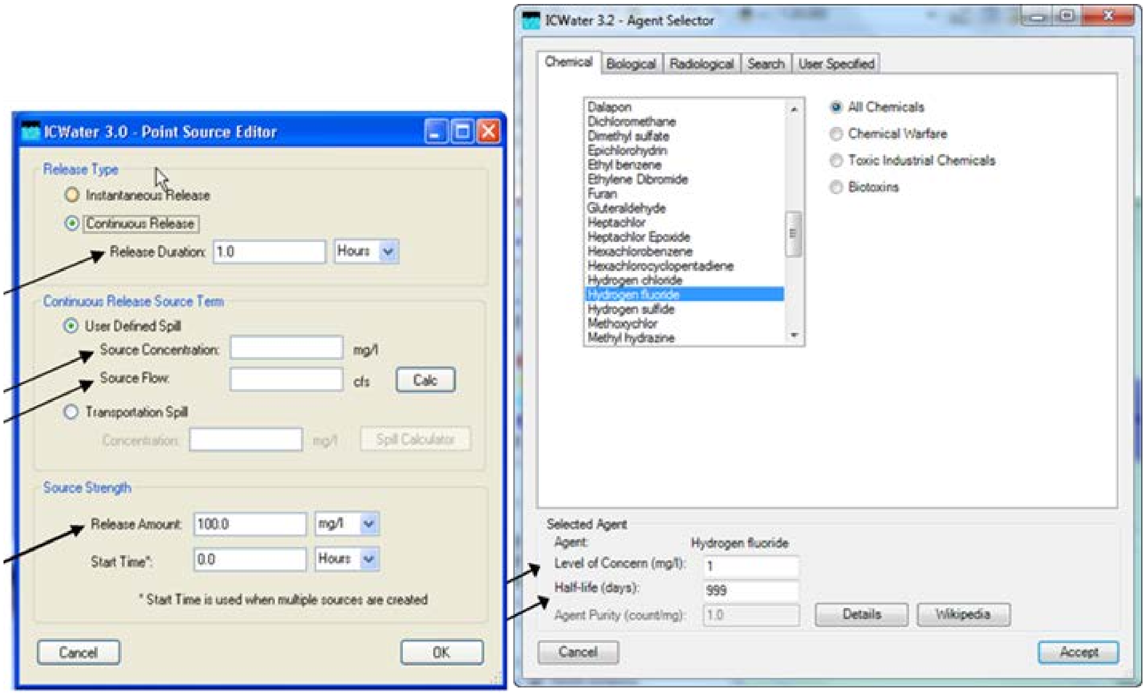
[2] A more in-depth discussion of ICWater that includes general limitations and strengths related to its being a one-dimensional model is presented in IDA Document D-4742.



ICWater 3.0 - Point Source Editor

Release Type

○ Instantaneous Release
● Continuous Release

Release Duration: 1.0 Hours

Continuous Release Source Term

● User Defined Spill

Source Concentration: mg/l
Source Flow: cfs

○ Transportation Spill

Concentration: mg/l

Source Strength

Release Amount: 100.0 mg/l
Start Time*: 0.0 Hours

* Start Time is used when multiple sources are created

ICWater 3.2 - Agent Selector

Dalapon
Dichloromethane
Dimethyl sulfate
Epichlorohydrin
Ethyl benzene
Ethylene Dibromide
Furan
Gluteraldehyde
Heptachlor
Heptachlor Epoxide
Hexachlorobenzene
Hexachlorocyclopentadiene
Hydrogen chloride
Hydrogen fluoride
Hydrogen sulfide
Methoxychlor
Methyl hydrazine

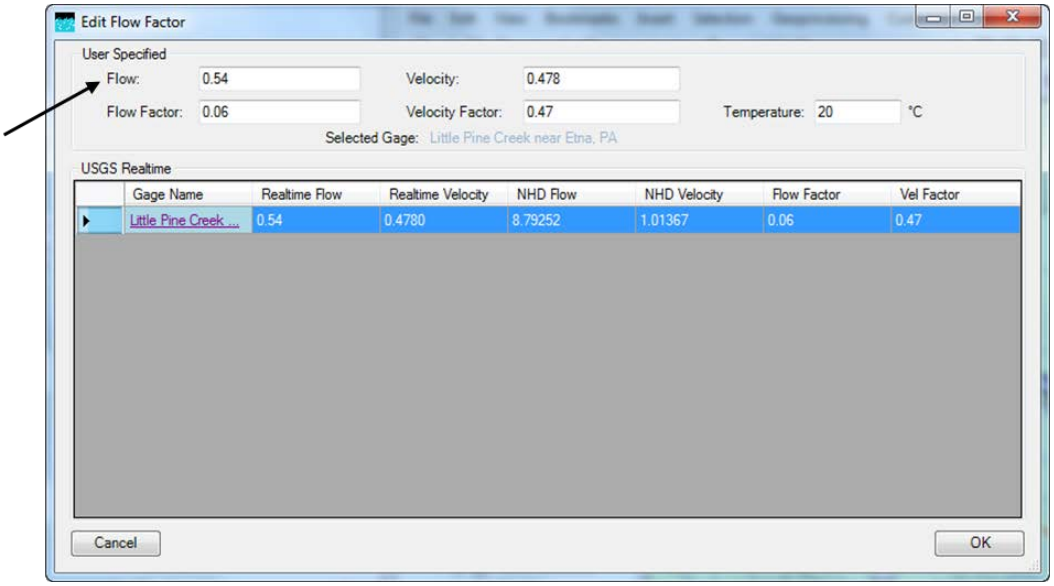
● All Chemicals
○ Chemical Warfare
○ Toxic Industrial Chemicals
○ Biotoxins

Selected Agent

Agent: Hydrogen fluoride
Level of Concern (mg/l): 1
Half-life (days): 999
Agent Purity (count/mg): 1.0

These graphical user interfaces allow the user to define the nature of the spill. User-defined parameters include the concentration of toxic material (left panel) and the contaminant being released (right panel).

Figure 1-1. GUI for Supplying Spill Parameters



Edit Flow Factor

User Specified

Flow: 0.54
Velocity: 0.478
Flow Factor: 0.06
Velocity Factor: 0.47
Temperature: 20 °C
Selected Gage: Little Pine Creek near Etna, PA

USGS Realtime

	Gage Name	Realtime Flow	Realtime Velocity	NHD Flow	NHD Velocity	Flow Factor	Vel Factor
▸	Little Pine Creek ...	0.54	0.4780	8.79252	1.01367	0.06	0.47

By default, NHD mean values are used as input for flow and velocity. However, if the user wishes, default flow values can be modified using the Flow Factor GUI pictured above. If the user does not wish to use gauge data, he or she can choose to define his or her own flow values by entering in a new value in the flow box. Once new flow is set, ICWater automatically updates velocity.

Figure 1-2. Flow Factor GUI

D. Report Outline

This paper contains three additional chapters as well as appendixes. Chapter 2 provides details on the USGS Yellowstone field study used as part of IDA's independent assessment of ICWater's predictive capabilities. Chapter 3 discusses the present model evaluation results in detail. This chapter also explores several factors that could cause ICWater to deviate from observations made in the field. Chapter 4 summarizes the results and conclusions presented in Chapter 3. Chapter 4 also reviews the operational implications of IDA's findings and suggests potential future areas of assessment that are still needed for ICWater. Appendix A provides sample tables and references for the time-concentration data reported in the USGS Yellowstone River dye study. Appendix B presents alternative velocity-flow equations that could be considered for future versions of ICWater. Finally, Appendix C reviews how USGS gauges work and how flow is calculated.

E. References

1. *Operational Requirements Document (ORD) for Joint Effects Model (JEM)*, 28 May 2004.
2. Institute for Defense Analyses, *Initial Assessment of Waterborne Hazardous Material Transport and Dispersion Prediction Tools for DoD Applications*, IDA Document D-4742, 2013.
3. McCarthy, P. M., *Travel Times, Streamflow Velocities, and Dispersion Rates in the Yellowstone River, Montana*, U. S. Geological Survey Scientific Investigations Report 2009-5261, 2009.
4. Bahadur, R., Samuels, W. B., Monteith, M., *NHD-Based River Spill*, Esri International User Conference, July 25-29, 2005.

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2. U.S. Geological Survey Yellowstone River Dye Study

A. Field Study Selection Criteria

Our first step in this study was to perform a comprehensive literature review and identify suitable field studies that could be used to verify ICWater output. The USGS Yellowstone River dye experiments were ultimately selected for IDA's comparative study for three main reasons.

First, this study provides both the necessary inputs (i.e., river flow and velocity values at the time of the dye experiments and the amount of dye released into the river) and outputs (i.e., time-concentration data giving the dye arrival times and concentration measurements at specified sites) needed for running the simulations and comparing the results.

Second, the developers had not previously used Yellowstone to calibrate the model. Furthermore, Yellowstone is in a different hydrologic region of the United States than the previous sample cases tested in the earlier evaluation of the ICWater. These qualities allow for an independent assessment of ICWater's predictive capabilities in a real-world environment.

Third, the Yellowstone River serves as a primary source for irrigation and recreation, is a municipal-water supply for several cities, and is a primary transportation corridor in Montana. These traits and a complex infrastructure make the river critical to the region and particularly vulnerable to accidental spills from tanker cars or trucks. Therefore, the Yellowstone River represents a plausible environment in which a toxic spill might occur, thus allowing IDA to draw reasonable operational conclusions about ICWater's predictive performance in an important hydrologic region of the western United States.

B. USGS Yellowstone River Dye Study Background

In late September and early October 2008, the USGS conducted a dye-tracer study to determine in-stream travel times, stream-flow velocities, and dispersion rates for the Yellowstone River from Lockwood to Glendive, Montana. In total, the studied area extended approximately 266 river miles downstream to the West Bell Street Bridge in the city of Glendive. Four dye injection sites are located at bridges near Lockwood, Myers, Cartersville, and Miles City, Montana (Figure 2-1 and Table 2-1). Dye concentrations were measured at three to four sites downstream from each dye injection site (Table 2-2). Dye travel time and concentration measurements were made during a 48-hour window after dye injection.

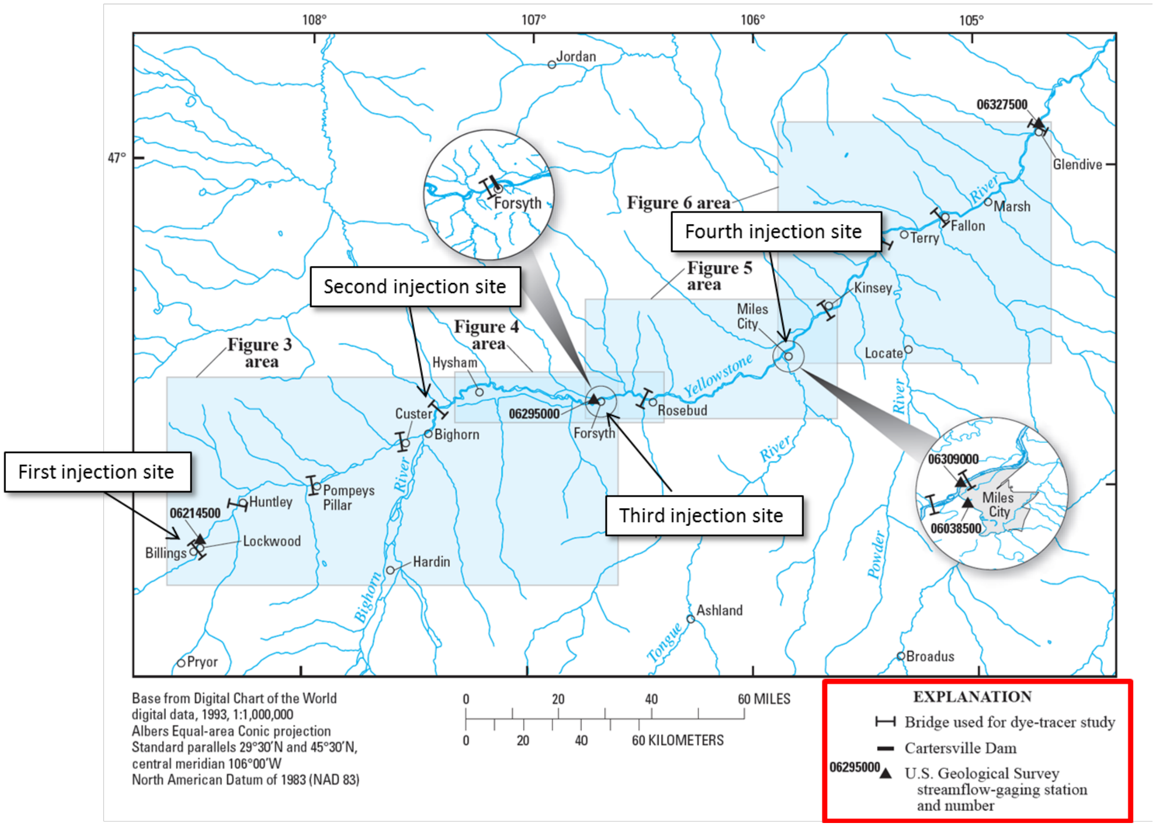

Figure 2-1. Map of the USGS Yellowstone River Dye Study Area and Injection Sites

For the experiment, the fluorescent dye Rhodamine WT was released at the selected injection sites. Rhodamine WT is a reddish-orange dye commonly used in tracer studies because it does not easily degrade in water and is non-toxic at the concentrations used in these studies. As with other fluorescent dyes, Rhodamine fluoresces when exposed to light. This property allows the dye to be detected at the µg/L range using a fluorometer. Although some physiochemical factors can affect fluorescent dyes, Rhodamine WT is considered to behave as a conservative constituent[1] (i.e., the dye is minimally adsorptive and has high chemical stability). Therefore, changes in dye concentration are realistically attributable to transport and dispersion processes that should be captured by the ICWater model. (If desired, further information on Rhodamine WT and dye fluorometry is provided in References 1-4.)

Steady stream flow conditions prevailed at the time of the USGS study. Specific information on the injection site locations, the date of the dye injection, the mass of dye released, the agent level of concern (LOC) and half-life,[2] and the river flow and velocity at

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[1] In general, some dye loss can occur as a result of deterioration from exposure to sunlight (photodecay) and sorption onto the river banks or river bottom. This is expected to be minimal for Rhodamine WT dye.

[2] Agent LOC and half-life were set to 999 in the ICWater simulations since the Rhodamine WT dye used in the experiment is nontoxic and, as explained above, is considered a conservative constituent.

the injection site are given in Table 2-1. Table 2-2 provides the latitude and longitude of the downstream sites where dye concentration measurements were made. A report summarizing the data collected at each of the measurement sites between Lockwood and Glendive was produced by USGS as a final product of their dye-tracer study [5]. This report is the source of data used by IDA during the present evaluation of ICWater (Appendix A).

Table 2-1. Injection Sites and Key Parameter Values

Injection Site Name	Injection Site Lat/Lon	Date of Injection	Release amt (lbs)	Flow (cfs)	Velocity (ft $^{s-1}$)	LOC and ½ Lift
Lockwood (near Billings)	45.7973N/ -108.4694E	Oct 6, 2008	174	3500	3.83	999
Myers (near Custer)	46.2544N/ -107.3455E	Sept 29, 2008	54	6750	3.42	999
Catersville (near Forsyth)	46.275N/ -106.6797E	Sept 26, 2008	84	6860	3.55	999
Miles City	46.4208N/ -105.860E	Sept 23, 2008	132	7420	3.75	999

Agent LOC and half-life were set to 999 since the dye is benign and is considered a conservative constituent.
Release amount, flow, LOC, and half-life are input by the user via ICWater's graphical user interfaces (GUIs).
Measurements up to 48 hours after dye injection are used in the study.

Table 2-2. Injection and Measurement Site Locations

Injection Site Name	Injection	1st Measurement	2nd Measurement	3rd Measurement	4th Measurement
Lockwood (near Billings)	45.797348N/ -108.469416E	45.903889N/ -108.31975E	45.996667N/ -108.009521E	46.142222N/ -107.548889E	46.254444/ -107.345556
Myers (near Custer)	46.254444N/ -107.345556E	46.264466N/ -106.696086E	46.275N/ -106.67972E	46.274722N/ -106.464722E	NA
Cartersville (near Forsyth)	46.275N/ -106.67972E	46.274722N/ -106.464722E	46.398346N/ -105.895779E	46.531631N/ -105.714054E	NA
Miles City	46.420833N/ -105.860E	46.531631N/ -105.71405E	46.779697N/ -105.411308E	46.855556N/ -105.116501E	47.105683N/ -104.71918E

Measurements up to ~48 hours after a dye injection are used in the study.
Over this 48-hour period, USGS took three to four measurements per dye injection.
The arrival time and the peak concentration of the dye at these locations are compared to ICWater output.
The measurement sites above span from Huntley to Glendive, Montana.

C. References

1. *Water Tracing, In Situ Dye Fluorometry and the YSI 6130 Rhodamine WT Sensor*, White paper, YSI Environmental, 2001.
2. Smart, P. L. and Laidlaw, I. M. S., *An Evaluation of Some Fluorescent Dyes for Water Tracing*, Water Resources Research, Vol. 13, pp. 15-33, 1977.
3. Field, M. S., *The QTRACER2 Program for Tracer-Breakthrough Curve Analysis for Tracer Tests in Karstic Aquifers and Other Hydrologic Systems*, U.S. Environmental Protection Agency, National Center for Environmental Assessment, Washington D.C., p. 179, 2002.
4. Sabatini, D.A. and Austin, T.A., “Characteristics of Rhodamine WT and Fluorescein as Adsorbing Ground-Water Tracers,” *Groundwater*, Vol. 29, pp. 341-349, 1991.
5. McCarthy, P. M., *Travel Times, Streamflow Velocities, and Dispersion Rates in the Yellowstone River, Montana*, U. S. Geological Survey Scientific Investigations Report 2009-5261, 2009.

3. Evaluation of the Incident Command Tool for Drinking Water Protection

In this chapter, we document IDA's assessment of a revised version of ICWater: one with a software patch installed to resolve two bugs identified by IDA; otherwise, it is the same as ICWater 3.2. Prior to installing the software patch, we discovered that ICWater 3.2 would not properly run in the Yellowstone region. Consequently, it is important to note that all the results provided below were obtained using the patched version of ICWater 3.2.

The purpose of this phase of model evaluation is to provide further information on ICWater's expected capability for predicting spills in real-world rivers. This includes assessing the code's strengths and limitations regarding its operational use or relevancy. For this analysis, IDA first compared ICWater's output to the USGS dye study data from the Yellowstone River. This comparative portion of the analysis proceeded in three stages.

In the initial set of simulations, the values for river flow[1] and dye mass were set equal to the values reported by the USGS at the time of the dye injection (see Table 2-1). This approach to setting up a simulation is assumed to be the approach a first responder would use in the event of a hazardous material release into the river. As discussed below, several discrepancies between the model output and the field data were apparent in these first set of simulations.

Because of the disagreement between the base case model results and field observations, IDA ran a second and third set of simulations to attempt to determine the reasons for discrepancies and to identify potential solutions. The second set of simulations looked at the effects of indirectly increasing model velocity.

The third set of simulations looked at the extent by which dye mass would have to be increased in the model to allow simulated concentration values to match measured values. Even with the adjustments to velocity and dye mass, ICWater was unable to fully reproduce the USGS reported time-concentration curves. Because of the model's failure to reproduce the field observations, we also investigated possible explanations for the observed discrepancies. As an outcome, we identified the velocity-flow relationship used in ICWater as a probable source for the observed model discrepancies.

In summary, this chapter covers the following material:

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[1] Note that in ICWater only flow can be input or adjusted by the user. Velocity is automatically calculated from flow based on hard-coded parameters. See Chapter 1 for more details.

- Results from simulations for which flow and dye mass values were set equal to values reported in the USGS study
- Results from simulations for which flow values were set higher than values reported in the USGS study
- Results from simulations for which both dye mass and flow values were set higher than values reported in the USGS study
- Possible explanations for model discrepancies.

A. ICWater Simulation Results

In this section we summarize the key findings, results, and recommendations arising from the present IDA assessment of waterborne hazardous material transport and dispersion prediction tools for DoD applications. The section is broken into four parts: (1) a discussion of results from a set of base case simulations in which input values for flow and dye mass were set equal to values reported in the USGS study; (2) a discussion of results from a set of simulations in which model flow was increased such that model velocity equaled measured velocity; (3) a discussion of results from a set of simulations in which model dye mass was increased along with flow; and (4) a discussion of the implications arising from IDA's present work.

1. Results from a Basic Set of Simulations (Base Case)

For the first set of simulations run by IDA, input values for flow and dye release amount were set equal to the values reported in the USGS study (given in Table 2-1). Results from these simulations were plotted as time-concentration curves from which the times of arrival for the leading edge, peak concentration, and trailing edge at each measurement site can be obtained (see Table 2-2 for the location of the measurement sites). Figure 3-1 gives the time-concentration curves for each of the four dye experiments conducted by the USGS in their Yellowstone River study. The initial injection sites were located at Lockwood, Myers, Cartersville, and Miles City. For each injection, three to four downstream measurements were made (represented by the different curves in each panel of Figure 3-1). Blue curves represent the data collected during the USGS dye study. Green curves represent the travel times and concentration levels predicted by ICWater. Solid, dotted, dashed, and dash-dotted lines represent results associated with the first, second, third, and fourth measurement sites, respectively. A red line indicating the LOC for the nerve agent soman[2] was also included in the plots for additional illustrative purposes.

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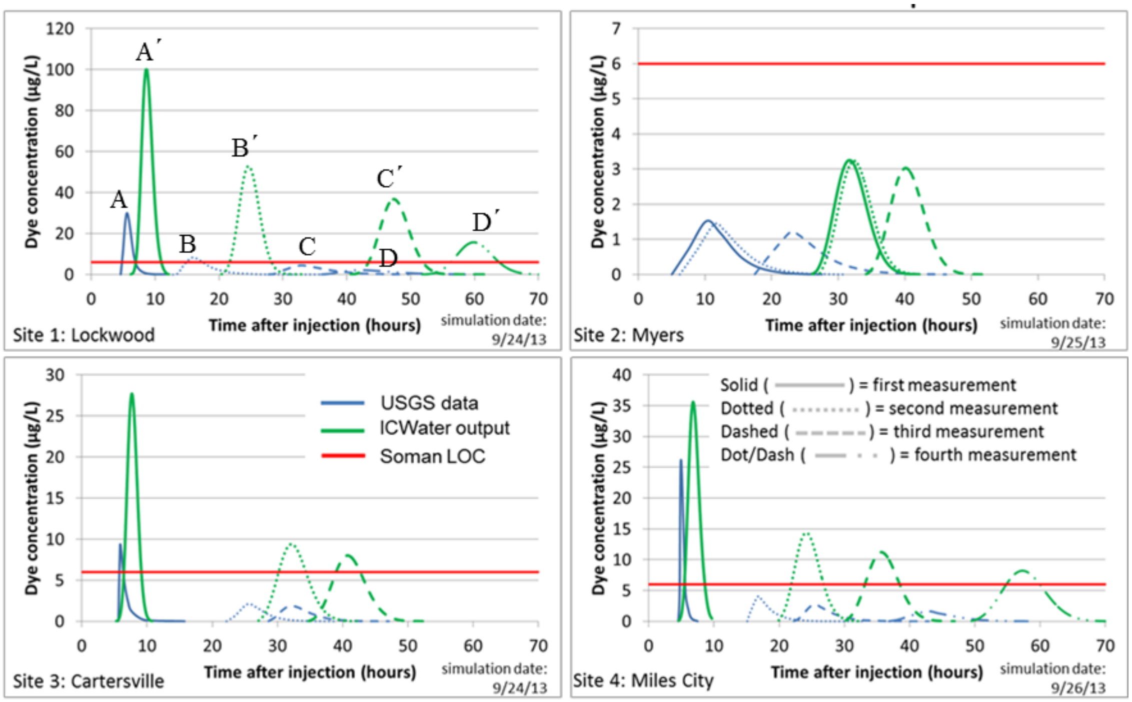
[2] Soman is moderately soluble in water. Following release of soman into water, a population can be exposed by drinking contaminated water or getting contaminated water on their skin [1]. The LOC for soman is reported in the ICWater database as 6 μg/L. We note that dye release amount between 54 and 174 pounds could be considered as an approximate surrogate for small-scale releases of a nerve agent in the river.



Letters indicate corresponding curves. For example, "A" indicates the first USGS measurement site and "A′" indicates the ICWater output for that measurement site.[3] The lack of alignment between the corresponding peaks signifies a mismatch between USGS and ICWater concentration levels and arrival times at the site.

Figure 3-1. USGS Field Measurements versus ICWater Output

The results illustrated in Figure 3-1 show three points for which significant discrepancies exist between the USGS field data and model output:

1. Arrival times of the dye plume are significantly delayed in the model with respect to the observed plume arrival times. This delay can be longer than the observed plume duration (i.e., the arrival time of the dye plume predicted by ICWater is after the departure time observed by the USGS).
2. The durations[4] of the dye plumes tend to be shorter in ICWater.
3. ICWater consistently over predicts peak concentrations at the measurement sites.

Accurate knowledge of the time of arrival and time of passage of waterborne contaminants is vital for protecting local populations who draw water from the river or use it for recreational purposes. To be a useful planning tool, ICWater must allow users to

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[3] The first panel in Figure 3-1 has the additional labels A, A', etc., to help the reader interpret the connection between the USGS and ICWater curves. To avoid clutter in the graphs, this labeling is not continued in subsequent panels. However, curves in all panels are related in the same manner.

[4] Duration of the plume can be defined as the time when concentration exceeds some prescribed threshold of interest. In these simulations, we used the soman LOC indicated by red lines in Figures 3-1 and 3-3.

safely prepare for the arrival of a contaminant. In particular, the delayed plume arrival times are problematic for the operational use of ICWater.

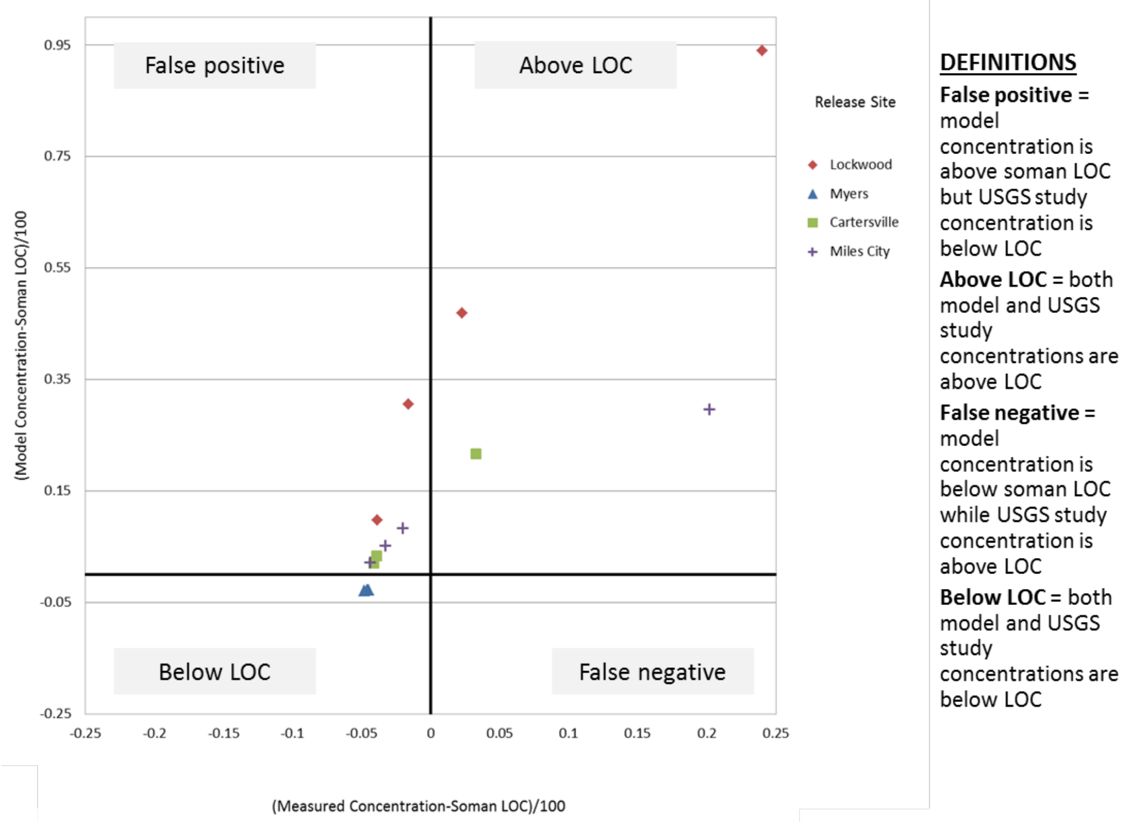
Potential consequences of the prediction of arrival times that are later than actual arrival times are that those responsible for mitigating the consequences of a spill may not close water intakes in time to allow the contaminant to safely pass by, or they may not issue timely warnings to the affected population. While correctly predicting the duration of a plume is also important, in the event of a spill, a monitoring system will likely be put in place to verify when the contaminant plume has past. Therefore, with regard to plume timings provided by ICWater, it is likely more important that the model be able to predict arrival times accurately.

In addition to problems of predicting plume arrival and departure times, ICWater does not correctly provide peak concentrations. Because ICWater tends to estimate higher dye concentration levels than those observed in the field, this could result in a number of false positives in a real spill scenario. Although it was not observed during the present evaluation, if ICWater consistently misestimates concentration levels, false negatives are also a possibility.

Traditionally, a false positive indicates that the model concentration is above some level of concern while the measured concentration is below this level of concern. Similarly, a false negative indicates that model concentration is below some level of concern while the measured concentration is above this level. However, IDA notes that false positives and false negatives can also be related to arrival times. When predicted plume arrival times are delayed, this can result in a false negative in the sense that hazardous material will arrive at a location before it is expected. Similarly, predicted early arrival times could be viewed as false positives since responders would anticipate hazardous material at a location prior to its arrival. Therefore, although ICWater provides false positives in relation to concentration values, the model also provides false negatives when considering arrival times.

The potential problems associated with overestimating the peak concentration can be illustrated by assuming that soman was released into the river instead of Rhodamine WT dye. Model concentration levels exceed the soman LOC of 6 μg/L (indicated by the red lines in Figure 3-1) at seven points. However, at these same points, the measured concentration remains below the LOC – resulting in a number of false positives (Figure 3-2). This thought experiment illustrates that, due to significant differences between predicted and actual plume concentrations, there can be instances in which the model could produce false positives or false negatives. Figure 3-2 suggests that if soman nerve agent had been released into the Yellowstone River during the time of the USGS study, ICWater's predicted concentration values would have resulted in false positives at 7 of the 14 measurement sites.

The primary detriment of false positive declarations related to the concentration levels is that they can result in unnecessary actions being taken during a spill event. In a similar fashion, it is also important to note that the false negatives related to arrival times may convince a user that no additional response is needed at that present stage and the local population may not receive timely warning. In the cases reviewed during this study, the false negatives associated with incorrect plume arrival times were more significant because of the potential for delayed response efforts. Nevertheless, costly consequences can still be associated with the false positives in terms of unnecessary resources being used to respond to a perceived threat.



DEFINITIONS

False positive = model concentration is above soman LOC but USGS study concentration is below LOC

Above LOC = both model and USGS study concentrations are above LOC

False negative = model concentration is below soman LOC while USGS study concentration is above LOC

Below LOC = both model and USGS study concentrations are below LOC

A comparison of measured and simulated concentration values to the soman LOC. This plot illustrates the possibility of false positive or false negative declarations.

Figure 3-2. False Indications Related to Concentration Provided by Model Output

A possible explanation for the discrepancy between ICWater output and the USGS field data is that velocity in ICWater is computed based on the expression [2]:

$$V = aQ^b \tag{3-1}$$

where *V* is velocity and *Q* is flow. The parameters *a* and *b* are specific to river regions.[5] Parameters, *V*, *a*, and *b* cannot be directly altered by the user. The user can only specify flow by changing the default value for *Q* in ICWater's Flow Factor GUI (Figure 1-2). Based on the user-supplied value for *Q* and the values set internally by ICWater for *a* and *b*, the model computes a velocity value for each part of the river. As shown in Table 3-1, in the case of this study, the computed ICWater model velocities are consistently lower than the USGS-measured river velocities. Based on this observation, IDA conducted a second set of simulations to explore the effects of velocity on model output.

Table 3-1. USGS Flow and Velocity versus Model Flow and Velocity

Injection Site	USGS Q (ft^3/s) **Measured**	USGS V (ft/s) **Measured**	Input V (ft/s) Determined from **$V = aQ_{USGS}^b$**	**Dye Release Date**
Site 1	3500	3.83	2.796	Oct 6, 2008
Site 2	6750	3.42	1.816	Sept 29, 2008
Site 3	6860	3.55	2.660	Sept 26, 2008
Site 4	7420	3.75	2.690	Sept 23, 2008

ICWater input velocities are consistently lower than those observed in the study.

Lower model velocity is possible explanation for the delayed dye travel times.

To investigate the degree to which velocity affects travel times in the model, IDA ran a second set of simulations in which input velocity was increased. The increased velocity was set to match the measured.

2. Results from a Set of Simulations with Increased Model Velocity

The second set of simulations was used to investigate the extent to which model velocity affects the dye concentration levels and plume travel times output by ICWater. For these simulations, we increased the input *Q* until the velocity values in the Flow Factor GUI matched those reported in the USGS study. In Table 3-2 we see that matching initial model velocities to USGS-measured velocities requires the user to set *Q* to values much higher than the measured flow.

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[5] Parameter *b* values differ based on the hydrologic region. For the Yellowstone region, the parameter *b* is set to 0.230375. Depending on injection site, ICWater's values for *a* vary from 0.23690 to 0.42422.

Table 3-2. Model Input Flow Required to Match USGS Measured Velocity

Injection site	USGS Q (ft^3/s) *Measured*	User adjusted Q (ft^3/s)	USGS V (ft/s) *Measured*	Input V (ft/s) *Determined from* $V = aQ_{USGS}^{b}$	Dye Release Date
Site 1	3500	14176.898	3.83	3.83	Oct 6, 2008
Site 2	6750	112400	3.42	3.42	Sept 29, 2008
Site 3	6860	24736.961	3.55	3.55	Sept 26, 2008
Site 4	7420	32470.370	3.75	3.75	Sept 23, 2008

Now agrees with USGS study measurements

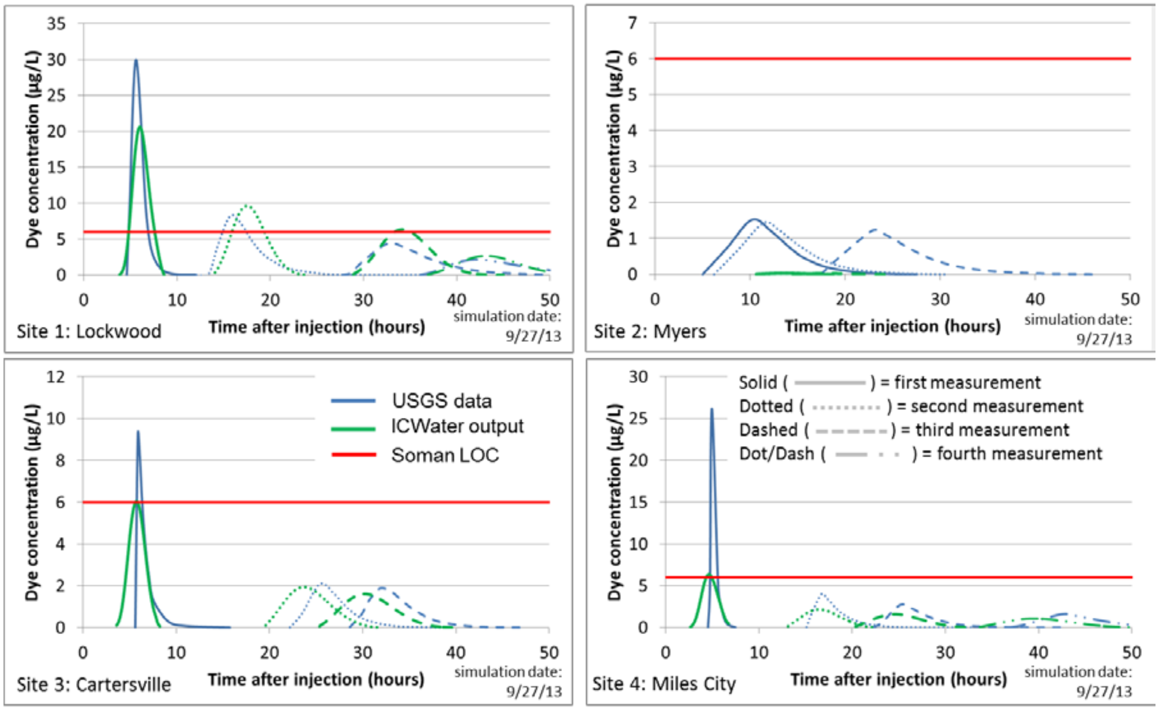
User must set Q to higher than observed in USGS study to match measured velocity values

Approach:

Instead of using the USGS measured values for initial Q, IDA entered a flow value that results in an input velocity equal to the USGS dye study velocity.

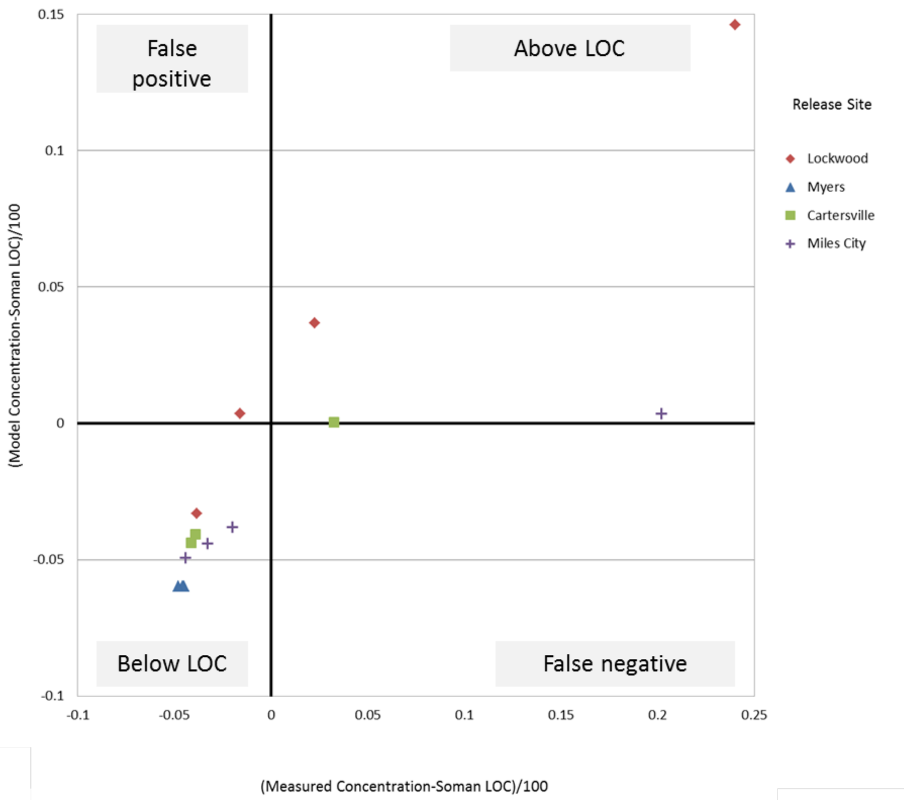
All other input values are the same as the ones used in the first set of simulations already presented.

As with the first set of simulations, results are displayed in the time-concentration curves below (Figure 3-3). After increasing the initial model velocities to make them equal to the USGS-reported velocities, the differences between predicted and measured arrival times, which were observed in the initial base case simulations, were notably reduced. Overall, better agreement exists between measured and predicted values in this set of simulations. However, durations over which dye is detected at measurement locations are still somewhat shorter in ICWater than in the field study. In addition, the model is now more likely to underestimate the peak concentration levels. Because of the lower concentrations predicted by the model, the likelihood of obtaining false positive declarations is greatly reduced in this particular scenario (shown in Figure 3-4). The seven false positives in the previous set of simulations have been reduced to one false positive. In this case, ICWater's tendency to under predict the dye concentration levels did not cause any false negatives. However, false negatives remain a possibility whenever model concentration is significantly underestimated.



Time-concentration curves for Rhodamine WT dye released at four injection sites in the Yellowstone River: Lockwood, Myers, Cartersville, and Miles City. For each injection, three to four downstream measurements were made as represented by the curves above. Blue curves represent data collected during the USGS dye study. Green curves represent predicted travel times and concentration levels output by ICWater. Solid, dotted, dashed, and dash-dotted lines represent results associated with the first, second, third, and fourth measurement sites, respectively. By increasing the initial model flow reported by the USGS, initial model velocities were made to match USGS measured velocities. This approach reduced discrepancies previously observed (Figure 3-1) in dye plume arrival times and duration. The red lines indicate the soman level of concern. Letters indicate corresponding curves.

Figure 3-3. USGS Field Measurements versus ICWater Output



DEFINITIONS

False positive = model concentration is above soman LOC but USGS study concentration is below LOC

Above LOC = both model and USGS study concentrations are above LOC

False negative = model concentration is below soman LOC while USGS study concentration is above LOC

Below LOC = both model and USGS study concentrations are below LOC

A comparison of measured and simulated concentration values to the soman LOC. The reduced number of false positives relative to Figure 3-2 is due to increasing initial model velocities until they match USGS measured velocities. To match velocities, model flow had to be greatly increased over the measured values. Although not the case here, this approach to improving model results could lead to an increase in false negatives.

Figure 3-4. False Indications Provided by Model Output

Finally, in an attempt to address the mismatch between model and measured dye concentrations, IDA conducted a third set of simulations to explore the effects of agent release amount on model output. This final set of simulations uses the same flow values as the second set of simulations, but assumes that increased amounts of dye were released.

3. Results from a Set of Simulations with Increased Model Dye Mass

Assuming the parameters set in the second set of simulations, IDA used the third set of simulations to investigate the amount of additional dye mass that would have to be added in the model in order to have the predicted peak concentration levels approximate the measured values. Although this approach is not a recommended solution for attempting to resolve model discrepancies, it does help further illustrate the degree to which ICWater could incorrectly estimate the dispersion of material in a riverine environment. A larger difference between model and actual dye mass translates to a larger discrepancy in concentration levels.

The data in Table 3-3 show that anywhere from 1.5 to 50 times more dye mass must be added to the model for initial predicted peak concentration levels to agree with observed values. In addition, as shown in the time-concentration curves below (Figure 3-5), increasing the dye mass in the model greatly improves agreement between predicted and measured concentration values only at the *first* measurement site. As the dye moves away from the release locations, differences between model and measured concentration values again become apparent.

Table 3-3. Model Input Flow Required to Match USGS Measured Velocity

Injection Site	Input Q (ft^3/s) User Selected	Input V (ft/s) Determined from $V = aQinput^b$	Increased Release Amt (lbs) Cincr	Flow Ratio Qi_{nput}/QUSGS	Velocity Ratio V_{input}/V_{USGS}	Release Ratio Cincr/$_{CUSGS}$
Site 1	14176.898	3.830	261	4.050	1.0	1.5
Site 2	112400	3.420	2700	16.652	1.0	50
Site 3	24736.961	3.550	126	3.606	1.0	1.5
Site 4	32470.370	3.750	528	4.376	1.0	4

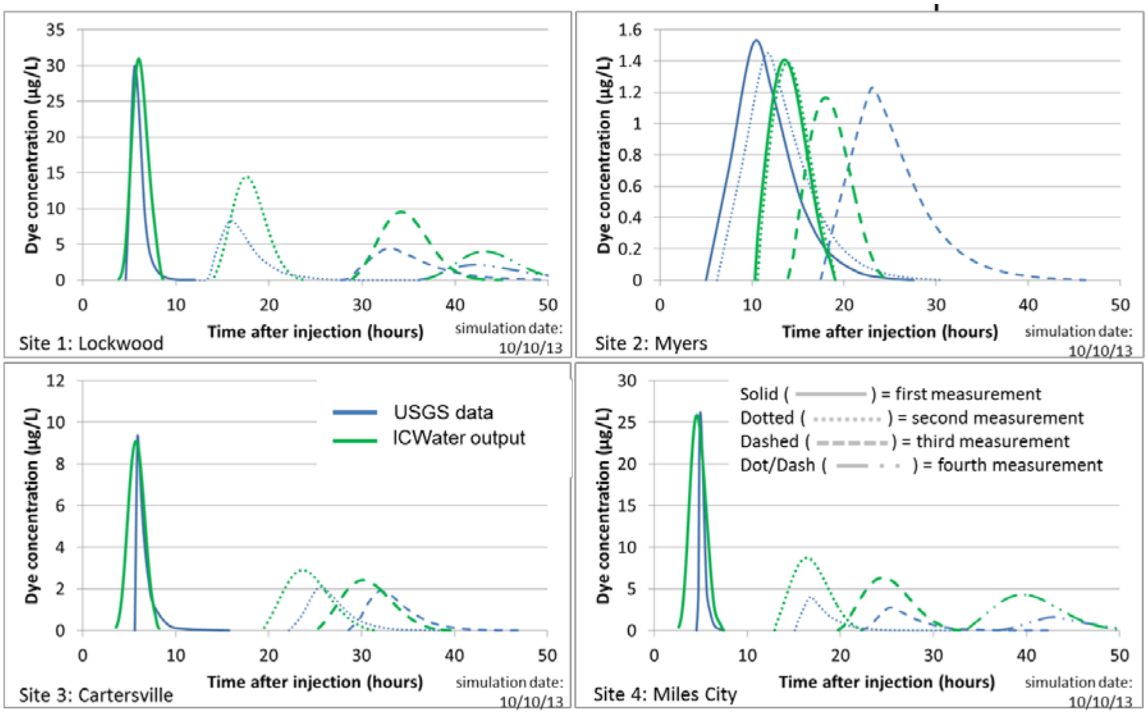
Approach:

Instead of using the USGS measured values for Q, input a flow value, Q_{input}, that results in an input velocity, V_{input}, that is equal to the USGS dye study velocity, V_{USGS}.

Next, increase the initial dye release amount, C_{incr}, such that ICWater peak concentrations approximate the peak concentrations, C_{USGS}, observed at the measurement sites.

All other input values are the same as the ones used in the first set of simulations.

Compare new output to field data to see how well differences previously observed are reconciled by this approach.



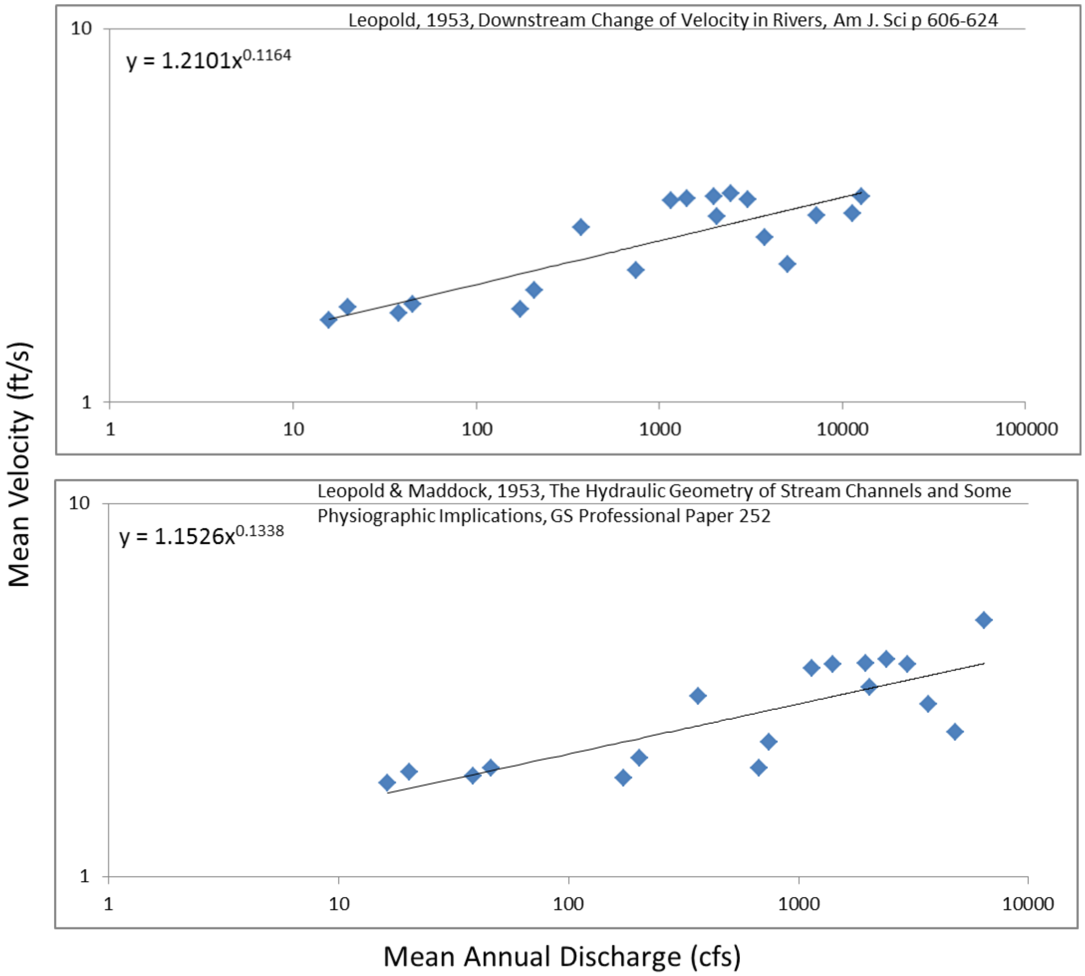
Time-concentration curves for Rhodamine WT dye released at four injection sites in the Yellowstone River: Lockwood, Myers, Cartersville, and Miles City. For each injection, three to four downstream measurements were made as represented by the curves above. Blue curves represent the data collected during the USGS dye study. Green curves represent the predicted travel times and concentration levels output by ICWater. Solid, dotted, dashed, and dash-dotted lines represent results associated with the first, second, third, and fourth measurement sites, respectively. By increasing the model flow and released dye amount above that reported by the USGS, discrepancies originally observed (Figure 3-1) in peak concentrations are somewhat reduced.

Figure 3-5. USGS Field Measurements versus ICWater Output

B. Implications of the Model Velocity-Flow Equation Used by ICWater

From the three sets of simulations reviewed above, the primary conclusion is that it may be difficult for operational models to accurately predict the transport and dispersion of materials in many real-world rivers and streams. Based on the work in this study, it appears that the best way to correct model predictions is to directly use measured velocity data instead of approximating velocity from flow (see Appendixes B and C for further discussion on the topic of flow versus velocity). Unfortunately, the USGS does not typically report velocity. Unless velocity data become widely available, ICWater developers will likely have to rely on identifying other factors responsible for model discrepancies. Isolating these responsible factors likely requires a closer look at the equations and assumptions used in the model [2].

Additional data in the hydrology literature may yield more robust relationships or expressions that could be used by ICWater developers [e.g., 3-6]. The source and values for parameters *a* and *b* should similarly be investigated. As part of a study investigating downstream changes of velocity in rivers, Leopold and Maddock [3] and Leopold [4] organized and reported a large amount of data on river velocities made at stream-gauging stations. They also presented comparisons of how velocity varies with discharge (i.e., flow) in the Yellowstone, Bighorn, Missouri, and Mississippi rivers. As shown in Figure 3-6, plotting these velocity-versus-discharge data and finding the best fit to the data, suggests alternative *a* and *b* values for the Yellowstone River system. The parameter values suggested by the Leopold and Maddock [3] and Leopold [4] data differ from the values that are presently hardcoded into ICWater. For the region, ICWater uses $b = 0.230375$ rather than the literature values of $b = 0.1164$ or 0.1338. Depending on injection site, ICWater's values for *a* vary from 0.23690 to 0.42422 versus ~1.2 in the literature.

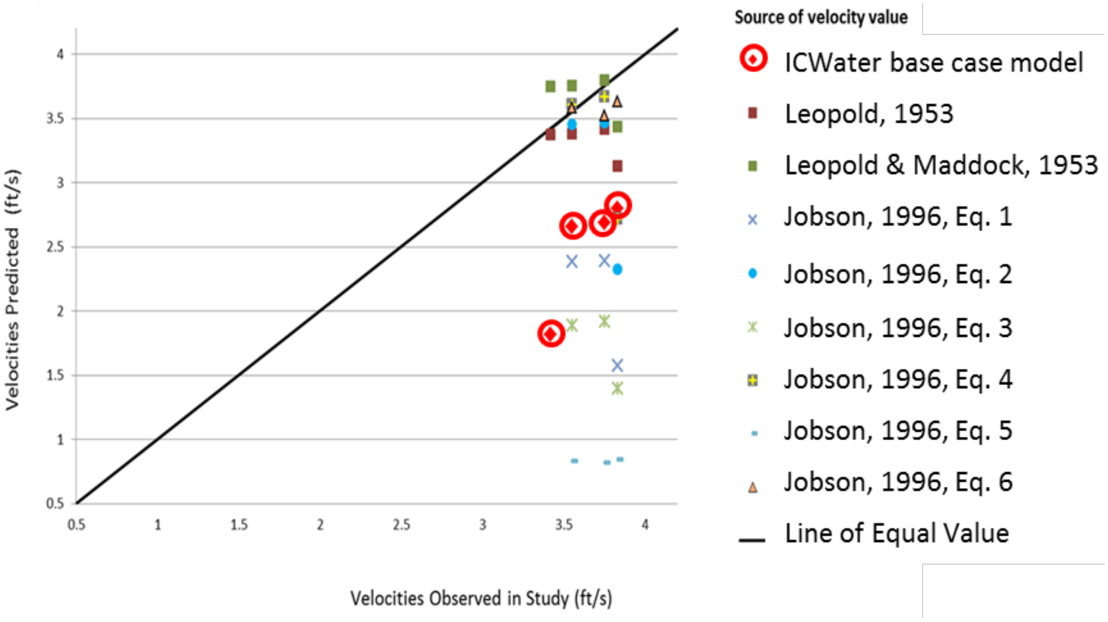


The plotted data are taken from References 3 and 4. These values suggest *a* and *b* values that differ from those used in ICWater calculations.

Figure 3-6. Relation of Mean Velocity to Discharge in the Yellowstone River

A report by Jobson [5] is specifically focused on effectively estimating travel times and dispersion in streams and rivers. He correctly acknowledged that even excellent models cannot be used confidently without calibration and verification to a particular river reach first. To try to help address this problem, Jobson [5] provides extensive data on time of travel and dispersion. More than 980 subreaches for about 90 different rivers were analyzed by Jobson. Using his data, he developed a series of prediction equations based on the drainage area, the reach slope, the mean annual discharge, and the discharge at the time of the measurement. These equations are explained and reproduced for the reader in Appendix B.

As illustrated in Figure 3-7, USGS-measured velocity values can be compared to the values computed by ICWater and those predicted from the literature. In this case, by inserting their values for *a* and *b* into ICWater's velocity-flow equation, Leopold [4] and Leopold and Maddock [3] are able to improve upon ICWater's default base case predictions. Similarly, some of Jobson's equations [5] do a better job than ICWater of predicting the velocity during the time of the USGS Yellowstone dye study. Clearly, a better approach may exist for modeling the velocity-flow relationship. However, a more systematic investigation into ICWater's modeling approach was not conducted. This is a potential area for future study. Another possible avenue would be to work with the USGS to determine the possibility of obtaining both measured velocity and flow data. This could be useful since having direct access to velocity data appears the easiest and most reliable way to improve model predictions.



Points falling closest to the line of equal value (solid black line) indicate the best agreement with the USGS field data recorded during the Yellowstone River dye experiment. Base case ICWater predictions (red diamonds) are not as accurate as several of the predictions taken from the literature. This indicates that alternative velocity-flow equations or updated parameters may be needed in ICWater. The Jobson equations referenced in the legend are given in Appendix B.

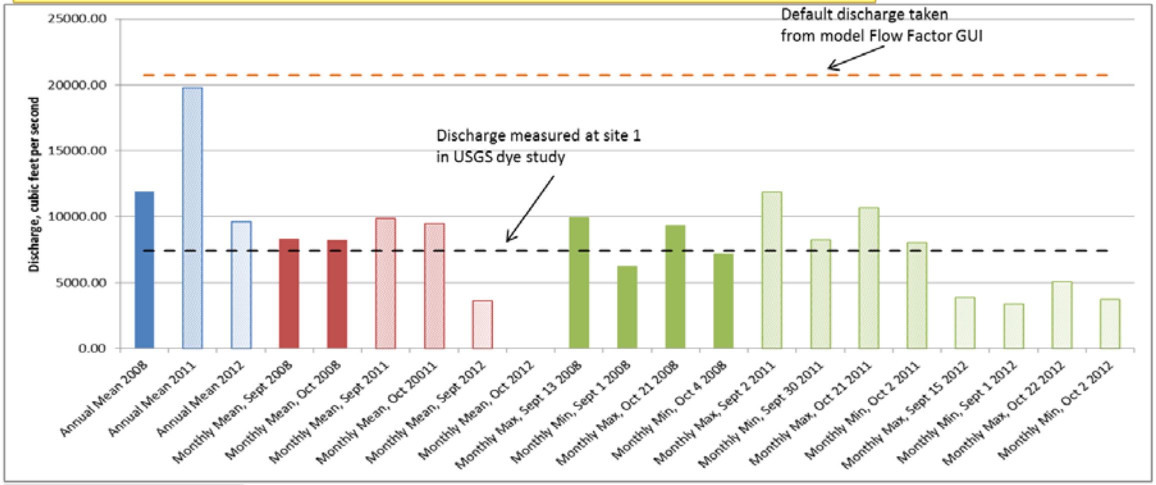
Figure 3-7. Comparison of ICWater and Literature Predicted Velocities to USGS Measurements

C. Other Considerations: Annual and Seasonal Variations in Flow

Other factors that could contribute to inaccurate predictions are temporal variations in flow resulting from changes in seasons, droughts, or flood years. As one example of these variations, average annual, monthly, and daily flow values at Miles City, Montana are shown in Figure 3-8. The plotted data were obtained from USGS gauge data archived online and easily accessible by the public. The annual data provided in Figure 3-8 are from 2008 (the year of the USGS Yellowstone River dye study), 2011, and 2012 (at the time of this study, 2012 was the most recent year with complete historic gauge data in the online database). Monthly and daily data are from September and October of those years. Again these data were selected because they are representative of the season during which the dye experiments were conducted.

- The default flow values reported in ICWater's Flow Factor GUI (dashed orange line) appear most similar to annual means provided by USGS (blue bars, particularly 2011 data).
- The annual mean/ICWater default values are notably higher than the USGS 2008 data (dashed black line).
- In this case, monthly (red bars) and daily (green bars) averages better approximate the USGS data.

Legend
Solid (▩) = data from 2008
Striped (☐) = data from 2011
Dotted (☐)= data from 2012
Blue = annual mean
Red = monthly mean
Green = monthly max/min



Site 4 - Miles City

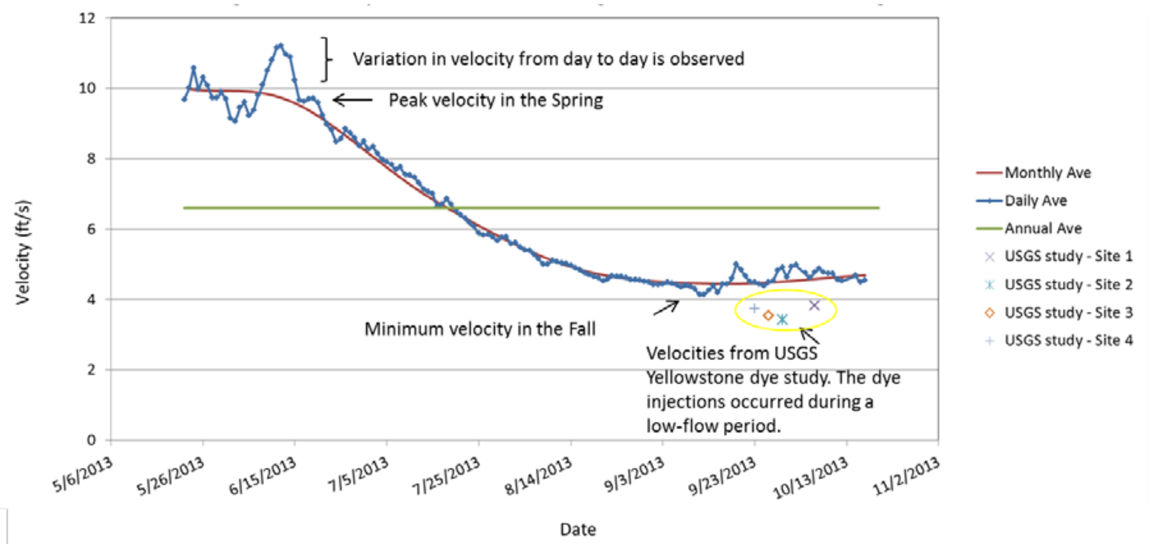
Average annual, monthly, and daily flow (discharge) values for 2008, 2011, and 2012 at the Miles City dye-injection site are shown above. The represented months of September and October were chosen since they correspond with the season of the USGS Yellowstone River dye study. These data were obtained from historic USGS gauge data. These historic values can be compared to the values measured during the USGS dye-tracer study (black dashed line) and the default value given in the ICWater Flow Factor GUI (orange dashed line). It appears that the ICWater default data during the time of the IDA evaluation may have been from a comparatively high flow year (e.g., 2011).

Figure 3-8. Average Annual, Monthly, and Daily Flow in the Yellowstone River

Looking at Figure 3-8, the potential fluxes in flow are obvious. Most notably, 2011 appeared to be a comparatively high flow year while the following year was lower. The orange dashed line in Figure 3-8 shows the default flow value taken from ICWater's Flow Factor GUI. The black, dashed line shows the value measured by the USGS during the dye study. ICWater's default value agrees well with the 2011 annual value. Conversely, the 2008 and 2012 historic data are in better agreement with what was actually observed. This example suggests that if ICWater accesses default flow data from a year that was significantly higher or lower than the flow at the time of the spill being modeled, problems with model accuracy could arise. The user needs to be aware that default values in ICWater may not always be the best values to use and real-time measurements of both flow and velocity may be the best means of improving model accuracy.

In addition to annual variations, there are seasonal variations in flow. For example, in the spring, snow and ice melt will result in increased river velocity. Conversely, by the end of a dry summer, flow will have diminished. Unfortunately, there is only one USGS site in the Yellowstone River for which real-time velocity data are provided online (typically only real-time flow is available). This gauge is located near Livingston, Montana. Figure 3-9 gives the velocity data reported from May through October 2013. The curve illustrates the general trend of flow peaking in the spring and then declining through the summer. The green horizontal line in Figure 3-9 provides the average annual velocity at this location in the Yellowstone River and the four symbols toward the bottom right show velocity at the time of the USGS dye study. Obviously, the dye study occurred during a seasonal low-flow period falling below the annual average velocity. This further suggests that using annual averages as default values in the model could lead to under- or overestimating transport and dispersion processes if a spill occurs during a high-flow or low-flow season. Furthermore, from this observation of flow fluctuations, it follows that using real-time velocity and flow measurements could be a key means of improving model predictions for plume arrival times and peak concentrations.

Of course, the limited online availability of real-time and historic velocity data prevents a more broad statement about the effects of temporal flow variations. However, these variations do appear to be an important consideration for this particular hydrologic region of the United States. Other regions may have additional or different factors that need to be considered. As future work, IDA could examine velocity-flow equations, parameter values, and flow variations in more detail and over a wider range of hydrologic regions.



Variation in velocity from day to day is observed

Peak velocity in the Spring

Minimum velocity in the Fall

Velocities from USGS Yellowstone dye study. The dye injections occurred during a low-flow period.

Real-time velocity data provided by one USGS gauge in the Yellowstone River. Data from May 2013 to October 2013 was available online at the time of this study. These data show seasonal and daily fluctuations related to snow melt, rain, or seasonal dry periods.

Figure 3-9. Velocity Data from the Yellowstone River

D. References

1. Organization for the Prohibition of Chemical Weapons, http://www.opcw.org/about-chemical-weapons/types-of-chemical-agent/nerve-agents/.
2. Samuels, W. B. et al., “RiverSpill: A National Application for Drinking Water Protection,” *J. Hydraulic Engineering*, 132, 393-403, 2006.
3. Leopold, L. B. and Maddock, T., “The Hydraulic Geometry of Stream Channels and Some Physiographic Implications,” *Geological Survey Professional Paper* 252, 1953.
4. Leopold, L. B., “Downstream Change of Velocity in Rivers,” *Am. J. Sci.* 251, 606-624, 1953.
5. Jobson, H. E. *Prediction of Traveltime and Longitudinal Dispersion in Rivers and Streams*, 1996, https://water.usgs.gov/osw/pubs/disp/dispersion.pdf.
6. McCarthy, P. M., “A Computer Program for Estimating Instream Travel Times and Concentrations of a Potential Contaminant in Yellowstone River, Montana,” *U. S. Geological Survey Scientific Investigations Report* 2006-5057, 2006.

4. Summary of Conclusions and Future Work

A. ICWater Assessment Summary

This report provides details on IDA's continued evaluation of the waterborne T&D model ICWater. This work represents part of an ongoing effort to provide DTRA Reachback with input on the utility of this code for predicting the transport, fate, and effects of CBRN materials. While earlier work was focused on the basic usability of the code (i.e., the technical documentation was sufficient for guiding users in the setup and running of simulations, and the code worked correctly without any evident errors), this study focused on independently assessing the accuracy of model predictions. In the present study, we compared ICWater output to data collected during a USGS dye study in the Yellowstone River.

As a result of IDA's current study, the following conclusions were reached:

- ICWater version 3.2 should not be used without installing the software patch provided by Leidos. Without this patch, ICWater should not be expected to operate correctly when used in modeling the western United States.
- The velocity-flow equation used in ICWater does not appear to be broadly applicable. The use of the current expression in the model likely contributes to notable discrepancies between model output and actual observations in the field.
- Annual or seasonal variations in flow could also affect model predictions if default values in ICWater are used without verification.
- Velocities calculated from flow measurements often fail to match observed or measured values. Mismatches between computed velocities and real-world velocities can result in simulated plume arrival times that are later than actual arrival times.
- For the reasons cited above, it may be difficult to get predictions from ICWater that accurately reflect the transport and dispersion of materials in many real-world rivers and streams.
- Improving the model in the future will require a systematic approach for addressing differences between output and real-world observations. This approach should include a method for correctly capturing velocity (e.g., using measured velocity data directly or a better approach for estimating velocity).
- At present, the operational relevancy of ICWater might be limited.

The simulation results that led to the development the above key conclusions are summarized in the table below.

Table 4-1. Summary of Key Simulation Results

Nature of Mismatch	Case 1: Default or Base Case Simulations	Case 2: Simulations with Modified Velocity	Case 3: Simulations with Modified Velocity and Increased Dye Mass
Correct arrival times?	No, delayed.	Yes, notable improvement.	Similar to case 2
Correct peak concentration?	No, overestimate.	No, underestimate.	Yes, but only for first measurement site
Correct plume duration?	No, too short	Yes, notable improvement	Similar to case 2

An important gain from the above conclusions is that the model's assumed correlation between flow and velocity will strongly affect predicted contaminant arrival times and concentration values at arrival. ICWater's failure to accurately predict transport and dispersion in a real-world river indicates the possibility that local populations may be falsely warned of a threat, warned late, or not warned at all. A possible solution to this model limitation would be to use measured velocity values directly in the model instead of computing it from flow. Doing so would likely help correct predictions of arrival times. However, the availability of velocity data is beyond the control of ICWater developers and would likely need to be provided by the USGS.

Although ICWater version 3.2 appears to operate per specification, it does not appear ready for broad military use because of limitations associated with the model's velocity-flow relationship. The findings enumerated above were communicated to ICWater developers at Leidos in January 2014. During the briefing, developers informed IDA that they were working on the next version of ICWater in which changes would address some of the IDA-identified limitations. As of this writing, IDA has not reviewed the latest version of the code. Based on our findings, we conclude that continued work with developers at Leidos would be beneficial for verifying that the necessary issues are being addressed.

B. Implications for Operational Relevancy

The Defense Threat Reduction Agency – Joint Science and Technology Office has the primary responsibility for ensuring implementation and availability of T&D modeling capabilities. These capabilities are identified as necessary for providing all warfighters with the ability to accurately simulate and predict the time-phased effect of CBRN and

Toxic Industrial Chemical/Material events. The T&D modeling capability requirements are provided in the Operational Requirements Document (ORD) for the Joint Effects Model (JEM)[1] [1]. As specified in the ORD, there are two main components to waterborne transport and dispersion modeling. The first component is the capability to predict hazard areas and effects on littoral and coastal areas. The second part pertains to riverine settings and a capability to predict the hazards and effects of waterborne contamination for surface water bodies and simple municipal water systems and aquifers. Some of the specific requirements given for waterborne hazard prediction are:

1. Accuracy and speed to reduce the likelihood of falsely warning people or of falsely not warning people[2]
2. Determination of the toxic hazard for a given exposure or protection level
3. Prediction of a combination of civilian as well as military fatalities and incapacitation, both initial and delayed (up to 180 days)
4. Access to relevant datasets.

As it presently stands, ICWater has limited utility for military applications. The model clearly failed to produce accurate predictions in the Yellowstone River case examined here. It may be demonstrated in the future that ICWater 3.2 only works for hydrologic regions in which the model was calibrated. In addition, there is no mechanism for calculating militarily relevant metrics (e.g., casualties or illness levels). ICWater is only able to report whether a concentration at a point is above or below a certain level of concern. There is no way to evaluate the implications of being above the level of concern (i.e., the seriousness of or exact consequences arising from that level of exposure). Complicating the issue of evaluating the implications of exposure, crucial waterborne lethality data are missing. This last issue is not a limitation of ICWater in the sense that the model's assumptions or equations need to be modified. However, the utility of the model does rely on these data eventually being collected and made available to the ICWater agent database.

C. Future Areas for Evaluation

IDA has not evaluated several capability features of ICWater 3.2. These capabilities include:

- Upstream traces
- Atmospheric deposition and surface runoff
- Simulating spills outside of the United States.

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[1] The Joints Effects Model is intended as the DoD-wide transport and dispersion model used to simulate CBRN release events.

[2] We note that the accuracy requirement is usually applied to predictions of concentration. As this study has shown, a temporal component should be considered as well to ensure people receive warning *before* a contaminant plume arrives.

In addition to following an agent downstream from its release location, ICWater is intended to help locate the source of a spill by also navigating upstream. In this mode, ICWater partitions the upstream watershed into zones based on either upstream distance or travel time. ICWater's upstream calculations should be evaluated just as the downstream traces were.

In addition, the current version of ICWater has the ability to model atmospheric deposition of contaminants and subsequent runoff into rivers and streams. To simulate atmospheric deposition and runoff, ICWater couples a methodology for determining surface runoff of contaminants with atmospheric deposition calculations from JEM. Both the surface runoff methodology and the coupling with JEM should be tested in the future.

Finally, ICWater has been offered as a tool for investigating spills occurring in rivers and streams outside the United States. For spills occurring in U.S. waterways, ICWater can access real-time flow (USGS gauges) and river network data (NHDPlus). Since little data are available for river networks outside the United States, ICWater's ability to provide realistic estimates of a contaminant's location, concentration, and arrival times should be independently assessed for when the model does not have access to abundant river and stream data.

The simulation results presented in Chapter 3 also generate several interesting questions that could be further reviewed. First, although the overarching reason for why ICWater predictions do not agree with observations seems to be connected to the way velocity and flow are linked in the model, IDA notes that model discrepancies are worse at the Myers site. Why this is true is unclear. It could be related to environmental conditions at Myers, smaller dye concentrations, poor flow estimates (see Table 3-3), or a combination of all these issues. Furthermore, during the course of this study, IDA did not attempt to rigorously define an acceptable discrepancy between model results and USGS measurements. Consequently, IDA could attempt to more quantitatively outline acceptable differences between model and measurement.

Besides evaluating the above features and issues, the current study can be built upon to better determine sensitivity to temporal variations in flow. It would also be advisable to evaluate any newer versions of ICWater in a manner similar to that which has been done for version 3.2. This would allow changes to the code to be tested and verified and any new or remaining issues to be identified. Also useful would be further identifying and, when possible, collecting data required for enhancing the model's operational relevancy (e.g., waterborne lethality data).

D. References

1. *Operational Requirements Document (ORD) for Joint Effects Model (JEM)*, 28 May 2004.

Appendix A
USGS Yellowstone Dye Study Data Tables

For the reader's reference and benefit, we reproduce here some available time-concentration data obtained by the USGS during the Yellowstone River dye study. An example of each injection and measurement site referenced in the main text is provided in the tables. The measurement sites given in the tables indicate site names at which data were collected. Similarly, the given injection sites indicate the name of the location from which dye was released. RWT is the abbreviation for Rhodamine WT dye. Because of the amount of data collected during the study, these tables only provide a sample of the data reported by the USGS. Complete tables can be found at http://pubs.usgs.gov/sir/2009/5261/. These data were used for producing the measured time-concentration curves for Rhodamine WT dye used in this report.

Table A-1. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 1		Huntley Bridge		Measurement Site 2		Pompeys Bridge	
Injection Site 1		Lockwood Bridge		Injection Site 1		Lockwood Bridge	
Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)	Entry number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)
25	2008:10:06	19:02:01	4.50	380	2008:10:07	4:31:01	4.23
26	2008:10:06	19:02:31	5.03	386	2008:10:07	4:34:01	4.64
27	2008:10:06	19:03:01	5.15	387	2008:10:07	4:34:31	4.74
29	2008:10:06	19:04:01	5.80	388	2008:10:07	4:35:01	4.71
31	2008:10:06	19:05:01	7.10	389	2008:10:07	4:35:31	4.77
32	2008:10:06	19:05:31	7.84	390	2008:10:07	4:36:01	4.93
33	2008:10:06	19:06:01	7.80	391	2008:10:07	4:36:31	5.07
34	2008:10:06	19:06:31	8.36	392	2008:10:07	4:37:01	5.11
35	2008:10:06	19:07:01	9.10	393	2008:10:07	4:37:31	5.18
36	2008:10:06	19:07:31	9.30	394	2008:10:07	4:38:01	5.16
37	2008:10:06	19:08:01	10.02	395	2008:10:07	4:38:31	5.27
38	2008:10:06	19:08:31	10.71	396	2008:10:07	4:39:01	5.38
39	2008:10:06	19:09:01	11.33	397	2008:10:07	4:39:31	5.45
40	2008:10:06	19:09:31	11.74	398	2008:10:07	4:40:01	5.54
41	2008:10:06	19:10:01	12.40	399	2008:10:07	4:40:31	5.58
42	2008:10:06	19:10:31	12.74	400	2008:10:07	4:41:01	5.60
43	2008:10:06	19:11:01	13.19	401	2008:10:07	4:41:31	5.70
47	2008:10:06	19:13:01	15.15	402	2008:10:07	4:42:01	5.78

Table A-2. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 3		Custer Bridge		Measurement Site 4		Myers Bridge	
Injection Site 1		Lockwood Bridge		Injection Site 1		Lockwood Bridge	
Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)	Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)
733	2008:10:07	19:45:31	1.35	1094	2008:10:08	3:30:01	0.51
734	2008:10:07	19:46:01	1.36	1102	2008:10:08	3:31:21	0.55
736	2008:10:07	19:47:01	1.42	1103	2008:10:08	3:31:31	0.60
737	2008:10:07	19:47:31	1.32	1104	2008:10:08	3:31:41	0.56
738	2008:10:07	19:48:01	1.38	1106	2008:10:08	3:32:01	0.52
739	2008:10:07	19:48:31	1.35	1107	2008:10:08	3:32:11	0.60
740	2008:10:07	19:49:01	1.41	1108	2008:10:08	3:32:21	0.46
742	2008:10:07	19:50:01	1.39	1109	2008:10:08	3:32:31	0.51
743	2008:10:07	19:50:31	1.46	1110	2008:10:08	3:32:41	0.53
779	2008:10:07	20:19:01	2.05	1111	2008:10:08	3:32:51	0.52
780	2008:10:07	20:19:31	2.04	1112	2008:10:08	3:33:01	0.52
781	2008:10:07	20:20:01	2.14	1113	2008:10:08	3:33:11	0.51
782	2008:10:07	20:20:31	2.14	1114	2008:10:08	3:33:21	0.56
787	2008:10:07	20:23:01	2.07	1115	2008:10:08	3:33:31	0.54
790	2008:10:07	20:24:31	2.26	1116	2008:10:08	3:33:41	0.52
791	2008:10:07	20:25:01	2.24	1117	2008:10:08	3:33:51	0.58
793	2008:10:07	20:26:01	2.39	1118	2008:10:08	3:34:01	0.53
805	2008:10:07	20:32:01	2.42	1119	2008:10:08	3:34:11	0.53

Table A-3. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 1		Forsyth Bridge		Measurement Site 2		Cartersville Dam	
Injection Site 2		**Myers Bridge**		**Injection Site 2**		**Myers Bridge**	
Entry Number	**Date**	**Time (hr:min:sec)**	**RWT dye concentration (µg/L)**	**Entry Number**	**Date**	**Time (hr:min:sec)**	**RWT Dye Concentration (µg/L)**
707	2008:09:30	14:37:01	1.39	2306	2008:09:30	14:46:31	1.34
708	2008:09:30	14:37:31	1.38	2307	2008:09:30	14:47:01	1.15
709	2008:09:30	14:38:01	1.44	2308	2008:09:30	14:47:31	1.44
710	2008:09:30	14:38:31	1.43	2309	2008:09:30	14:48:01	1.23
711	2008:09:30	14:39:01	1.51	2310	2008:09:30	14:48:31	1.24
712	2008:09:30	14:39:31	1.54	2311	2008:09:30	14:49:01	1.46
713	2008:09:30	14:40:01	1.53	2312	2008:09:30	14:49:31	1.33
714	2008:09:30	14:40:31	1.47	2313	2008:09:30	14:50:01	1.55
715	2008:09:30	14:41:01	1.45	2314	2008:09:30	14:50:31	1.53
717	2008:09:30	14:42:01	1.55	2315	2008:09:30	14:51:01	1.39
718	2008:09:30	14:42:31	1.52	2316	2008:09:30	14:51:31	1.31
721	2008:09:30	14:44:01	1.57	2317	2008:09:30	14:52:01	1.41
726	2008:09:30	14:46:31	1.57	2318	2008:09:30	14:52:31	1.33
729	2008:09:30	14:48:01	1.53	2322	2008:09:30	14:54:31	1.50
730	2008:09:30	14:48:31	1.50	2324	2008:09:30	14:55:31	1.34
732	2008:09:30	14:49:31	1.57	2325	2008:09:30	14:56:01	1.16
733	2008:09:30	14:50:01	1.60	2327	2008:09:30	14:57:01	1.27
739	2008:09:30	14:53:01	1.56	2329	2008:09:30	14:58:01	1.20

Table A-4. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 3		Rosebud Bridge	
Injection Site 2		Myers Bridge	
Entry Number	Date	Time (hr:min:sec)	RWT dye Concentration (µg/L)
1823	2008:10:01	0:19:01	1.07
1824	2008:10:01	0:19:31	1.01
1825	2008:10:01	0:20:01	0.99
1826	2008:10:01	0:20:31	1.02
1827	2008:10:01	0:21:01	0.99
1828	2008:10:01	0:21:31	0.96
1829	2008:10:01	0:22:01	1.06
1830	2008:10:01	0:22:31	1.04
1831	2008:10:01	0:23:01	1.01
1832	2008:10:01	0:23:31	1.06
1833	2008:10:01	0:24:01	0.94
1835	2008:10:01	0:25:01	1.04
1836	2008:10:01	0:25:31	1.00
1837	2008:10:01	0:26:01	1.04
1838	2008:10:01	0:26:31	1.04
1839	2008:10:01	0:27:01	1.02
1840	2008:10:01	0:27:31	0.92
1841	2008:10:01	0:28:01	0.98

Table A-5. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 1		Rosebud Bridge		Measurement Site 2		Fort Keogh Bridge	
Injection Site 3		Cartersville Dam		Injection Site 3		Cartersville Dam	
Entry Number	Date	Time (hr:min:sec)	RWT dye concen-tration (µg/L)	Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)
301	2008:09:26	15:49:01	7.07	1121	83.673229	0.49028935	2.30
302	2008:09:26	15:49:31	5.48	1122	83.673229	0.49063657	2.21
307	2008:09:26	15:52:01	8.08	1123	83.673229	0.4909838	2.23
308	2008:09:26	15:52:31	8.57	1124	83.673229	0.49133102	2.11
309	2008:09:26	15:53:01	8.84	1125	83.673229	0.49167824	2.13
310	2008:09:26	15:53:31	8.28	1126	83.673229	0.49202546	2.13
311	2008:09:26	15:54:01	8.72	1127	83.673229	0.49237269	2.22
312	2008:09:26	15:54:31	9.28	1128	83.673229	0.49271991	2.13
313	2008:09:26	15:55:01	9.90	1129	83.673229	0.49306713	2.21
314	2008:09:26	15:55:31	9.94	1130	83.673229	0.49341435	2.03
315	2008:09:26	15:56:01	10.14	1131	83.673229	0.49376157	2.05
316	2008:09:26	15:56:31	9.87	1132	83.673229	0.4941088	2.01
318	2008:09:26	15:57:31	10.10	1133	83.673229	0.49445602	2.03
319	2008:09:26	15:58:01	10.23	1134	83.673229	0.49480324	2.10
320	2008:09:26	15:58:31	10.39	1135	83.673229	0.49515046	1.96
321	2008:09:26	15:59:01	10.12	1136	83.673229	0.49549769	1.92
322	2008:09:26	15:59:31	10.00	1137	83.673229	0.49584491	2.06
323	2008:09:26	16:00:01	9.59	1138	83.673229	0.49619213	2.02

Table A-6. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 3		Kinsey Bridge	
Injection Site 3		Cartersville Dam	
Entry number	Date	Time (hr:min:sec)	RWT Dye Concentration (µg/L)
2108	2008:09:27	21:55:01	0.79
2109	2008:09:27	21:55:31	0.74
2110	2008:09:27	21:56:01	0.76
2111	2008:09:27	21:56:31	0.75
2112	2008:09:27	21:57:01	0.73
2113	2008:09:27	21:57:31	0.75
2114	2008:09:27	21:58:01	0.81
2120	2008:09:27	22:01:01	0.73
2121	2008:09:27	22:01:31	0.69
2122	2008:09:27	22:02:01	0.65
2123	2008:09:27	22:02:31	0.63
2124	2008:09:27	22:03:01	0.71
2125	2008:09:27	22:03:31	0.65
2126	2008:09:27	22:04:01	0.72
2127	2008:09:27	22:04:31	0.74
2129	2008:09:27	22:05:31	0.66
2130	2008:09:27	22:06:01	0.74
2131	2008:09:27	22:06:31	0.68

Table A-7. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 1		Kinsey Bridge		Measurement Site 2		Calypso Bridge	
Injection Site 4		Miles City Bridge		Injection Site 4		Miles City Bridge	
Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)	Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)
224	2008:09:23	15:04:31	24.75	592	2008:09:24	2:39:01	9.91
225	2008:09:23	15:05:01	24.41	593	2008:09:24	2:39:31	12.55
226	2008:09:23	15:05:31	23.74	594	2008:09:24	2:40:01	12.36
227	2008:09:23	15:06:01	23.30	596	2008:09:24	2:41:01	12.18
228	2008:09:23	15:06:31	22.90	609	2008:09:24	2:47:31	9.67
229	2008:09:23	15:07:01	22.59	617	2008:09:24	2:51:31	10.25
230	2008:09:23	15:07:31	21.84	625	2008:09:24	2:55:31	10.55
231	2008:09:23	15:08:01	21.49	626	2008:09:24	2:56:01	7.62
232	2008:09:23	15:08:31	21.37	627	2008:09:24	2:56:31	8.94
233	2008:09:23	15:09:01	20.84	628	2008:09:24	2:57:01	10.02
234	2008:09:23	15:09:31	20.23	629	2008:09:24	2:57:31	7.52
235	2008:09:23	15:10:01	19.64	630	2008:09:24	2:58:01	8.61
236	2008:09:23	15:10:31	19.40	631	2008:09:24	2:58:31	7.49
237	2008:09:23	15:11:01	19.17	632	2008:09:24	2:59:01	6.92
238	2008:09:23	15:11:31	18.82	633	2008:09:24	2:59:31	6.03
239	2008:09:23	15:12:01	18.27	634	2008:09:24	3:00:01	7.28
240	2008:09:23	15:12:31	17.62	635	2008:09:24	3:00:31	6.32
241	2008:09:23	15:13:01	17.62	636	2008:09:24	3:01:01	7.05

Table A-8. Time-Concentration Data Collected during the USGS Dye Study

Measurement Site 3		Fallon Bridge		Measurement Site 4		Glendive Bridge	
Injection Site 4		Miles City Bridge		Injection Site 4		Miles City Bridge	
Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)	Entry Number	Date	Time (hr:min:sec)	RWT Dye Concen-tration (µg/L)
1159	2008:09:24	10:59:31	2.83	2021	2008:09:25	1:29:01	1.10
1165	2008:09:24	11:02:31	3.00	2022	2008:09:25	1:29:31	1.11
1167	2008:09:24	11:03:31	2.92	2023	2008:09:25	1:30:01	1.15
1168	2008:09:24	11:04:01	3.01	2024	2008:09:25	1:30:31	0.94
1169	2008:09:24	11:04:31	3.07	2026	2008:09:25	1:31:31	1.04
1170	2008:09:24	11:05:01	2.85	2027	2008:09:25	1:32:01	1.02
1172	2008:09:24	11:06:01	2.82	2028	2008:09:25	1:32:31	1.07
1173	2008:09:24	11:06:31	2.94	2029	2008:09:25	1:33:01	0.98
1175	2008:09:24	11:07:31	2.98	2030	2008:09:25	1:33:31	1.09
1176	2008:09:24	11:08:01	3.09	2031	2008:09:25	1:34:01	1.06
1177	2008:09:24	11:08:31	2.83	2032	2008:09:25	1:34:31	0.93
1178	2008:09:24	11:09:01	3.05	2033	2008:09:25	1:35:01	1.00
1180	2008:09:24	11:10:01	2.86	2034	2008:09:25	1:35:31	0.97
1182	2008:09:24	11:11:01	3.01	2035	2008:09:25	1:36:01	0.98
1183	2008:09:24	11:11:31	3.10	2036	2008:09:25	1:36:31	0.90
1186	2008:09:24	11:13:01	2.94	2037	2008:09:25	1:37:01	0.95
1188	2008:09:24	11:14:01	3.05	2038	2008:09:25	1:37:31	1.13
1189	2008:09:24	11:14:31	3.05	2039	2008:09:25	1:38:01	1.10

Appendix B
Alternative Velocity-Flow Relationships from the Literature

As discussed in Section B of Chapter 3, the literature provides alternative velocity-flow relationships that could be used in ICWater. Here we discuss and reproduce the six equations given in Jobson [1]. These six equations were used in producing the velocity comparison plot (Figure 3-7).

The purpose of Jobson's study was specifically to develop prediction equations that could be used either to calibrate a model or to make travel time and concentration predictions directly. In his paper, Jobson shows that the time required for a tracer to reach a specific point in a river determines the concentration that will occur. He further points out that river velocity depends on many factors including the general morphology of the river and the amount of ponding caused by dams or other manmade works. To improve travel time prediction, Jobson derives several alternatives to the standard velocity-flow equation used in ICWater ($V = aQ^b$).

The velocity of the peak concentration and associated hydraulic data for more than 980 subreaches for about 90 different rivers in the United States representing a wide range of river sizes, slopes, and geomorphic types are compiled in the report. Four variables were available in sufficient quantities for regression analysis. These were the drainage area (D_a), reach slope (S), mean annual river discharge (Q_a), and discharge at the section at time of the measurement (Q). Based on 939 data points, Jobson determined that the most accurate prediction equation for peak velocity (V) is:

$$V = 0.094 + 0.0143 \times (D'_a)^{0.919} \times (Q'_a)^{-0.469} \times (S)^{0.159} \times {}^{Q}/_{D_a} \qquad \text{(B-1)}$$

Since during a spill response the conditions resulting in the highest probable concentration are often desired, Jobson also provides an equation for the maximum probable velocity:

$$V = 0.25 + 0.02 \times (D'_a)^{0.919} \times (Q'_a)^{-0.469} \times (S)^{0.159} \times {}^{Q}/_{D_a} \qquad \text{(B-2)}$$

For when data are more limited, Jobson next provides the best equation for the velocity of the peak concentration that does not include slope as a variable:

$$V = 0.020 + 0.051 \times (D'_a)^{0.821} \times (Q'_a)^{-0.465} \times {}^{Q}/_{D_a} \qquad \text{(B-3)}$$

Similarly, the maximum probable velocity without slope as a variable is given as:

$$V = 0.20 + 0.093 \times (D'_a)^{0.821} \times (Q'_a)^{-0.465} \times {}^{Q}\!/_{D_a} \qquad \text{(B-4)}$$

The best equation for the velocity of the peak concentration using only drainage area is:

$$V = 0.152 + 8.1 \times (D''_a)^{0.595} \times {}^{Q}\!/_{D_a} \qquad \text{(B-5)}$$

Last, the maximum probable velocity using only drainage area is:

$$V = 0.20 + 40.0 \times (D''_a)^{0.595} \times {}^{Q}\!/_{D_a} \qquad \text{(B-6)}$$

In the above equations, D'_a, D''_a, and Q'_a are defined as:

$$D'_a = {}^{D_a^{1.25} \times \sqrt{g}}\!\Big/_{Q_a} \qquad \text{(B-7)}$$

$$D''_a = {}^{D_a^{1.25} \times \sqrt{g}}\!\Big/_{Q} \qquad \text{(B-8)}$$

$$Q'_a = {}^{Q}\!/_{Q_a} \qquad \text{(B-9)}$$

Referring back to Figure 3-7, of the six velocity-flow equations above, Jobson's equations for maximum probable velocity (i.e., Eqs. B2, B4, and B6) best predict the Yellowstone River velocities at the time of the USGS dye study. In addition, inclusion of the extra variables of slope and mean annual river discharge does not seem to significantly improve the predictions (i.e., Eq. B-6 does not produce the outliers seen with Eqs. B-2 and B-4, thus, in general, Eq. B-6 seems to provide the best fit to the USGS Yellowstone velocity data). Although the values offered by Jobson's maximum probable velocity equations are an improvement to the ICWater predictions, Leopold [2] and Leopold and Maddock [3] offer the best agreement to the Yellowstone data. This suggests two possible approaches to improving the velocity calculations in ICWater. First, new equations could be introduced into ICWater. These more robust equations would need to consider river morphology or other environmental factors. Second, ICWater maintains its current velocity-flow expression, but its database of *a* and *b* parameter values could be improved or expanded using data such as that provided by Leopold and Maddock [3]. Further study is required to determine which, if either, of these approaches would work best in general.

E. References

1. Jobson, H. E. *Prediction of Traveltime and Longitudinal Dispersion in Rivers and Streams*, 1996, https://water.usgs.gov/osw/pubs/disp/dispersion.pdf.
2. Leopold, L. B., “Downstream Change of Velocity in Rivers,” *Am. J. Sci.* 251, 606-624, 1953.
3. Leopold, L. B. and Maddock, T., “The Hydraulic Geometry of Stream Channels and Some Physiographic Implications,” *Geological Survey Professional Paper* 252, 1953.

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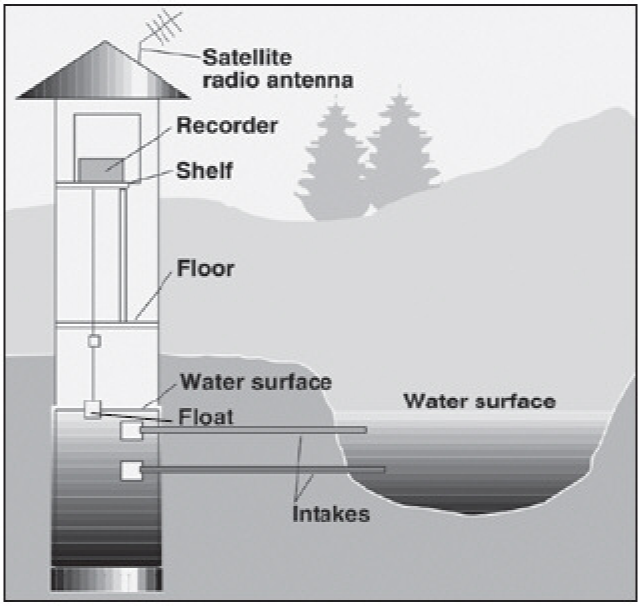
Appendix C
USGS Gauge Measurements

Here, we briefly review how USGS real-time stream flow and velocity information is obtained. The USGS uses stream gauges to measure the amount of water flowing in a river or stream at a given time. This flow is also known as discharge. Discharge is the volume of water moving down a stream or river per unit of time, commonly expressed in cubic feet per second. The first step for obtaining flow is to record water level. This level is also referred to as stage or gauge height. Measuring the relative height of a stream or river is done using an underwater tube contained in the stream gauge (Figure C-1). Gas is pushed from the tube into the water. As the depth of water above the tube opening increases, the pressure required to push the gas through the opening also increases. Based on the level of pressure, the height of water above the tube opening can be calculated. In other words, changes in pressure are recorded as changes in height or stage [1].



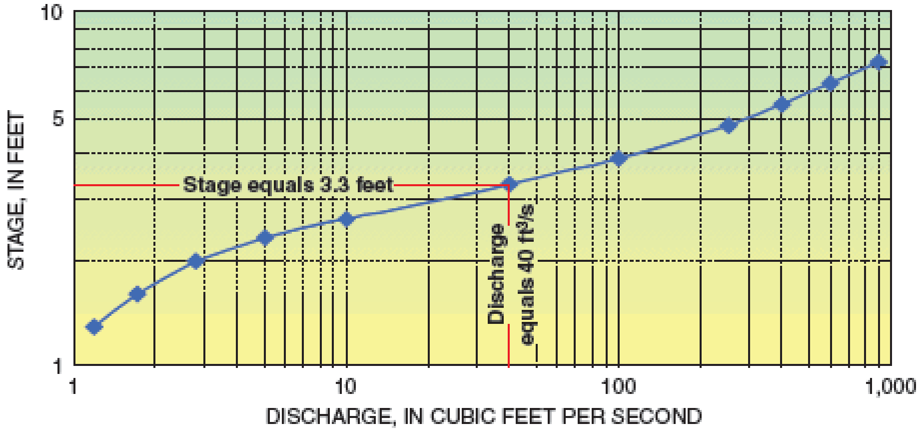
Source: http://water.usgs.gov/edu/streamflow1.html

Diagram of a typical USGS gauge used to measure the water level (i.e., stream stage). The underwater tubes or intakes shown in the diagram are used to determine the height of water above the tube opening.

Figure C-1. USGS Stream Gauge

In general, USGS gauges make stage measurements about every 15 minutes. These stage data are stored by the gauges for 1-4 hours before being transmitted back [1, 2]. Most

USGS gauges transmit stage data by satellite to USGS computers. Although stage can be valuable information, the water science community is largely interested in knowing river discharge. Therefore, once stage data are obtained, they are converted to flow by applying a site-specific rating curve (Figure C-2). Rating curves are used because it is not possible to directly measure the flow of rivers and streams using gauge data (n.b., discharge must be calculated from velocity and cross-sectional area of a river channel). However, rating curves are produced and updated as regularly as is feasible for every site.



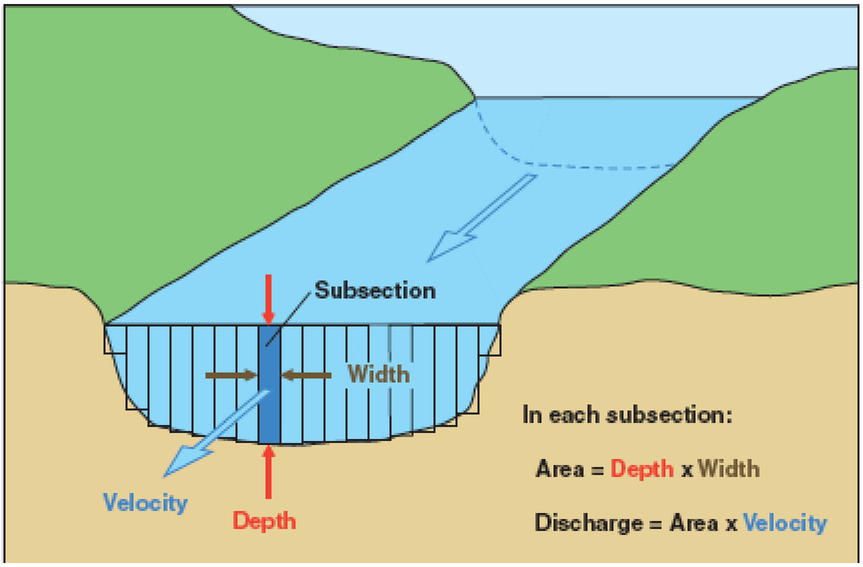
Source: http://water.usgs.gov/edu/streamflow3.html

Example of a typical rating curve providing the stage-discharge relation. Once stage is recorded by a gauge, the curve is used to determine flow. For example, on the plot above for a stage equal to 3.3 feet, the river discharge is 40 ft^3/s. The dots on the curve represent concurrent measurement of stage and discharge. For each measurement of discharge, there is a corresponding measurement of stage.

Figure C-2. Rating Curve

The stage-discharge relationship depends on the shape, size, slope, and roughness of the channel at each gauge and is different for every gauge [2, 3]. Consequently, stage-discharge relations must be continually checked on an ongoing basis because stream channels are constantly changing. Changes in stream channels are often caused by erosion or deposition of streambed materials, seasonal vegetation growth, debris, or ice.

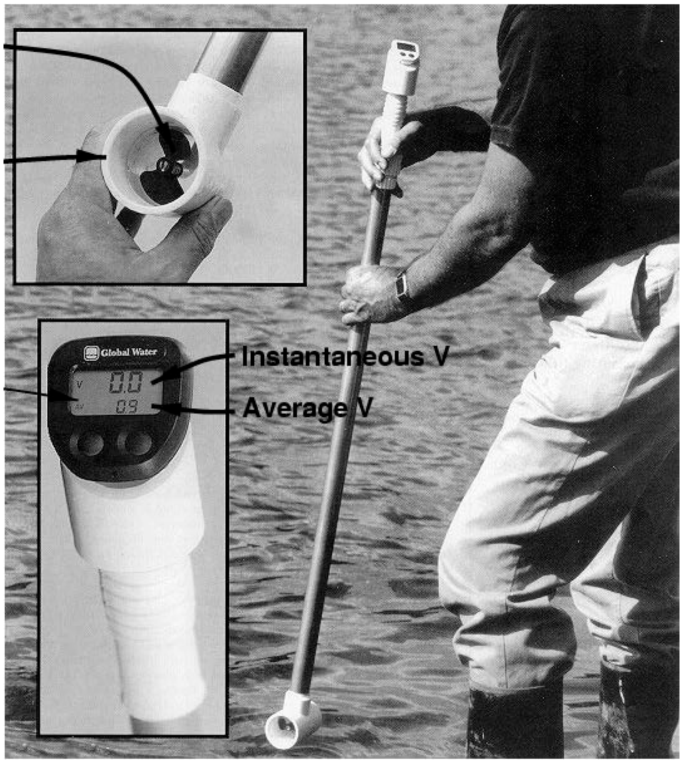
Rating curves are typically developed by physically measuring the velocity of a river or stream with a mechanical current meter at a wide range of stages (i.e., low flow to flood conditions). The stream channel cross section is divided into numerous vertical subsections (Figure C-3). In each subsection, the area is obtained by measuring the width and depth of the subsection, and the water velocity is determined using a current meter. The current meter may be used to measure a vertical profile of water velocity at several points across the channel to obtain an average reading. The meter determines velocity according to the number of revolutions of a propeller or rotor over a given time interval (Figure C-4) [4].



Source: http://water.usgs.gov/edu/streamflow2.html

River discharge is computed by multiplying the area of water in a channel cross section by the average velocity of the water in that cross section.

Figure C-3. Diagram of a River Channel Cross Section



Source: https://www.utdallas.edu/~brikowi/Teaching/Hydrogeology/OutdoorLabs/Gauging_Background.html

Figure C-4. Example of a Current Meter

At the same time the velocity measurements are made, the depth of the water is also measured. Typically, the USGS takes measurements at 25-30 regularly spaced locations across the river or stream [1]. The discharge in each subsection is computed by multiplying the subsection area by the measured velocity. The total discharge is then computed by summing the discharge of each subsection. To keep the curves up-to-date, USGS researchers visit gauges every 6-8 weeks to measure velocity and stream height directly [3].

USGS flow and gauge-height data are available to users over the Internet at http://water.usgs.gov/nwis/ or http://waterdata.usgs.gov/nwis/rt. Additional details on obtaining stage, velocity, and flow data are provided in the references listed below.

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4. *A Citizen's Guide to Understanding and Monitoring Lakes and Streams*, Washington State Department of Ecology, 1991, http://www.ecy.wa.gov/programs/wq/plants/ management/ joysmanual/5meter.html.

Appendix D
List of Illustrations

Figures

Tables

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Appendix E
Acronyms and Abbreviations

CBRN	chemical, biological, radiological, and nuclear
DoD	Department of Defense
DTRA	Defense Threat Reduction Agency
GUI	graphical user interface
ICWater	Incident Command Tool for Protecting Drinking Water
IDA	Institute for Defense Analyses
IT	information technology
JEM	Joint Effects Model
LOC	level of concern
NHDPlus	National Hydrography Database Plus
ORD	Operational Requirements Document
RWT	Rhodamine WT
SAIC	Science Applications International Corporation
SDWIS	Safe Drinking Water Information System
SHARC	System for the Hazard Assessment of Released Chemicals
T&D	transport and dispersion
USGS	United States Geological Survey

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Nathan Platt, Project Leader

14. ABSTRACT

As part of a multi-phase study, we have continued evaluating the predictive capabilities and performance of the waterborne transport and dispersion model known as the Incident Command Tool for Protecting Drinking Water (ICWater). The overarching goal of the study is to provide DTRA with information on the predictive reliability of this software package. In this second-year report, we compare ICWater simulation results to field measurements collected by the USGS during a series of dye experiments conducted in the Yellowstone River. The key conclusions arising from the study are that the velocity-flow expression used in ICWater causes the model to predict late plume arrival times and over predict peak concentration levels. It is suggested that the velocity-flow equation be improved or that real-time velocity be used instead of a velocity inferred from flow. Recommendations for future work are also discussed.

15. SUBJECT TERMS

waterborne transport and dispersion, verification and validation, V&V, Yellowstone River, dye studies, USGS, ICWater

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