General comments of Referee #2

During the last few years, an increasing number of studies have focused on contaminant transport in surface water system with transient storage models. As a result, the topic of this paper is timely and appropriate. The authors present an interesting study of a numerical model for contaminant transport along an 1D channel with transient storage zones and performed various model verifications. First of all, it is important to acknowledge how difficult and time consuming the development of a complex numerical algorithm is. At the same time, it can be difficult to publish work in the field of environmental modeling that focuses on increased abilities to handle complex problems. The authors tend to overrate the novelty of their work and miss to cite relevant previous works which are quite similar or more advanced than the model suggested in the paper. Considering that the authors suggest a “comprehensive” model, the question "what is scientifically new?" arises. The authors may want to take the opportunity to further highlight advances made by this development (e.g., the flexibility, applicability and robustness of their model). Therefore, the paper is on the borderline in my view from Major Revision to Rejection. I believe the author should be allowed to respond to the reviews and strongly improve the clarity of the scientific contributions.

1) English-editing is required to improve the quality of this paper. 2) The manuscript needs in general more discussion on the novelty of the work. 3) How could the method presented in the paper solve real-world problems (i.e., complex river networks)? 4) The authors should provide more in-depth discussion on the efficiency, applicability and robustness of this method.

Answers to General comments of Referee #2

Thank you for allocating your time to review this manuscript. You have mentioned valuable points, we really appreciate.

It is necessary to mention a few points in response to your comments:

- As you mentioned, several approaches have been proposed to simulate the solute transport in rivers with storage areas, in recent years. But, most of them are multi-dimensional models, whereas the presented model is 1D and the superiority of 1D models in practical engineering works, is obvious (with fewer inputs and easier setup, someone can get reliable results).
- Currently, OTIS is the only available model for solute transport simulation with transient storage, but it has some shortcomings, that mentioned in table 1. Such as limitation on the

number of input parameters, inability in calculation of irregular cross-sections and unsteady flow characteristics. While the presented model, does not have the above mentioned defects.

- We believe that the main novelty of our work is the use of a robust third-order numerical method in model structure (QUICK scheme), which can handle the advection-dominant problems better than the other ones. It is interesting because in mountain rivers and streams where the transient storage often observed in such areas, higher slopes lead to higher velocities and as a result the advection will be a dominant mechanism.

About the last paragraph of your comments we can say that:

1-English-editing will be done in revised version, definitely.

2-The discussion about this issue will be added to the revised version.

3- Yes, the real-world problems could be simulated by the presented model, because it takes into account the effect of irregularity in cross-sections and the unsteadiness in flow regime. For river network that you mentioned, the presented model can be implemented for each branch of the river, separately.

4- The discussion about this issue will be added to the revised version.

Specific comments of Referee #2

1-Slide 2, Line 21: Please provide the dimensions or units for each of the parameters in all the equations used in the paper.

Answer:

The dimensions for each of the parameters in all the equations will be added to the revised version.

2-Slide 3, Lines 26_28: Please provide references related to the real-world applications of the TSM.

Answer

These references already given in slide 4, lines 1-4.

-D'Angelo, D., Webster, J., Gregory, S., and Meyer, J.: Transient storage in Appalachian and Cascade mountain streams as related to hydraulic characteristics, J. N. Am. Benthol. Soc., 12, 223–235, 1993.

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- Morrice, J. A., Valett, H., Dahm, C. N., and Campana, M. E.: Alluvial characteristics, groundwater–surface water exchange and hydrological retention in headwater streams, Hydrol. Process. 11, 253–267, 1997.

- Czernuszenko, W., Rowinski, P.-M., and Sukhodolov, A.: Experimental and numerical validation of the dead-zone model for longitudinal dispersion in rivers, J. Hydraul. Res., 36, 269–280, 1998.
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- Laenen, A. and Bencala, K. E.: transient storage assessments of dye-tracer injections in rivers of the Willamette basin, Oregon, J. Am. Water Resour. As., 37, 367–377, 2001.
- Fernald, A. G., Wigington, P., and Landers, D. H.: Transient storage and hyporheic flow along the Willamette River, Oregon: field measurements and model estimates, Water Resour. Res., 37, 1681–1694, 2001.
- Keefe, S. H., Barber, L. B., Runkel, R. L., Ryan, J. N., Mcknight, D. M., and Wass, R. D.: Conservative and reactive solute transport in constructed wetlands, Water Resour. Res., 40, W01201.
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- Ensign, S. H. and Doyle, M. W.: In-channel transient storage and associated nutrient retention: evidence from experimental manipulations, Limnol. Oceanogr., 50, 1740–1751, 2005.
- Van Mazijk, A. and Veling, E.: Tracer experiments in the Rhine Basin: evaluation of the skewness of observed concentration distributions, J. Hydrol., 307, 60–78, 2005.
- Gooseff, M. N., Hall, R. O., and Tank, J. L.: Relating transient storage to channel complexity in streams of varying land use in Jackson Hole, Wyoming, Water Resour. Res., 43, W01417, doi: 10.1029/2005WR004626, 2007.
- Jin, L., Siegel, D. I., Lautz, L. K., and Otz, M. H.: Transient storage and downstream solute transport 5 in nested stream reaches affected by beaver dams, Hydro. Process. 23, 2438–2449, 2009.

3-Slide 4, Line 5: "comprehensive" needs to be reworded since the 1D model has limitations on solving complex problems.

Answer:

From the point of view of dealing with 1D, 2D or 3D it is correct that the 1D model has its limitations compared to the other ones but as you see in the manuscript, the word "comprehensive" refers to the ability of model to simulate solute transport problem in both with and without transient storage conditions under steady and unsteady flow regimes in rivers with irregular cross-section (without limitation in section number), just in 1D model. We kindly ask you, if you still feel it is better to use another word, we are pleased to have your suggestion in this regard.

4-Slide 4, Line 19: Since TSM suggested in this paper is somewhat similar to previous works (see additional references), I believe that Table 1 is highly misleading. Therefore, the model comparison part should be thoroughly reworked.

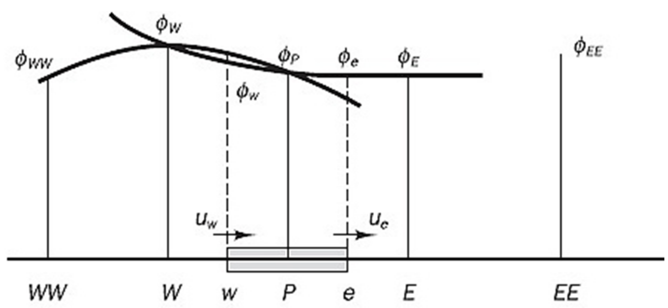
Answer:

In table 1 we tried to demonstrate and compare the features of two well-known software products and the presented model studied in this paper. Now, you may ask "why we select these models and not the other ones". The answer is that we select them because they have some features in common with our presented model. MIKE 11 is the most powerful and applicable software for simulating of flow and transport problems in rivers under wide variety of conditions (complex geometry, different flow regimes, etc.). Also, OTIS is the only model for simulating of solute transport with TS which has been presented. However, if you think it is necessary, we can add another table describing other previous works as well.

5-Slide 5, Line 7: What is the "QUICK" scheme?

Answer:

The quadratic upstream interpolation for convective kinetics (QUICK) scheme of Leonard (1979), is one of the well- known numerical methods. This method uses a three-point upstream-weighted quadratic interpolation for cell face values. The face value of ϕ is obtained from a quadratic function passing through two bracketing nodes (on each side of the face) and a node on the upstream side (figure below).



Quadratic profiles used in the QUICK scheme

For example, when $u_w > 0$ and $u_e > 0$ a quadratic fit through *WW*, *W* and *P* is used to evaluate ϕ_w, and a further quadratic fit through *W*, *P* and *E* to calculate ϕ_e. For $u_w < 0$ and $u_e < 0$ values of ϕ at *W*, *P* and *E* are used for ϕ_w, and values at *P*, *E* and *EE* for ϕ_e. It can be shown that for a uniform grid the value of ϕ at the cell face between two bracketing nodes *i* and *i* – 1 and upstream node *i* – 2 is given by the following formula:

$$\phi_{face} = \frac{6}{8}\phi_{i-1} + \frac{3}{8}\phi_i - \frac{1}{8}\phi_{i-2}$$

$$\text{if} \quad u_w > 0: \qquad \phi_w = \frac{6}{8}\phi_W + \frac{3}{8}\phi_P - \frac{1}{8}\phi_{WW}$$

$$\text{if} \quad u_e > 0: \qquad \phi_e = \frac{6}{8}\phi_P + \frac{3}{8}\phi_E - \frac{1}{8}\phi_W$$

The diffusion terms may be evaluated using the gradient of the approximating parabola. It is interesting to note that on a uniform grid this practice gives the same expressions as central differencing for diffusion, since the slope of the chord between two points on a parabola is equal to the slope of the tangent to the parabola at its midpoint:

$$\left(\frac{\partial \phi}{\partial x}\right)_w = \frac{\phi_P - \phi_W}{\Delta x}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_e = \frac{\phi_E - \phi_P}{\Delta x}$$

For more details please see:

-Versteeg, H. K. and Malalasekera, W. (2007), *An introduction to computational fluid dynamics: the finite volume method*, Pearson Education.

- Leonard, B. P.: A stable and accurate convective modelling procedure based on quadratic upstream interpolation. Computer methods in applied mechanics and engineering, 19**,** 59-98, 1979.

6-Slide 10, Line 1: I believe that Equation (18), 1D discretization matrix, does not provide valuable information because it is a trivial matrix form for the 1D discretization.

Answer:

One of the most important steps in numerical solution of every partial differential equation is obtaining the final pattern of coefficient matrix (tridiagonal, pentadiagonal or block matrix), which determine the solution method of system of discretized equations. Hence, the authors thought it might be worth to give the form of matrix the discretized equations.

7- Section 3.1: The verification results (Tables 5, 6, 7 and 8) should be discussed further. Did authors mean the grid size of the simulation domain is 1 m and the time step size is 30 seconds? If so, are they optimized conditions for your model verifications? Since the grid and time step sizes affect simulation results, further discussion is necessary on this point.

Answer:

Basically, in every numerical simulation, one of the parameters that may be affect the results is grid size. Hence to ensure that the results doesn't depend on grid size, we carried out a mesh independency analysis (which is a common test in numerical studies), that is as follows: at first a large mesh was chosen (large time and space steps) and the model was implemented with this values and results obtained; then the amounts of time and space steps gradually reduced, and simulation was repeated until the results do not show significant changes. The corresponding values of time and space step selected as final grid size at simulations.

8- Section 3.2: What is the definition of the "flow sub-model"? Did authors mean that 1D surface flow simulations were performed to obtain the initial conditions? If so, what kind of the flow model was applied? It should be detailed in the manuscript.

Answer:

The part of model which solves 1D unsteady flow equations (Saint-Venant equations) and provides the values of flow velocity and depth at each computational node is called as "flow sub-model". In this paper Saint-Venant equations have been solved with Preissmann scheme and a numerical code developed for it.

9- Section 4: Please provide information about "CTQS, CTCS and BTCS." Again, further discussion is necessary on the simulation settings (i.e., grid and time step sizes). Generally, the oscillations of concentrations in the concentration profiles can be removed if the grid and time step sizes are very small.

Answer:

- CTQS CTCS and BTCS are abbreviations of Centered Time – QUICK Space, Centered Time – Centered Space and Backward Time – Centered Space, respectively. The detailed information about these methods is given in table 2. Also, discussion about simulation settings has been given in answer of comment 7.
- In theory, numerical results may be obtained that are indistinguishable from the 'exact' solution of the transport equation when the number of computational cells is infinitely large, irrespective of the differencing method used. But it should be noted that, in practical calculations we can only use a

finite – sometimes quite small – number of computational cells. On the other hand in complex problems such as simulation of solute transport in rivers with irregular cross-sections under unsteady flow regime, when we solve flow and transport equations simultaneously, finer mesh lead to extremely high computational cost, that is not desirable.

10- Slide 15, Lines 8_11: It is hard to see that the suggested model performs better than the other models. Further discussion is also necessary on this statement. Section 4.2: Again, the results of the model comparison should be discussed further.

Answer:

Further discussion will be added to revised version.

11- Slide 16 Lines 4_6: Authors should explain about the statement that "MIKE 11 model has a little flaws." It is hard to believe that MIKE 11 has defects based on the simulation results.

Answer:

Yes, you are right, it will be modified in the revised version.

12- Section 4.3: Since reactive solute transport was performed in Section 4.4, Section 4.3 (conservative solute transport) is not necessary.

Answer:

The aim of this example is to show the effect of transient storage mechanism on downstream transport, specifically. However, this section will be removed from the revised version.

13- Slide 24 Lines 6_8: There are several papers that worked on the issues. Please refer to additional references attached in the review comments.

Answer:

Thank you for introducing new and relevant works, we really appreciate it. Some of them are very new and were not available at the time of writing this paper. We will add them to the revised version.