Further Development of an Instream Salt Transport Model for IQQM

A.J. Davidson and **I. Salbe**

Centre for Natural Resources, NSW Department of Sustainable Natural Resources, Parramatta, Australia.

Abstract: The Murray Darling Basin is home to a large proportion of Australia's agriculture and many unique and environmentally significant features, many of which are subject to international treaties. The 1999 Basin Salinity Audit showed salt, that was previously stored in the landscape, is now being mobilised on a massive scale by land-use changes raising water tables. The Murray Darling Basin Commission and the States within the basin have set end of valley salinity targets to address this trend. The New South Wales Department of Sustainable Natural Resources is developing a suite of computer models to evaluate actions designed to meet the targets, such as land-use change and salt interception schemes. The Integrated Quantity Quality Model (IQQM) is an instream model, principally developed to evaluate quantity issues such as the auditing of the Murray Darling Basin Ministerial Council's cap on usage. This paper describes an upgrade of the IQQM's salinity routing scheme, designed to allow the sound scaling up of actions at a sub-catchment level to basin level. The IQQM uses a fully mixed storage assumption combined with a series of lag storages to model the instream transport of water quality constituents. Problems with the schematisation of the flow and salinity time series had to be resolved in order for a correct application of the governing equation to be made, and a suitable numerical solution had to be chosen before it could be implemented. Trouble was encountered with discontinuities in the solution caused by special cases, such as a reach drying out, and these had to be dealt with by the developed solution. The paper concludes with a description of the proposed improvements that will be made to the IQQM's transport model to allow for a better representation of the transport processes in the IQQM.

Keywords: *IQQM; Salinity; Transport; Modelling*

1. INTRODUCTION

1.1. The Integrated Quantity Quality Model (IQQM)

The IQQM is a water resources system model that has been developed by the NSW Department of Sustainable Natural Resources (DNSR) to simulate reservoir and river behaviour at a valley level (Simons et al. 1996). The IQQM uses input data and, most commonly, produces output at a daily time-step. Internally the IQQM divides a day into a user specified number of computation time-steps.

The IQQM has been developed by the DNSR for the following main purposes. 1. Auditing compliance with policy objectives such as the Murray Darling Basin Ministerial Council's (MDBMC) cap on diversions to 1993/94 levels. 2. Help river management committees in their input into Water Sharing Plans (a NSW government initiative to help farmers in their investment decisions by fixing resource-sharing rules for a ten-year period). 3. Provide information for NSW Inter-state sharing management with Queensland and Victoria. 4. Help plan better operating strategies and new infrastructure.

1.2. Need for the IQQM in Salinity Modelling

The IQQM is a part of a suite of models used by the DNSR to predict the effects of land-use change or system management on in-stream salinity. The IQQM's role in this suite is to allow the predictions made at a sub-catchment level, by CATSALT (Vaze et al. in press) for example, to be projected to downstream locations.

The models are required for two main policy objectives. These are the NSW salinity strategy and the Murray Darling Basin Commission's (MDBC) Basin Salinity Management Strategy. Both strategies are designed to address increased dryland and river salinity due to increases in agriculture, industrial, and urban activities.

1.3. Description of the Current IQQM Salinity Routing Model

The IQQM uses a series of nodes and links to represent the layout of the components of a basin's water resource system. Flow routing in the IQQM is represented by the links and is carried out using storage routing--either Muskingum (McCarthy 1938) or rout and lag (Linsley et al. 1949). The IQQM uses a concentrated routing storage with a power relationship between the storage volume and its discharge. The IQQM has the facility to vary the parameters of the routing store for different flow regimes; the different ranges of flow pass through parallel routing and lag storages.

The current IQQM salinity transport model uses an identical schematisation as the flow routing model. As this paper is concerned with modifications to it, only a brief description will be given of the current model. A full description of the model can be found in Javam et al. (2000). It is assumed that the routing store acts as continuously stirred tank reactor and the translation stores each add a time-step's delay to the passage of the salt.

The mass balance for salt in a continuously stirred tank reactor is given by (Chapra 1997, p.287):

$$\frac{dM}{dt} = Q_{in} c_{in} - Q_{out} \frac{M}{V} + L \qquad (1)$$

Where M is the mass of salt in the store (M), Q_{in} is the inflow rate ($M^3 T^{-1}$), Q_{out} is the outflow rate, c_{in} is the salinity concentration of the inflow ($M L^{-3}$), L is the nett external loading rate ($M T^{-1}$), V is the volume of water in the store (L^3), and t is time (T).

2. MODIFICATIONS MADE TO THE EXISTING MODEL

2.1. Schematisation of Concentration Time Series

The total mass of salt that has passed a point in a stream is calculated from:

$$M' = \int Q(t) c(t)\, dt \qquad (2)$$

Where M' is the mass of salt (M), $Q(t)$ the flow rate at time t ($M^3 T^{-1}$), $c(t)$ is the salinity concentration at time t ($M L^{-3}$), and t is time (T).

The result of equation 2 depends upon the relationship that flow and concentration have with time. Two possible assumptions that could be used are; a linear relationship between time and the variables, with the model outputs being considered as instantaneous values at the end of the time-step; or the variables are constant over a time-step and the model outputs are averages for the time-step.

As the IQQM already uses the second assumption for flow routing, the salinity routing code was rewritten to use the average for a time-step assumption. This means, for the IQQM, equation 2 can be rewritten as:

$$M' = \sum \overline{Q}_t \overline{c}_t \Delta t \qquad (3)$$

Where $\overline{Q}_t$ it the average flow for time-step t ($L^3 T^{-1}$), $\overline{c}_t$ is the corresponding average salinity concentration ($M L^{-3}$), and Δt is the time step (T).

2.2. Solution of the Equation

Originally the IQQM used the method presented by Medina et al. (1981) to solve equation 1. However, that method only has direct solutions for two different assumptions of the form of the inflows and outflows, neither of which match the assumptions used in the IQQM. A numerical solution of the governing ordinary differential equation (ODE) 1 was adopted.

The `odeint` function from Press et al. (1992) was adopted to solve equation 1 in the IQQM. This function uses an adaptive step size control to drive a fifth-order Runge-Kutta solution and is warmly recommended by its authors for use on "garden-variety ODEs", such as Equation 1.

Equation 1 is solved for a time step using the assumption that Q_{in}, c_{in}, L, and Q_{out} are constant over the time step but M and V vary. From the value of M at the end of the time step the average outflow concentration is calculated from:

$$\overline{c}_{out} = \frac{\overline{Q}_{in} \overline{c}_{in} \Delta t + L' - M_t + M_{t-1}}{\overline{Q}_{out} \Delta t} \qquad (4)$$

Where M_t is the mass of salt in the store at the end of this time step (M), M_{t-1} is the mass of salt in the store at the end of the last time step (M), $\overline{Q}_{in}$ is the average inflow ($L^3 T^{-1}$), $\overline{Q}_{out}$ is the average outflow ($L^3 T^{-1}$), $\overline{c}_{in}$ is the average inflow salinity concentration ($M L^{-3}$), $\overline{c}_{out}$ is the average outflow salinity concentration ($M\,L^{-3}$), L' is the nett external source (M), and Δt is the time step (T).

It can be seen from equation 4 that the solution of c_{out} for reaches with large residence times is very dependent upon the relatively small change from M_t to M_{t-1} requiring a high level of accuracy when solving equation 1. In the IQQM a tolerance of 10^{-6} was adopted. This means that, except where M is close to zero, the solution for M is accurate to one part in a million. It was found that solving the salinity routing equations consumes 11% of the running time of a typical application of the IQQM.

The modification to the solution of equation 1 made it necessary to add the salt load in a reach to the variables output by IQQM, for later processing. Previously it was assumed that the concentration in the reach was equal to the concentration of the outflow at the end of the time-step. This assumption was correct for the instantaneous value assumption, but is not correct for the average assumption or where a lag was specified.

2.3. Drying Out of Reaches

If evaporation from the reaches is not modelled, then it is not possible for the salinity concentration anywhere in the model to rise higher than the concentrations of the inflows. If evaporation is modelled, the salinity concentrations will generally increase downstream as water is removed from the system by the evaporation. This can lead to unrealistically high salinity concentrations being produced by the model, especially when a reach ceases to flow. One possible solution to this problem is to assume a small volume of dead storage in each reach, which cannot evaporate, as done in Bigmod (Close 1996). Another solution would be to arbitrarily cap the salinity concentration at some predetermined level. We decided that the unrealistically high salinity levels would be left as an indication to the modeller that the range of applicability of the model had been exceeded. A natural channel is likely to dry to a chain of pools but in the model the channel dries out when the stream stops flowing. As a river channel dries out, some of the salt would be deposited on the banks, unlike the model that concentrates the salt in the remaining water.

For the solution routines it was necessary to test for the case of the reach drying out to prevent problems with solving equation 1.

2.4. Refilling Dry Channels

When a reach has dried out and still contains salt it will cause numerical problems when the reach next has water introduced to it. At the first instant of contact with water $\frac{dM}{dt} \rightarrow \infty$. This causes a discontinuity that most numerical solutions cannot handle. To avoid this problem we added a case, to the solution routines, to detect this happening and to reintroduce the deposited salt over the time-step, removing the discontinuity.

2.5. Results of Modifications

The modifications made to IQQM removed the mass-balance errors that were experienced with the older code. In a test case based on the Border Rivers IQQM, for example, the mass-balance error was eliminated (Figure 1).

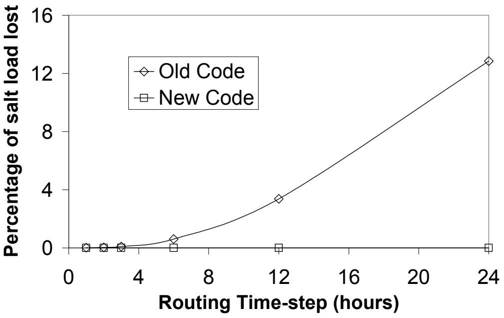

Figure 1: Relationship between calculation time-step and mass balance error.

The lack of a mass-balance error with the new code was expected, as the governing equations had been recast to ensure mass-balance. To test the effect of time-step on the results of the model the Border Rivers test case was run, using synthetic input data, with time-steps ranging from 1 hour to 24 hours and the results compared on a daily time-step. The results show (Figure 2) that the output depends on the time-step used. The pattern of the differences is closely related to the differences between the flow-rates, at the two time-steps, indicating that most of the change is explained by the change in the flow-routing.

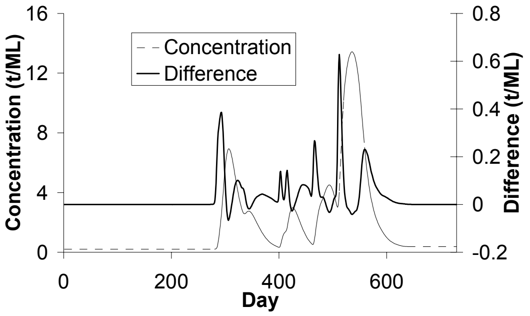

Figure 2: Difference between 1 hour and 24 hour calculation time-step, over a 2 year period.

3. PROPOSED MODIFICATIONS TO THE MODEL

3.1. Addition of a Travel Time Parameter

As the IQQM salinity routing model is currently formulated there are no calibration parameters, the amount of travel-time and dispersion obtained are a function of the flow routing parameters used. In order to model both travel times and wave celerity it will be necessary to modify the flow routing used in IQQM. We propose to adopt a scheme similar to that used in Bigmod (Close 1996).

Wave celerity in a reach is a function of the slope of the storage-discharge relationship, but the travel time in a reach is a function of the absolute storage in a reach. By adding a storage offset to a reach, as a calibration parameter, it will become possible to vary the travel time while keeping the wave speed the same. This storage offset is a combination of dead-storage and compensation for the underestimation of how steep the storage-discharge relationship is below the flow range that you have calibration data for.

3.2. Adoption of a Langrangian Approach to Model Dispersion

With the current IQQM salinity routing model the longitudinal dispersion is a function of the size of the flow routing store. To allow variation of the longitudinal dispersion, the salinity routing store should be independent from the flow routing store. One alternative arrangement is to link a series of continuously stirred tank reactors, such as used by Stefan and Demetracopoulos (1981), and Banks (1974), with the number of stores as the calibration parameter. The principal problem with the cells in series model is the fixed relationship between the number of stores and the travel time and dispersion (Rutherford, 1994 p.223).

The alternative chosen for the IQQM is a Lagrangian transport model. Fischer (1972) developed the original Lagrangian box model and McBride and Rutherford (1984), Schoellhamer (1988) and Jobson (2001) have developed others. Lagrangian models effectively eliminate numerical dispersion and solution oscillation problems (Sobey 1984). Schoellhamer (1985) reports that very simple Lagrangian algorithms can be very accurate compared to relatively complex Eulerian algorithms.

A Lagrangian model uses a reference frame that is moving with the mean velocity of flow, which eliminates the advection term. The dispersion can then be modelled using the Fickian analogy using (Jobson 1980):

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial \xi^2} \qquad (5)$$

Where c is concentration (M L^{-3}), t time (T), D is the longitudinal dispersion coefficient (L^2 T^{-1}) and ξ is distance on the Lagrangian reference frame (L).

Equation 5 can then be solved using an explicit finite difference scheme. For the case where the longitudinal dispersion coefficient is zero the resulting flow becomes plug flow and equation 6 can be solved at any time-step chosen by the modeller. For non-zero dispersion Jobson (1980) suggests that maximum accuracy is obtained when D_f, from equation 6, is equal to 0.2, and is not seriously eroded in the range 0.05 to 0.3.

$$D_f = \frac{D}{U^2 \Delta t} \qquad (6)$$

Where D_f is the diffusion factor (ratio), D is the longitudinal dispersion coefficient (L^2 T^{-1}), Δt the time-step (T) and U the average velocity (L T^{-1}).

The time-step for the salinity routing will need to be much shorter than that used for flow routing. From equation 6, and data from Rutherford (1994), time-steps for natural rivers would be in the range of 2 min-2.5 hours, with a median of 0.2 hours. For the Murray River, as an example, there could be up to 30 000 parcels of water being tracked at any one time. This means that for every time step 30 000 parcels of water would be advected down the system and 30 000 equations solved sequentially—to model the dispersion between the parcels.

4. CONCLUSIONS

The IQQM salinity routing model was improved by adopting a superior numerical solution technique and clarifying the schematisation used. The robustness of the routing model was improved by adding code to deal with the problems caused by reaches drying out and refilling.

To improve the salinity routing model it is planned to add three new features to the model. Adding a storage offset to the storage-discharge relationships will allow for calibration of travel times. Changing to a Langragian transport model, from the continuously stirred tank reactor model, will allow the modelling of plug-flow. The addition of a dispersion component will allow us to be able to model transport in streams where dispersion is significant.

The proposed salinity transport model is at present only at a preliminary stage. It is based on schemes used by others successfully but a pilot study will have to be carried out to see if it improves the results we obtain for New South Wales rivers. Further investigation will need to be carried out to see if dispersion modelling is required, as the computation expense may be large.

5. REFERENCES

Banks, R.B. 1974, 'A mixing cell model for longitudinal dispersion in open channels', *Water Resources Research*, vol. 10, no. 2, pp. 357-358.

Chapra, S.C. 1997, *Surface Water-Quality Modeling*, WCB/McGraw-Hill, Boston, Massachusetts.

Close, A.F. 1996, 'A new daily model of flow and solute transport in the River Murray', *23rd. Hydrology and Water Resources Symposium*, Institution of Engineers, Australia, Canberra, pp. 173-178.

Fischer, H.B. 1972, *A Lagrangian Method for Predicting Pollutant Dispersion in Bolinas Lagoon, Marin County, California*, Geological Survey Professional Paper 582-B, U.S. Department of the Interior, Washington.

Javam, A., Podger, G., Boddy, J. & Beecham, R. 2000, 'Modelling of instream salt transport processes', Hydro 2000 3rd International Hydrology and Water Resources Symposium, Institution of Engineers, Australia, Canberra, pp. 727-732.

Jobson, H.E. 1980, Comment on 'A new collocation method of the convection-dominated transport equation', *Water Resources Research*, vol. 16, no. 6, pp. 1135-1136.

Jobson, H.E. 2001, *Modeling Water Quality in Rivers using the Branched Lagrangian Transport Model (BLTM)*, U.S.G.S Fact Sheet FS-147-00, U.S. Department of the Interior, Washington.

Linsley, R.K., Kohler, M.A & Paulhus, J.L.H. 1949, *Applied Hydrology*, McGraw-Hill, New York.

Medina, M.A., Huber, WC & Heaney, JP 1981, 'Modeling stormwater storage/treatment transients: theory', *Journal of the Environmental Engineering Division*, vol. 107, no. EE4, pp. 781-797.

McCarthy, G.T. 1938, The unit hydrograph and flood routing, Paper presented to the Conference of the North Atlantic Division, U.S. Army Corps of Engineers, New London, Connecticut, June 24, quoted in Clark, C.O. 1945, 'Storage and the unit hydrograph', *Transactions ASCE*, vol. 110, pp. 1419-1488.

McBride, G.B. & Rutherford, J.C. 1984, 'Accurate modeling of river pollutant transport', *Journal of Environmental Engineering*, vol. 110, no. 4, pp. 808-827.

Press, W.H., Teukolsky, S.A., Vetterling, W.T. & Flannery, B.P. 1992, *Numerical Recipes in FORTRAN*, 2nd edn, Cambridge University Press, Cambridge, England.

Rutherford, J.C. 1994, *River Mixing*, John Wiley and Sons Ltd, Chichester, England.

Schoellhamer, D.H. 1985, Discussion of 'Numerical alternatives in transient stream response', *Journal of Hydraulic Engineering*, vol. 111, no. 8, pp. 1214-1215.

Schoellhamer, D.H. 1988, 'Lagrangian transport modeling with QUAL II kinetics', *Journal of Environmental Engineering*, vol. 114, no. 2, pp. 368-381.

Simons, M., Podger, G. & Cooke, R. 1996, 'IQQM—a hydrologic modelling tool for water resource and salinity management', *Environmental Software*, vol. 11, nos. 1-3, pp. 185-192.

Sobey, R.J. 1984, 'Numerical alternatives in transient stream response', *Journal of*

Hydraulic Engineering, vol. 110, no. 6, pp. 749-772.

Stefan, H.G. & Demetracopoulos, A.C. 1981, ‘Cells-in-series simulation of riverine transport’, *Journal of the Hydraulics Division*, vol. 107, no. HY6, pp. 675-697.

Vaze, J., Barnett, P., Beale, G.T.H., Dawes, W., Evans, R., Tuteja, N.K., Murphy, B., Geeves, G. & Miller, M. in press, ‘Modelling the effects of landuse change on water and salt delivery from a catchment affected by dryland salinity’, *Hydrological Processes*.