On the Numerical Solution of the ADZ Model

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Abstract
The ADZ model is a simple and effective tool for simulating solute transport in rivers. The study reported here concerns the model's numerical algorithm. Tracer data from the Murray Burn in Edinburgh is used to compare the performance of three alternative formulations. The theoretical advantages of a new algorithm are borne out by simulations of the tracer data, although improvements in simulations, compared to those obtained with the standard algorithm, are probably only significant when the problem is poorly resolved in time. Nevertheless, the new algorithm can be recommended on the grounds that little extra effort is required to use it and simulations so obtained are generally more robust.

1. Introduction
The Aggregated Dead Zone (ADZ) model is an alternative approach to the Advection-Dispersion Equation (ADE) for simulating solute transport in rivers (Rutherford, 1994). Since the model's inception, little attention has been paid to the model's numerical algorithm. The aim of this paper is to draw readers' attention to this aspect of the model. This is achieved by showing how the algorithm is derived, and by exploring some straightforward alternatives. The performance of three algorithms is illustrated by applying the model to tracer data collected in the Murray Burn, which is a small stream that runs through the Heriot-Watt University Campus at Riccarton in Edinburgh.

The following sections present relevant details of the ADZ model, its application to the Murray Burn, presentation and discussion of illustrative results and, finally, some conclusions.
2. The ADZ Model

2.1 Background
The ADZ model originated in the work of Beer and Young (1983), where it was described within the framework of the physically-based ADE model (Rutherford 1994). In that era, possibly the major disadvantage of the ADE model was that it did not explicitly account for the action of transient storage (TS) on the transport of solutes in rivers. It had been postulated that transient storage in dead zones was responsible for the elevated tails of, and the persistence of skewness in, observed concentration profiles that were not catered for by the ADE model. However, although (a) it was relatively straightforward to include transient storage caused by dead zones in the ADE model (Bencala and Walters 1983) and (b) as a result better agreement with observations could be obtained, two additional model coefficients were introduced that were difficult to relate to measurable physical features.

More recently, this ADE+TS model has become more popular (Hart 1995, Rowiński et al. 2004). However, since transient storage may occur not only through the action of re-circulating flow within dead zones, but also through exchange with the hyporheic zone (Marion et al. 2003, Worman et al. 2002), the physical significance of the model coefficients remain a subject of debate (Czernuszenko and Rowiński 1997, Hart 1995, Schmid 2002).

In the ADZ model, in contrast to simulating the action of a complex system of physical interactions, a conceptually simpler (but less well physically-based) approach is taken. Several matters are simplified, but crucially dispersion is modelled as if it were created by the action of a single transient storage zone that represents the aggregated effect of all the physical dispersive mechanisms taking place in a reach. Previous studies (Wallis et al. 1989) have shown the benefits of this rather radical approach. Interestingly, the ADZ model coefficients have a simple physical interpretation, and have generally been found to be robust.

2.2 Derivation
Under steady flow conditions, the ADZ model is based on the following reach scale dynamic solute mass balance equation:

\[
\frac{dS(t)}{dt} = \frac{Q}{V} [u(t) - y(t)]
\]

where \( V \) is the volume of water in a reach, \( S(t) \) is the reach average solute concentration, \( Q \) is the flow rate of water through the reach, \( u(t) \) is the cross-sectional average solute concentration at the upstream boundary of the reach, \( y(t) \) is the cross-sectional average solute concentration at the downstream boundary of the reach and \( t \) is time.

To model dispersion in the reach by the action of a (single effective) transient storage zone, the reach is represented by a continuously stirred tank (Chapra 1997). With this, any solute that enters the tank is immediately and uniformly mixed throughout the entire tank volume such that any change in the input concentration causes an immediate change in the output concentration. As it stands, this is not a
good representation of solute transport in a river, however, because there is no delay to
represent the time it takes for the leading edge of a solute cloud to be advected through
a reach. Similarly, if the continuously stirred tank is assumed to contain the same vol-
ume of water as the reach this is also inconsistent with reality, because it is certainly
not the case that all the water in a reach is so well mixed longitudinally that the solute
concentration in it is uniform.

Both the above difficulties are overcome by assuming that the continuously stirred
tank contains only a fraction of the total reach volume, and that the remaining water is
contained in a plug flow tank (Chapra 1997) in series with the continuously stirred
tank. With the plug flow tank there is no longitudinal mixing, but it introduces the
required advective time delay.

If \( \gamma \) is the fraction of the reach volume contained in the continuously stirred
tank, and \( \tau \) is the time delay associated with the plug flow tank, Eq. (1) can be modified by
(a) replacing \( S(t) \) with \( \gamma S(t) \) and (b) moving the origin of \( u(t) \) forward in time by \( \tau \).
Thus the ADZ model equation that describes advection and dispersion is:

\[
\frac{dy(t)}{dt} = \frac{1}{T} [u(t - \tau) - y(t)]
\]

where \( T \) is the residence time of the transient storage zone (\( = \gamma V/Q \)). A moment analy-
sis (Wallis 1994) reveals that:

\[
\bar{T} = T + \tau
\]

where \( \bar{T} \) is the reach travel time \( (V/Q) \). \( \gamma \) is termed the dispersive fraction.

2.3 Numerical algorithms

Equation (3) can be used to predict the temporal solute concentration profile at the
downstream boundary of a reach assuming that the model coefficients (\( T \) and \( \tau \)) and
the corresponding temporal solute concentration profile at the upstream boundary of
the reach are known. Since the latter is usually in discrete form, a numerical solution
algorithm for Eq. (2) is required.

There are many numerical methods that are appropriate for such a straightforward
ordinary differential – delay equation, including the well-known Euler and Runge-
Kutta algorithms. The approach used here, however, comes from linear dynamical
systems theory (Schwarzenbach and Gill 1984). Consider, initially, the general first
order linear dynamical system equation (with no time delay) shown below:

\[
\frac{dY(t)}{dt} = \alpha Y(t) + \beta U(t)
\]

where \( Y(t) \) is the system output, \( U(t) \) is the system input and \( \alpha \) and \( \beta \) are constant coef-
ficients. A general numerical solution for this equation that relates the output at time
\( t + \Delta t \) to the output at time \( t \) (where \( \Delta t \) is a short time interval or time step) is:

\[
Y(t + \Delta t) = Y(t) e^{\alpha \Delta t} + \int_0^{\Delta t} e^{\alpha (\Delta t - \lambda)} \beta U(\lambda) d\lambda.
\]

where \( \lambda \) is a dummy integration variable. Applying these ideas to Eq. (2) gives:
\[
\alpha = -\beta = -\frac{1}{T} \tag{6}
\]

The accuracy of Eq. (5) depends on how \( U(\lambda) \) is approximated over \( \Delta t \) and on the product \( \alpha \Delta t \). Three treatments of \( U(\lambda) \) are now considered for the ADZ model.

The simplest (and most natural) treatment of the input is to assume that it is constant over a time step and that it takes the value corresponding with the start of the time step, i.e. \( u(t) \). Using this, Algorithm 1 (the standard algorithm) for Eq. (2) is:

\[
y_{k+1} = ay_k + bu_{k-\delta} \tag{7}
\]

where:

\[
a = \exp(-\Delta t/T) \tag{8}
\]

\[
b = 1 - a \tag{9}
\]

\[
\delta = (\tau/\Delta t) - 1 \tag{10}
\]

and \( y_{k+1} \) is the downstream concentration at the time \((k+1)\Delta t\), \( y_k \) is the downstream concentration at the time \( k\Delta t \) and \( u_{k-\delta} \) is the upstream concentration at an earlier time corresponding to a time delay of \( \tau \). Note that Eq. (10) allows for the fact that Eq. (7) automatically introduces a time delay of one time step. An equally valid treatment of the input assumes that it is constant over a time step and that it takes the value corresponding with the end of the time step, i.e. \( u(t+\Delta t) \). Hence, Algorithm 2 is defined by Eqs. (7)–(9), but the time delay is now defined as:

\[
\delta = (\tau/\Delta t) \tag{11}
\]

A theoretically better treatment of the input would consider its variation over the time step. The simplest variation is a linear one, i.e.:

\[
U(\lambda) = u(t) + \left[ u(t + \Delta t) - u(t) \right] \frac{\lambda}{\Delta t} \tag{12}
\]

Using this, Algorithm 3 for Eq. (2) is:

\[
y_{k+1} = ay_k + bu_{k-\delta} + cu_{k+1-\delta} \tag{13}
\]

where:

\[
a = \exp(-\Delta t/T) \tag{14}
\]

\[
b = -a + T/\Delta t - a T/\Delta t \tag{15}
\]

\[
c = 1 - T/\Delta t + a T/\Delta t \tag{16}
\]

\[
\delta = (\tau/\Delta t) \tag{17}
\]

Differences in simulations obtained with these three algorithms are discussed below in relation to observed solute transport in the Murray Burn, which is a small stream running through the Heriot-Watt University Campus in Edinburgh.
3. Application to the Murray Burn

Data were available from a series of tracer experiments (Burke 2002). Each experiment consisted of the (gulp) injection of a known mass of Rhodamine WT dye followed by the measurement of tracer concentration-time profiles at up to four measurement sites. The profiles were obtained by measuring tracer concentrations in water samples (from the stream centre) using a calibrated Turner Designs fluorometer.

The three ADZ model algorithms were used to simulate the solute transport in the reach between the first and second sampling sites. This reach is 137 m long with a mean width of 3.7 m, a mean longitudinal slope of 0.025 and a bed covered with cobbles of nominal size between the order of 1 cm and the order of 15 cm. In applying the algorithms, the values of $T$ and $\tau$ were adjusted until an optimum agreement was found between predicted and observed tracer data at Site 2, under the constraint provided by Eq. 3 (reach travel times were evaluated as the time delay between the centroids of the tracer data at the two sites). Note also that with the ADZ model, values of $\tau$ are constrained to be integer multiples of the time step. Eighteen experiments provided reliable data: experiments containing incomplete profiles were not used.

4. Results and discussion

Some clear trends emerged from the simulations. For example, the peak concentration and the overall shape of the observed concentration-time profiles were generally reproduced well by all three algorithms for all eighteen experiments. However, simulations with Algorithm 1 tended to show a phase lead, simulations with Algorithm 2 tended to show a phase lag, while simulations with Algorithm 3 tended to show little phase error and were, therefore, consistently better. These features are illustrated well in Figs. 1 and 2. Table 1 shows a measure of the agreement between the observed and simulated concentration profiles for each algorithm, evaluated over all experiments. The data in the table are based on the coefficients of determination for each simulation, calculated as $1-(e/var)$, where $e$ is the mean square error and var is the variance of the observed concentration profile, respectively (a value of unity indicating a perfect agreement).

![Comparison of observed and simulated concentrations: experiment 24.](attachment:image.png)

Table 1: Coefficients of determination for each algorithm.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Coefficient of Determination</th>
</tr>
</thead>
<tbody>
<tr>
<td>Algorithm 1</td>
<td>0.9620</td>
</tr>
<tr>
<td>Algorithm 2</td>
<td>0.9445</td>
</tr>
</tbody>
</table>

Fig. 1. Comparison of observed and simulated concentrations: experiment 24.
fit). The table suggests that there is little to choose between Algorithms 1 and 2, but that Algorithm 3 is better. Of course, it is difficult to judge the significance of the differences between the values in Table 1, but the individual coefficients of determination shown on Figures 1 and 2 help to put them into perspective. In addition to these overall data, consideration of the individual experiments showed that in all but one experiment, Algorithm 3 produced the largest coefficient of determination.

Table 1

<table>
<thead>
<tr>
<th>Algorithm 1</th>
<th>Algorithm 2</th>
<th>Algorithm 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>Standard deviation</td>
<td>Mean</td>
</tr>
<tr>
<td>0.9686</td>
<td>0.0243</td>
<td>0.9668</td>
</tr>
</tbody>
</table>

The superiority of Algorithm 3 reflects its inherently more accurate treatment of the upstream concentration data. Also, Algorithm 3 is better suited to cases where there is some ambiguity in the time delay, $\delta$, due to $\tau/\Delta t$ not being close to an integer value. As would be expected, the differences between the simulations obtained with Algorithm 3 and those obtained with either of the other two algorithms reduced as (a) the temporal resolution of the problem increased and (b) the ratio $T/\Delta t$ increased. Since both of these parameters decrease with increasing river flow, it is probably more important to use Algorithm 3 for higher flow events. Alternatively, tracer experiments at high flows could be designed to employ a reduced sampling interval, as indeed had been attempted in the Murray Burn experiments.

5. Conclusions

This paper has focused attention on numerical algorithms for simulating solute transport in rivers with the ADZ model. Some advantages of using an algorithm that uses
two values of upstream concentration (Algorithm 3) in contrast to the standard algorithm that uses only one upstream concentration value have been discussed. Although Algorithm 3 generally provides better simulations, the differences are perhaps not significant unless the time step used is not matched satisfactorily to the river flow. On the other hand, the extra effort required to implement Algorithm 3 is negligible, so there is no impediment to using it, and by doing so ADZ model simulations would always tend to be more robust.

References


