MODELLING SOLUTE TRANSPORT
IN A SMALL STREAM USING DISCUS

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Abstract

This paper describes the main features of the DISCUS model for one-dimensional advection–dispersion computations in rivers, and describes its application to a short reach of The Murray Burn (a small stream in Edinburgh). DISCUS was calibrated using tracer data and an optimisation technique that uses a genetic algorithm. The optimised dispersion coefficients were found to increase from 0.25 to 2 m\textsuperscript{2}/s in the flow range 16-261 l/s. The model was validated using tracer data not used in the calibration stage. It appears that transient storage does not play a major role in the transport of solutes in the reach that was modeled.

Key words: solute transport, streams, numerical modelling, DISCUS, dispersion coefficients

1. INTRODUCTION

This paper concerns the simulation of solute transport in a small stream using a conservative semi-Lagrangian numerical model known as DISCUS. The model has evolved over the last decade and has previously been shown to provide robust and accurate results for several riverine water quality scenarios over a range of physical and discretisation scales (Manson and Wallis, 2000b; Manson \textit{et al.}, 2001).

The aims of the paper are (a) to describe the main features of the model and (b) to calibrate and validate it for a small stream, using a set of tracer data. In the next two sections, numerical modelling of solute transport in streams is reviewed, and details of
2. MODEL BACKGROUND

One-dimensional solute transport in rivers in the absence of transient storage may be described by the following solute mass conservation equation, which is usually called the Advection-Dispersion Equation (Rutherford, 1994).

\[ \frac{\partial (AC)}{\partial t} + \frac{\partial (AUC)}{\partial x} = \frac{\partial}{\partial x} \left( DA \frac{\partial C}{\partial x} \right). \]  

(1)

Here \( A \) is the cross-sectional area of the flow, \( C \) is the cross-sectionally averaged solute concentration, \( U \) is the cross-sectionally averaged longitudinal flow velocity, \( D \) is the longitudinal dispersion coefficient, \( x \) is the longitudinal spatial co-ordinate and \( t \) is time. In general, numerical solutions to eq. (1) are sought because there are few exact analytical solutions that can be applied to practical problems. Unfortunately, eq. (1) is not an easy equation to solve numerically (a) because of the quite different nature of the advection and dispersion terms (terms 2 and 3, respectively) and (b) because the advection term needs particular care. Over the last thirty years or so, however, workers have gradually developed some reliable methods.

In summary, these developments have led from the use of Eulerian low-order finite difference, finite element and finite volume methods, and have culminated in semi-Lagrangian high-order finite element and finite volume methods. Along the way, the potential problems of instability, numerical diffusion, unphysical oscillations and non-conservation of mass have been marginalized, so that robust and accurate numerical schemes are now relatively easy to construct. Many of the key ideas are described and discussed in, for example, Leonard (1979; 2002), Celia et al. (1990), Roache (1992), Leonard et al. (1995) and Russell and Celia (2002). A particularly important feature of the semi-Lagrangian method is that much larger time steps can be used compared to Eulerian approaches. This is particularly attractive because it enables model runs to be completed very quickly, thus making possible (a) the inclusion of parameter uncertainty in modelling studies using, for example, Monte Carlo techniques and (b) the use of sophisticated automatic model calibration procedures using parameter optimization algorithms.

One of the first of the latest breed of numerical schemes for one-dimensional solute transport in rivers was developed by the authors in the 1990s, and it is this model that is used in the current study. The model is called DISCUS (Domain of Influence Search for Convective Stability), and the main features of it are described in the following section with more detail being available elsewhere (Manson and Wallis, 2000a; Manson et al., 2001). Some further developments of the techniques used in DISCUS have been proposed recently by Cox et al. (2002) in their DOZER model.
3. **DISCUS**

DISCUS is a semi-Lagrangian, finite volume scheme. It is unconditionally stable, conserves mass and yields accurate results over wide ranges of discretisation scales. The latter property makes it equally as suitable to dealing with grid refinement in areas of highly non-uniform flow as it is to providing very efficient simulations using large time steps.

The basic idea of the semi-Lagrangian approach is illustrated in Fig. 1, which shows part of the computational grid on which the calculations are executed. It is important to appreciate that (a) the transport of solute along rivers is usually dominated by advection and (b) the success of any numerical scheme lies in the appropriate mapping of the domain of influence of a computed variable to the corresponding physical domain of influence in the river. With reference to Fig. 1, in order to accurately predict information between locations 1 and 2 (the “arrival” zone) in the future (time level $n+1$) it is essential that data from the corresponding domain of influence is used. This region is identified by following characteristic lines upstream from the arrival zone until they intersect the present (time level $n$), thus defining the “departure” zone. The characteristic lines are dependent only on the velocity field in the river, such that in regions of high velocity they have shallow gradients and in regions of low velocity they have steep gradients. Thus in advection dominated flows the departure zone is often a long way upstream of the arrival zone, and increasingly so as the time step used in the calculations ($\Delta t$) is made larger.

![Fig. 1. Illustration of the semi-Lagrangian concept: the river is flowing to the right.](image-url)
A further important feature of the semi-Lagrangian approach is that for pure advection, parameters remain constant along a characteristic line. Hence, advection can be modeled by equating a required value at time level \( n+1 \) to one interpolated from known values at time level \( n \). As well as its simplicity, this method of modeling advection has another advantageous feature, namely that it is unconditionally stable.

The basic idea of the finite volume numerical method is illustrated in Fig. 2 and by the corresponding Eulerian discretisation of eq. (1) given below.

\[
\frac{(AC)_{n+1} - (AC)_n}{\Delta t} + \frac{(UAC)_R - (UAC)_L}{\Delta x} = \frac{1}{\Delta x} \left[ \frac{DA}{\Delta x} \frac{\partial C}{\partial x} \right]_R - \left[ \frac{DA}{\Delta x} \frac{\partial C}{\partial x} \right]_L.
\]

Here \( \Delta x \) is the space step (or the length of the computational cell) used in the calculations (assumed here to be uniform) and the other symbols are as previously defined. The subscript \( i \) refers to the computational node at the centre of the computational cell and the subscripts \( R \) and \( L \) refer to the cell’s right-hand and left-hand faces, respectively. The double overbar indicates that a quantity is averaged over the length of the computational cell, while the single overbar indicates that a quantity is averaged over the time step. If the six average quantities in eq. (2) were evaluated exactly, then eq. (2) would give an exact representation of eq. (1). In practice, of course, this isn’t possible, but the more nearly a numerical scheme remains faithful to the finite volume concepts, the more likely it is to yield reliable results.

![Fig. 2. Finite volume grid for computational cell (shaded) centred at node \( i \).](image)

The semi-Lagrangian finite volume method on which DISCUS is based follows directly from the above by realizing that although the “top” of the computational cell remains centred at node \( i \), the “bottom” of it must be located in the corresponding
domain of influence. As a result the time step average values introduced above can be interpreted as values averaged along the characteristic lines. The simplest way of evaluating these averages is to use a "two-point $\theta$-weighted" algorithm. Although this technique is used for the dispersion term, it is not actually required for the advection term, because, assuming advection can be modeled in isolation from dispersion, the advection term can be evaluated more accurately and more simply using the idea introduced earlier, namely that advected quantities remain unchanged along characteristic lines. Hence eq. (1) can be represented by the following equation:

$$\frac{(AC)^{n+1} - (AC)^n}{\Delta t} + \left[ \frac{\partial (AUC)}{\partial x} \right]_f = (1 - \theta) \frac{\partial}{\partial x} \left( DA \frac{\partial C}{\partial x} \right)_f + \theta \frac{\partial}{\partial x} \left( DA \frac{\partial C}{\partial x} \right)_{*+1}.$$  (3)

Here, subscript $f$ indicates that the term is evaluated within the domain of influence of node $i$. Note that (a) the finite volume form of the advection term has been replaced by its differential form, as an indication that it is treated in a different way, although as is described below, the method used does in fact remain faithful to the finite volume approach and (b) it is assumed that the hydraulic variables required are available in the computational domain from supplementary computations or from measurements.

In DISCUS, the treatment of the dispersion term is approximated by taking $\theta = 1$. Although it would be more accurate and only a little more demanding to use $\theta = 0.5$, such a scheme is not as robust as the fully backward implicit approach (Manson et al., 2001). In practice, no disadvantages have been encountered from this when modelling advection dominated flows, and it has the added advantage of being unconditionally stable. At this stage, there are some advantages in (a) introducing a new variable, namely the solute mass per unit length $m (= AC)$, and (b) splitting the calculation into two steps, one for advection and one for dispersion. Hence eq. (3) becomes

$$\bar{m}_i = m_i - \Delta t \left[ \frac{\partial (mU)}{\partial x} \right]_f,$$  (4)

$$m_i^{*+1} = \bar{m}_i + \frac{\Delta t}{\Delta x} \left[ DA \frac{\partial C}{\partial x} \right]_r - \left( DA \frac{\partial C}{\partial x} \right)_{*+1},$$  (5)

where the curly overbar indicates the (cell-average) result of the advection step.

Turning our attention now to the solution of the advection step, recall that this consists of three parts: the generation of characteristic lines to locate the domain of influence, the interpolation of information within the vicinity of the domain of influence and finally the transfer of the interpolated values along the characteristic lines. Whereas the first and third of these are relatively straightforward, the second contains several potential difficulties. Interestingly, there are a number of apparently quite different approaches that might be used here that, perhaps surprisingly, can lead to the
same final algorithm. Indeed, several approaches have been used successfully during the development of DISCUS (Wallis and Manson, 1997; Wallis et al., 1998; Manson and Wallis, 2000a). Here, however, only the latest and most refined approach is described. The most significant difference between this and earlier approaches is that a cumulative solute mass distribution function is interpolated rather than the solute concentration. This enables the treatment of advection to be consistent with the finite volume method, whilst also retaining a satisfying elegance. Importantly, this treatment guarantees that solute mass is conserved by the numerical scheme.

In DISCUS, the hydraulics of the flow is represented in a cell-averaged fashion, achieved by spatially averaging hydraulic data over each computational cell. Thus the hydraulic parameters in the model are constant within each cell, see Fig. 3. Since the velocity field is represented in this cell-wise-constant manner, the characteristic lines take a cell-wise-linear form. Figure 3 shows how the left-hand and right-hand sides (l and r, respectively) of the domain of influence of the ith computational cell are located by tracking the characteristic lines from the faces of the cell. For pure advection, all of the solute mass in the domain of influence remains between the two characteristic lines while it is transported over the time step. Thus the solute mass in the ith computational cell at time level n+1 must be the same as the solute mass in its domain of influence. Hence, the advection step consists of determining the total solute mass between r and l, and dividing by ∆x to give the solute mass per unit length. Therefore,

\[ \tilde{m}_i = \frac{M_r - M_l}{\Delta x}, \]  

(6)

where \( M_r \) and \( M_l \) are cumulative solute masses at \( r \) and \( l \), respectively, which can be found by interpolation of the continuous cumulative solute mass distribution function, \( M(x) \), defined below:

\[ M(x) = \int_0^s m(s) \, ds. \]  

(7)

Here \( s \) is a dummy integration variable in the longitudinal co-ordinate direction. Assuming that solute concentration is represented in the same cell-averaged manner as the velocity and area, it too is cell-wise-constant, and so is \( m \) (see Fig. 3). Hence, in practice the integral above is replaced by the following summation.

\[ M_{i \Delta x} = \sum_{i=1}^j m_i \Delta x. \]  

(8)

So, for example, the cumulative solute mass at the right-hand face of the third computational cell is given by \( M_{3 \Delta x} = (m_1 + m_2 + m_3) \Delta x \). Clearly, the only places where the cumulative solute mass is known exactly are the faces of the computational cells. Hence the continuous cumulative solute mass distribution, \( M(x) \), as defined by eq. (7) is not available. Instead, it is found by fitting a continuous function through the discrete values of \( M_{i \Delta x} \), see Fig. 3.
Fig. 3. Illustration of: characteristic lines for the \( i \)th computational cell (panel 1); cell-average representation of hydraulic and solute parameters (panels 2-5); discrete (symbols) and continuous (dashed line) representations of the longitudinal solute mass distribution (panel 6).

Rather than fitting a single function through all the values of \( M_{j\Delta x} \) within the entire computational domain, however, \( M_r \) and \( M_l \) are interpolated from a local function for \( M(x) \) that is obtained by fitting a polynomial to neighbouring values of \( M_{j\Delta x} \) in the vicinity of \( r \) and \( l \) (i.e. in the interpolation zone, see Fig. 3). This procedure is then
repeated for each computational cell (Manson and Wallis, 2000a). The choice of interpolation scheme requires a lot of care. Firstly, it should be of a high enough order of accuracy to represent the local longitudinal distribution of cumulative solute mass, and secondly, any spurious local maxima that may be generated need to be “clipped” in order to preserve the convexity of the original distribution (Manson et al., 2001). Experience suggests that cubic interpolation gives a good compromise between accuracy and computational cost. The results presented later were in fact obtained using a symmetrical cubic Lagrange interpolation scheme, as described in Manson et al. (2001).

The characteristic lines that are tracked upstream from the first few computational cells intersect the upstream boundary of the computational domain before they have propagated for a time equal to the time step. In such cases spatial interpolation is replaced by temporal interpolation of the data that is available at the upstream boundary. Indeed, for some cells a mixture of temporal and spatial interpolation may be required to evaluate the total solute mass in the domain of influence (Manson and Wallis, 2000a).

Having obtained the cell-average solute mass per unit length for each computational cell using eq. (6), the dispersion step (eq. 5) is applied to each computational cell in turn. Next, the resulting equations are assembled into a tri-diagonal matrix and all the cell-averaged solute mass per unit lengths are found using an appropriate matrix solver. Finally, cell-averaged solute concentrations are recovered.

4. APPLICATION OF DISCUS TO THE MURRAY BURN

DISCUS was used to model solute transport in The Murray Burn, which flows through the Heriot-Watt University campus at Riccarton in Edinburgh, Scotland. Data were available from a series of tracer experiments that had been conducted in a 0.5 km reach of the stream (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 four sampling sites. The profiles were obtained by measuring tracer concentrations in water samples (collected from the central part of the stream) using a calibrated Turner Designs fluorometer. The sampling interval was matched to the stream flow of each experiment, with the aim of capturing well-resolved profiles. Typically, sampling intervals of 30 s, 60 s and 120 s were used for high, medium and low flows, respectively. A total of 26 experiments were conducted under steady flow conditions in the flow range 0-3 m$^3$/s.

DISCUS was applied to 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. Thirteen sets of complete tracer data were available (these covered the flow range 0-0.3 m$^3$/s). Ten of these were used to calibrate the model and three were used to validate it. For each data set, the tracer data at Site 1 were used as the
upstream boundary condition, and the model predicted the tracer data at Site 2. In all cases the reach was treated as a uniform channel (because no surveys of individual cross-sections were available), so that the cross-sectional area (represented by a dummy value, since it plays no part in uniform flow simulations), velocity $U$ and dispersion coefficient $D$ were constant throughout the computational domain, which consisted of 50 uniform space steps of length 2.74 m. In the calibration stage, the values of $U$ and $D$ were adjusted until an optimum agreement was obtained between the predicted and the observed tracer data at Site 2. Automatic optimization was undertaken using the genetic algorithm approach described in Manson and Wallis (2004). In the validation stage the model was used to predict the tracer data at Site 2, using values of $U$ and $D$ derived from the values found in the calibration stage.

5. RESULTS AND DISCUSSION

A summary of the optimized coefficients and other relevant data is shown in Table 1. The flows in column three were evaluated by applying dilution gauging to the tracer data from Site 1. Column six shows coefficients of determination that describe how well the optimized model output agrees with the tracer data at Site 2. Overall, the $R^2$ values are quite consistent, being between 0.93 and 0.98 (1.00 indicates perfect agreement). An indication of the quality of the agreement that these $R^2$ values represent is given in Figs. 4 and 5, which show tracer concentration-time curves from two of the calibrations. Generally the peak concentration and the width of the profile were captured well, with any lack of fit being confined to the leading and trailing edges. In Fig. 5, however, which is the worst resolved data set (highest flow) and the one with

<table>
<thead>
<tr>
<th>Tracer experiment number</th>
<th>Mass of tracer [g]</th>
<th>Flow, $Q$ [l/s]</th>
<th>Velocity, $U$ [m/s]</th>
<th>Dispersion coefficient, $D$ [m$^2$/s]</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.05</td>
<td>68.0</td>
<td>0.204</td>
<td>0.608</td>
<td>0.957</td>
</tr>
<tr>
<td>4</td>
<td>0.05</td>
<td>43.6</td>
<td>0.162</td>
<td>0.445</td>
<td>0.980</td>
</tr>
<tr>
<td>5</td>
<td>0.05</td>
<td>47.5</td>
<td>0.165</td>
<td>0.559</td>
<td>0.968</td>
</tr>
<tr>
<td>7</td>
<td>0.10</td>
<td>134.2</td>
<td>0.306</td>
<td>0.985</td>
<td>0.946</td>
</tr>
<tr>
<td>8</td>
<td>0.05</td>
<td>45.7</td>
<td>0.165</td>
<td>0.460</td>
<td>0.982</td>
</tr>
<tr>
<td>10</td>
<td>0.10</td>
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<td>0.187</td>
<td>0.563</td>
<td>0.955</td>
</tr>
<tr>
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<td>0.323</td>
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</tr>
<tr>
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</tr>
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<td>62.1</td>
<td>0.185</td>
<td>0.587</td>
<td>0.982</td>
</tr>
</tbody>
</table>
the smallest $R^2$, the peak is not particularly well matched. These figures also illustrate the similar nature of the concentration-time curves over the range of flows contained in the data set (Burke, 2002; Wallis, 2005).

Figures 6 and 7 illustrate the variation of the optimized coefficients with the flow $Q$. Clearly, $U$ shows the sort of non-linear increase with increasing $Q$ that would be expected (Fig. 6), with values that are commensurate with a small, steep stream carry-
ing the range of flows experienced. Further corroboration of these values was obtained by estimating the velocity from the centroids of the tracer curves, i.e. by using the method of moments (Rutherford, 1994). This data is also shown in Fig. 6 where there is excellent agreement at the low flows, but some divergence at the high flows, with the values derived from the centroids, $U_c$, being smaller. Indeed, closer inspection shows that in nine of the ten data sets $U$ is slightly greater than $U_c$; overall, the ratio of $U$ to $U_c$ varies between 0.99 and 1.06. It is not unexpected that generally $U$ is larger than $U_c$ because the effect of any transient storage in the river is included in $U$, but is not explicitly included in $U_c$. However, the optimized coefficients will compensate for the absence of transient storage in the model. It seems likely, therefore, that the optimized velocities are a few percent smaller than they would be if there were no transient storage zones in the river (see, for example, Czernuszenko and Rowiński, 1997).

![Fig. 6. Variation of velocity with flow rate.](image)

Figure 7 shows that the dispersion coefficient increases with flow, which is consistent with most previous work on dispersion in streams (Rutherford, 1994; Wallis and Manson, 2004). The values are very small, but this is consistent with the size of the stream (Rutherford, 1994). Similarly to the velocities, however, the optimized values will be affected by any transient storage in the river, tending to be overestimated during model calibration because they will compensate for the dispersion caused by transient storage not being explicitly included in the model (Czernuszenko and Rowiński, 1997).

Although transient storage could have been included in the model, there was little evidence in the tracer data that it was playing a significant role in the solute transport in the stream. For example, there were few cases where tell-tale elevated tails on tracer
concentration-time profiles were apparent. This judgement is consistent with the small velocity ratios commented on earlier and the generally good fits obtained in the model calibration (in the absence of transient storage). Further analysis of the data is planned that will investigate the role of transient storage in The Murray Burn in more detail.

To investigate the reliability of the model, the velocity and the dispersion coefficients for the three validation data sets were estimated from Figs. 6 and 7 using the individual flow rates corresponding to each data set. As before, these were obtained by applying dilution gauging at Site 1. To help estimate the coefficients, polynomial trend lines were fitted to the data obtained from the calibrations, see Figs. 6 and 7.

Fig. 7. Variation of dispersion coefficient with flow rate.

Figures 8 and 9 show the results of two of the validation runs. The agreement between the observed and the predicted concentration-time profiles is generally good. The higher flow case gives excellent agreement, but the lower flow case over-predicts the peak by about 10% (with no phase error). In both cases the predicted tail of the concentration-time profile matches the observations well, giving further support to the judgement that transient storage is not a major transport mechanism in the reach.

Finally, it is worth noting that with time steps, velocities and dispersion coefficients being in the ranges 30-120 s, 0.1-0.3 m/s and 0.3-2.0 m²/s, respectively, Courant numbers \( \frac{U \Delta t}{\Delta x} \) and diffusion numbers \( \frac{D \Delta t}{\Delta x^2} \) in the (optimum) calibration and validation runs were in the ranges 2-5 and 2-8, respectively. The high quality of the simulations throughout these cases illustrates the ability of DISCUS to yield reliable results not only for Courant numbers greater than 1, but also over a wide range of discretisation parameters. This robustness is an important feature when using automatic calibration procedures, since there are no threats to its satisfactory convergence from it exploring wide ranges of the parameter space. In other words, should the search for
the optimum parameter values require that very small or very large values be explored, stable and physically realistic simulations will always be found.

Fig. 8. Validation results: Experiment 6; flow rate 126 l/s, velocity 0.294 m/s, dispersion coefficient 0.950 m²/s.

Fig. 9. Validation results: Experiment 17; flow rate 17 l/s, velocity 0.095 m/s, dispersion coefficient 0.360 m²/s.

6. CONCLUSIONS
This paper has described the main features of the DISCUS model for simulating one-dimensional solute transport in rivers. The model was calibrated for a short reach of
The Murray Burn using the results of tracer experiments and by optimizing the velocity and dispersion coefficients. The resultant coefficient values are consistent with previous work, with the dispersion coefficient increasing from 0.25 to 2 m$^2$/s in the flow range 16-261 l/s. Validation runs of the model gave good agreement with observations. It appears that transient storage does not play a major role in the transport of solutes in the reach that was modeled. Further analysis of the complete tracer data set, however, is required to fully justify this judgement.

References


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