Comparing Two Numerical Models of Fluvial Transport: Parameter Exploration Using Stream Tracer Data with Combined Micro-Genetic Algorithm and Simplex Method

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Abstract:
The advection-dispersion equation with transient storage (ADE-TS) is fitted to observed stream tracer study data to elucidate stream transport characteristics. Two different numerical approaches to solving the ADE-TS are implemented. Differences between the predicted and observed data is minimized by use of multidimensional optimization techniques. Convergence of the parameter estimation technique, a micro genetic algorithm followed by a simplex method, is demonstrated. The data used in the simulation originated in a study used to obtain hydrodynamic parameters for streams in Scotland [7]. The numerical approaches are a Crank-Nicolson finite-difference scheme with tridiagonal solver [11] and a semi-Lagrangian method known as DISCUS [5]. Results suggest that DISCUS is better suited to fitting the observed data as evidenced by overall lower relative error in predicted concentrations compared to the traditional predictions.

1 Introduction

Estimation of parameters in the one dimensional transport equation with transient storage is conducted using two different numerical schemes. The Crank-Nicolson discretization is used in both models for the dispersion terms, giving unconditionally stable simulations. The models differ in their treatment of advection; the first approach treats advection in a traditional finite-difference Eulerian scheme with central differencing while the second uses a semi-Lagrangian technique [5] known as DISCUS. DISCUS is shown to perform slightly better than the traditional scheme. The parameter estimation utilizes a micro-genetic algorithm followed by a multidimensional simplex minimization.

Determining parameter values for models of transport of solutes in an open channel is a common task in hydrodynamics. Tracer experiments combined with numerical methods for solving partial differential equations offer a way to elucidate the coefficients in mathematical models describing the transport equation. Recent work in Scotland and Iceland involved such tracer experiments for exactly the purpose of quantifying hydrodynamic parameters in a one-dimensional advection-diffusion transient storage model and this data was available for our study. Two locations of a stream are selected to monitor the conductivity at regular time intervals. A slug dose of NaCl is then introduced to the stream upstream from the first sampling point. The pulse of conductivity caused by the salt solution provides the tracer in these studies. These two points on the stream represent boundary conditions for the equation modeling the transport of conserved quantities in open channel flow with transient storage (see Formulation for more details).

The most readily available method for finding parameters is by brute force; that is, by running a simulation with a guess for the unknown parameters and adjusting this set manually until an acceptable match is obtained. This trial-and-error approach is time consuming, so alternatives are often sought. For example, in the software OTIS-P, an algorithm called STARPAC uses a nonlinear squares iterative technique to approximate model parameters [11]. In recent work concerning the characteristics of a series of streams in Iceland, the simplex method was used to fit observations [8]. Optimizations for other engineering problems frequently use another method, the genetic-algorithm, which, unlike the previous two methods, is a stochastic search that does not require an initial guess [10,12]. Our approach combines the simplex method and genetic algorithm.

Compared to running simulations, tracer experiments are expensive. A modeler wishing to observe the fate of a different solute with a different set of initial boundary conditions can get a reasonable idea of the actual result as long as the model is accurate and applicable [3]. Many parameter search techniques require a “close-enough” guess to the optimal solution [9,11]. When a brute-force

approach is the only method available, using such schemes require the modeler to continue to guess successively better guesses in order to approach an optimal one. Manually adjusting a poor guess in order to improve the approximation is often inconvenient. The modeler will benefit from a convenient and, above all, accurate methodology for transforming tracer data into a reasonably accurate model. This study can be regarded as a step in that direction because starting without a reasonable initial solution, values that accurately describe the observed dynamics of each river are obtained. The need for a reasonable starting solution is eliminated by use of the genetic algorithm which searches a broad parameter space stochastically. Such genetic algorithm solutions are further improved by the subsequent application of the simplex method. A set of data from the experiments in Scotland was made available for the purpose of comparing spatial discretization schemes [7]. Results show that DISCUS was able to achieve a closer fit to the subset of tracer experiment data considered.

2 Formulation

2.1 Partial differential equation (PDE) for one-dimensional transport with transient storage region

It is assumed that the primary mechanisms governing the transport of open channel flows such as small streams with stony beds and/or aquatic plants are advection, diffusion, and transient storage. Concentration of the solute in the storage zone is not affected by advection, dispersion, or lateral inflow. The only physical process affecting the transient storage concentration is transient storage. The governing set of PDE's that represent transport of a conserved solute in an open channel are:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} + k_1(S - C) - q_{lateral}C \tag{1}$$

$$\frac{\partial S}{\partial t} = -\frac{k_1}{k_2}(S - C) \tag{2}$$

where U is the advective velocity, D is the dispersion coefficient, k_1 is the transient storage rate constant and k_2 is the ratio of cross sectional area of the storage zone to the cross sectional area of the main-channel. C represents the main channel concentration and S represents storage zone concentrations [8]. The concentration is specified for all time at the upstream boundary, and a zero diffusive flux is applied at the downstream boundary.

2.2 Model application

The physical basis for mass transport in open channel flows is derived ultimately from the Navier-Stokes equations in three dimensions [3]. Although the transport phenomenon is inherently three dimensional, a one dimensional approximation is often used in hydrodynamics for streams or other open channel flows [6,7,11]. Research has shown that simulating all three dimensions is critical in determining the fate of a transported solute only in the near-field zone (for example the region where the tracer solute is injected into the main channel). In the mid-field zone, a two dimensional approach can be used by averaging the concentrations over the depth of the channel. A one-dimensional approximation comes from averaging the width of the channel as well as its depth. The rationale for such averaging is that over a sufficient reach, the concentration of a conserved solute will be completely mixed in the transverse and vertical directions, and the unknown quantity becomes the concentration in the longitudinal direction. A popular application of such a one-dimensional approach is to quantify the dynamics in far-field regions where longitudinal mixing has not yet occurred. More information about these assumptions is available in reference 3.

The advection-diffusion equation is derived from the conservation of mass principle [3]. Mass is conserved during the exchange of solute between the main channel and the transient storage region. Without the presence of sorption or chemical reactions, no solutes are lost or converted to other substances. The equations given in (1) and (2) can be cast in the same terms as the equation governing transport used in OTIS by setting parameters for sorption and reaction to zero [11]. It can be shown that the two forms are equivalent except for some notational differences.

Tracer data collected from experiments are measured concentrations at the downstream location at each time step during the duration of the experiment. A control volume is selected to be a region of the channel where concentrations of a known amount of solute are well-mixed in vertical and lateral directions. Concentrations travel from the upstream location to the downstream location. For a series of M regularly occurring measurements at the downstream location there are M corresponding measurements of concentration values at the upstream end. The upstream values are also taken to be measurements at the same regular intervals. Figure 1 below shows an example of such data. The squares represent upstream concentrations taken at regular intervals. The triangles represent downstream values.

In (1) and (2), five parameters affect the outcome of the transported solute. Velocity of the flow within the main channel is given by U and is taken to be a constant across the length of the channel. It is measured from the upstream location (x=0) of the control volume and positive in the direction towards the downstream location of the control volume. The dispersion coefficient D is a measure of longitudinal dispersion due to the turbulence of the flow and is assumed to be constant. Transient storage parameters include k_1 and k_2. The constant k_1 is a measure of the flow rate between the main channel and the transient storage zone. The cross sectional area ratio of the transient storage zone to the main channel is represented by k_2. Lateral flow per main channel cross sectional area is measured by $q_{lateral}$; note that in all data sets, $q_{lateral}$ is known. Therefore, the values needed to evaluate (1) and (2) are the four parameters U,D, k_1, and k_2.

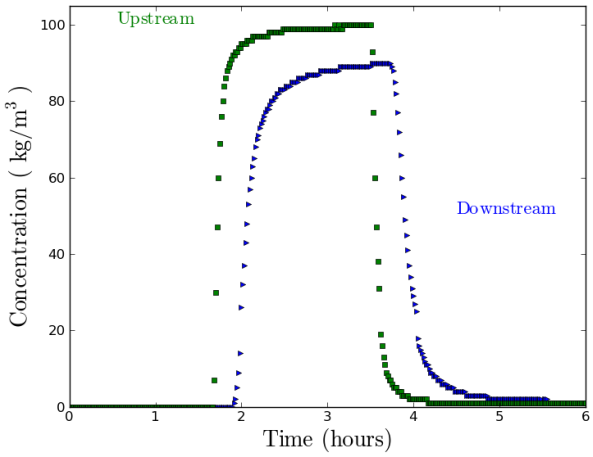

Figure 1 – Typical Tracer Experiment Data: Upstream and downstream concentrations at each time as measured for one of six streams. The upstream boundary is plotted as squares and the downstream as triangles for each of the measurements taken.

2.3 Discretization schemes considered

In order to solve the coupled system in (1) and (2), the finite-volume method is employed. The finite-volume method is a finite-difference scheme in which the nodes are centered inside cells representing discrete control-volumes. The continuous variables x and t are discretized onto a two-dimensional grid. Using such discretization schemes, spatial and temporal derivatives are approximated in order to integrate the second-order PDE [3]. Two such discretization schemes are used in this study; a central-difference approach and the DISCUS methodology.

2.3.1 Spatial central-difference approximation

Centered difference approximation is used on the spatial first and second derivative, corresponding to advection and diffusion, respectively. The method uses the second order accurate in time Crank-Nicolson scheme. This scheme is unconditionally stable, and avoids the severe oscillations that appear in a fully implicit method. Details concerning application of central-difference approximations Crank-Nicolson to the advection-diffusion transient storage model as in (1) and (2) are in reference 11.

2.3.2 DISCUS discretization scheme

The DISCUS method treats advection differently from the discretization used in the OTIS methodology. The DISCUS scheme estimates advection by using a third-order accurate treatment of advection. This is similar to the QUICKEST scheme [4]. In one-dimension, DISCUS is shown to be stable and accurate for arbitrary Courant numbers. The method employs a semi-Lagrangian treatment similar to a method of characteristics [5]. Diffusion terms are handled with the traditional central-difference approximation [6]. Recent work uses the Crank-Nicolson method, and this is the same scheme used for results in this study [8].

2.3.3 Comparison of schemes

Each channel and its associated transient storage region is considered to be L meters long, with x=0 denoting the upstream boundary and x=L denoting the downstream boundary. Let the the length L be divided into N cells of length dx = L/N and the total duration of the experiment T be divided by M time-steps of duration dt = T/M. Let C_i^j be the concentration of solute and S_i^j the concentration within transient storage at the *i*-th control-volume cell, where *i* is from 1 to N, and at the j-th time-step, where j is from 1 to M . After the Crank-Nicolson finite-difference scheme is applied, (1) takes the form of:

$$\alpha C_{i-1}^{j+1} + \beta C_i^{j+1} + \gamma C_{i+1}^{j+1} + \delta S_i^{j+1} = \rho_i \qquad (3)$$

$$\beta^S C_i^{j+1} + \delta^S S_i^{j+1} = \rho_i^S \qquad (4)$$

as discussed in [8]. This is reduced to a tridiagonal system of linear equations by solving for S_i^{j+1} in (4) and substituting into (3). Initial conditions in space, C_i^0 and S_i^0 for all i, are set to 0 because the baseline reading has been subtracted from the data set. Integrating the discretized PDE in time requires values for the upstream boundary C_1^j at each time t=jdt. Unlike the upstream condition, the downstream condition is defined as zero diffusive flux. This means the values of nodes N and N+1 are equal; hence, $C_N^j = C_{N+1}^j$ [11]. Evaluating the model gives C_N^j for all time-steps. This vector corresponds to the predicted concentration of the main channel at the downstream location over time.

The only difference between the two methods is the treatment of advection. In DISCUS, the treatment of advection is based on a third-order accurate in space discretization called QUICKEST [4].

As an improvement to QUICKEST, DISCUS uses the Courant number of the discretization in order to determine the correct finite-volume cell from which to advance the solute [5]. Although both methods are unconditionally stable, accurate solutions are bound by a time-step restriction. For the traditional central-difference method, a large time-step will produce inaccurate results. Both methods share the same time-step restriction due to the treatment of diffusion (see [6] for results regarding accuracy of DISCUS related to diffusion).

2.4 Parameter search approach

The parameter search for values of U, D, k_1 , k_2 in (1) and (2) above is conducted using two proven parameter search methods in succession. Note that the parameter $q_{lateral}$ is known for the data sets used. First, a micro genetic algorithm (mGA) is applied given a possible range of parameter values. After the mGA has successfully found a candidate set of parameters, these parameters are passed into a simplex method as an initial guess. The simplex method iteratively searches for a set of parameters that optimizes the objective function and is used to improve the solutions obtained from the micro-genetic algorithm.

2.4.1 Micro-genetic algorithm

Genetic algorithms solve mathematical optimization problems by employing the concepts of biological evolution. Members of the population are mathematical functions; in this case, the mathematical function governing concentration of a tracer solute. In the context of finding the values for the parameter vector corresponding to (1) and (2), the positive real values for parameters are used as genetic code [13]. For example, the value of U can be considered a trait of the stream representing the velocity of the flow. Possible values of U would then be encoded as discrete values to make up the genotype of the organism. This introduces the need for a maximum and minimum value for the values that each parameter can take. In the study from which the data sets originate, parameters were found to be between 0 and 1. Hence, this serves as guidance in defining the minimum and maximum values allowed by any one gene [8].

Whereas natural selection determines which organisms reproduce, a user-defined objective function defines which parameter vectors are recombined to produce offspring (see section 2.4.2). The offspring are composed of a recombination of the parents' chromosomes. This recombination, along with optional mutation rates, is the simple genetic algorithm's driving mechanism for searching parameter space for an acceptable solution [2].

The micro-genetic algorithm (mGA) is a variant of the simple genetic algorithm (SGA) in which many SGA simulations are run successively. Defining characteristics of an mGA are smaller than SGA population sizes and the insertion of the best member of the current population into the initial population of each new SGA run [10,12]. For problems that might require a population of about 100 to be successful in the SGA, mGA's have been designed that converge on a solution with a population of only 10. Mutation rates define the probability that a gene is mutated in a new offspring; this changes the value of a parameter. Elitism is used in some genetic algorithms to copy the fittest member of each generation when no fitter member is produced in the current generation [2,10].

Values for the number of populations per generation, number of members in a population, and other characteristics of the SGA determine how many possible solutions will be considered in total by the mGA. Although finding a global minimum is not guaranteed, researchers working on engineering problems have reported that the mGA is well suited to avoiding premature convergence to a local minimum [10]. Stopping criteria must also be decided, which can present a difficulty. In this application, the fitness value of the best population member was monitored for convergence (see Simulations for more information on mGA stopping criteria).

2.4.2 Objective function

The idea of the parameter search is to find values that minimize the error between the approximate model and the collected data. Therefore, the measure of absolute error was used as the objective function. The objective function can be described as the the 2-norm of the predicted data minus the observed data. Referring to the notation introduced in 2.3.3, it is expressed as:

$$G(U, D, k_1, k_2) = \sqrt{\sum_{j=0}^{M} (C_N^j - Y^j)^2} \tag{5}$$

where Y^j is the observed downstream concentration at time j. Note that unlike traditional mGAs, the lower this score, the more likely a member of the population is to produce offspring. Traditionally, the fitness score is considered superior to another fitness score if it is higher in value [2]. The software library used to implement the genetic algorithm search allows the user to define either minimization or maximization of a mathematical function as the goal of the simulation. Minimization was chosen, and the absolute error from observed data was conveniently used as the objective function [13].

2.4.3 Simplex method

Refinement of the parameter estimation is carried out by the Nelder-Mead simplex algorithm [9]. It is a method designed for multidimensional minimization problems where the minimum of a function of n variables may be zero or non-zero. The Nelder-Mead Simplex algorithm uses an initial set of parameter values and builds n+1 vertices to form an n-dimensional simplex. Geometrical transformations are applied by improving the worst vertex at each iteration. The objective function that determines the quality of a vertex is the same objective function used in the genetic algorithm, equation (5) above. Because this is a technique for minimization problems, the best vertex is the vertex that results in the lowest objective function value. These transformations change the overall size of the simplex at each iteration until either the maximum number off iterations have been reached or the size of the simplex is sufficiently small.

A benefit of the simplex method is that it may be used with no knowledge of the derivative of the objective function. Armed only with a scalar measure of how well a model predicts the transport phenomenon given a data set, a more accurate vector of parameters can be found. The simplex method is well suited to finding a local minimum of a n-dimensional minimization problem. However, it gives no guarantee of a global minimum. The discovery of a global minimum partially depends on how close in n-dimensional parameter space the initial parameter vector is to the global minimum. In our mGA/simplex approach, the optimization therefore depends on the mGA producing a population member that approximates the global minimum.

3 Simulations

3.1 Parameter search with mGA/simplex

We employ the free C++ library GAlib for the mGA. The library's simple genetic algorithm (SGA) was run 15 times in each mGA, passing the best member of the previous SGA as a member of the initial population in the current SGA. The initial SGA is populated completely randomly, with the genotype built from real numbers ranging from 0 to 1. The mGA was run with population sizes of 100 for all simulations. Then tournament selection is used which gives the fittest members of the population the highest probability to mate [2,13]. Mutation is set to 0.01 which means one percent of the offspring are randomly mutated such that one of their parameter values changes slightly. The crossover rate is 0.9, so roughly 10% of the offspring have a direct copy of one parents genetic code but 90% have a

random combination both parents' genetic code. Each SGA continues to produce new generations of offspring until the best fitness score does not change for 20 consecutive generations (up to a maximum of 100 generations). The best raw fitness score of every SGA and the corresponding parameters that produced them are recorded during the mGA. In this way, relative error can be calculated after each SGA (see figure 6).

The result from each mGA is passed to the simplex method as a vector of parameter values. We use the Nelder-Mead algorithm as implemented in the GNU Scientific Library (GSL) [1]. Multidimensional minimization is used by coding routines that define objective function and initial parameter vector. The simplex step size is 0.1, which determines the vertices that constitute the n-dimensional simplex. This is a measure of how far away from the original parameter vector the vertices will be generated. Simplex simulations run for a maximum of 1000 iterations, terminating when the simplex size reaches a value under 10^{-15}. The result of the simplex search is used as the model prediction for that stream and the relative error from observed data is recorded along with the parameter values for that run. At each iteration, the current best estimate is output so the progress of the simplex method can be observed (see figure 7).

The same objective function was used in both the mGA and the Simplex runs. Note that when using the objective function for either the genetic algorithm or the simplex method, partial and incomplete solutions must be quantified [1,13]. Floating-point computations may result in NaN or infinity for poor choices of U, D, k_1 or k_2. These values cannot be used by the mGA algorithm and should be converted to large values to indicate a poor model fit. The simplex method also must be defined for meaningless output of the objective function. The GSL allows the objective function to pass a constant GSL_NAN when results are meaningless [1]. Note that when the relative error is reported throughout, it has been recalculated from the model simulation output. This ensures that the error, and not the objective function, is used to evaluate the results.

Two sets of runs were conducted, each set consisting of 10 runs for each of six data sets, for a total of 120 runs. The two different numerical approaches were used, each corresponding to a set of 60 runs. From here on, when the central-difference approximation is used, it is referenced as OTIS for brevity. The label OTIS comes from the software of the same name that employs the traditional scheme [11]. When the DISCUS methodology is used as in reference 8, it is referenced as DISCUS. Parameter-estimation is undertaken for all six streams in this fashion ten times for each discretization. One run per spatial discretization would be insufficient because the mGA is a stochastic method.

3.2 Differences between numerical approaches

The best relative error measures were gained from DISCUS on the order of 0.02. Half of the best OTIS runs resulted in relative error over 0.1, and the other half were near 0.04. This shows DISCUS was better suited to predicting concentration values as observed in tracer experiments. The worst norms averaged about 0.1 for OTIS and for DISCUS. Typical results for each method can be found in figures 3 and 4 below. Figure 4 shows best results for both DISCUS and OTIS simulations in the region where the concentration over time is at its highest. Though both models clearly overestimate the observed data at many points, DISCUS demonstrates a closer fit.

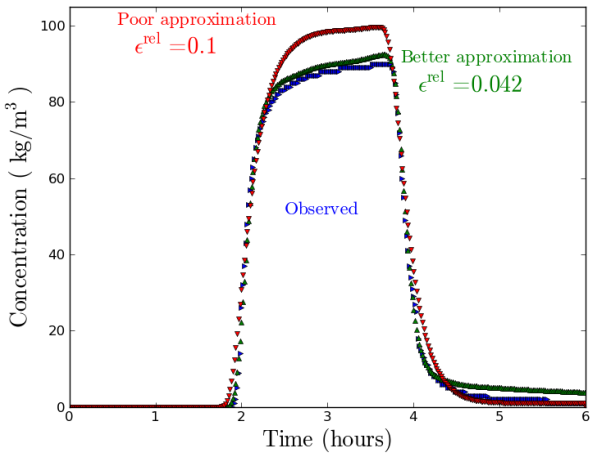

Figure 2 – OTIS Sample Result: Best and worst approximation for a selected stream for the OTIS scheme. Shown as downward pointing triangles is a downstream profile from simulation that results in a relative error of 0.1 from observations. The upward pointing triangles show a simulation that has a relative error of 0.042. The observed boundary concentrations are plotted as triangles pointing to the right.

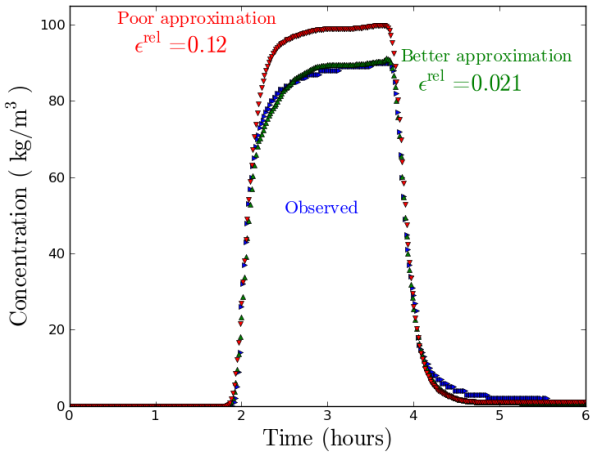

Figure 3 – DISCUS Sample Result: The observed concentration is plotted in right facing triangles for the same stream as depicted in figure 2. Plotted as down pointing triangles is an estimate resulting in relative error 0.12. Plotted as upward pointing triangles are the results with relative error 0.021.

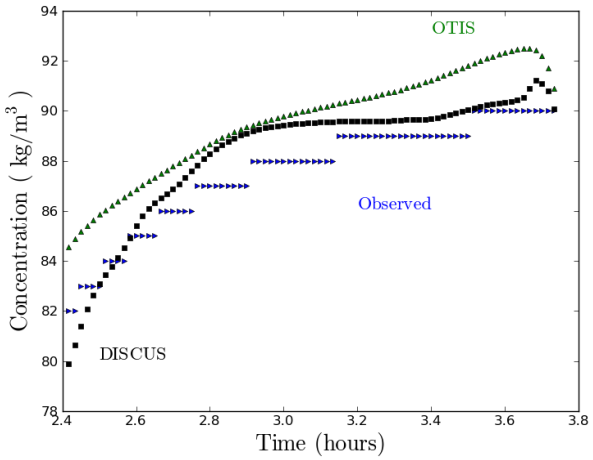

Figure 4 – Comparison of Predictions Near Peak Concentrations: A close-up of the region where the peak concentrations are overestimated. Both OTIS and DISCUS methods overestimate the concentrations at the peak. This error is common in both methods, but DISCUS results have the least error at or near the peak. This is typical of the best solutions obtained for all six streams.

The models behaved similarly, with DISCUS finding values that produced lower relative error measurements. Given the poorest approximations to the predicted data, both discretization techniques produce results that overestimate the peak of the concentration. Considering the best approximations attained, DISCUS consistently achieved a closer fit to the model than the OTIS style discretization. In the figure below, the relative error of the best solutions from the mGA/simplex technique are plotted for each data set.

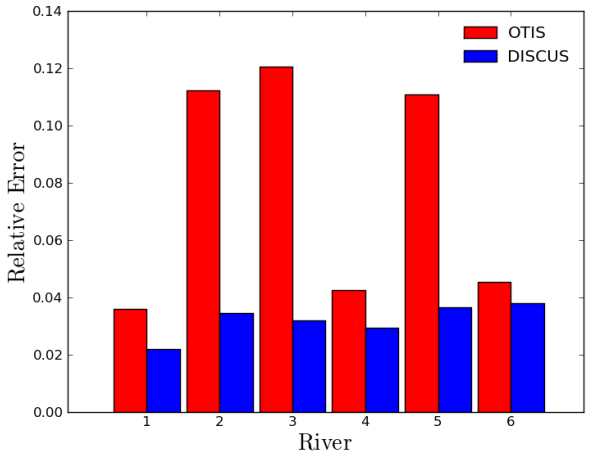

Figure 5 – Comparing Relative Error: For each set of tracer data from individual rivers, the lowest relative error obtained from each discretization is shown. All values obtained from DISCUS are clearly lower than those from OTIS which indicates a closer fit to tracer data in all cases.

3.3 Convergence of parameter estimation

In most of the 120 runs, poor results were obtained as shown by the downward pointing triangles that overestimate peak concentration in figures 2 and 3. In general, the relative error between observations and predictions progress as shown in figures 6 and 7 below. Initial random guesses for the mGA are poor, but rapidly improve. After the rapid improvement, most results do not improve until applying the simplex method. As shown in figure 7, the simplex method almost always improves the fit to model data. In one case, one of the least accurate solutions did not improve any as shown by the completely horizontal line at the top of figure 7. It always terminates before the maximum iteration count of 1000 because the simplex-size has been reduced below 10^{-15}. It is evident that the mGA quickly finds values near a local minimum of the objective function and remains nearby. Most solutions did not improve past the sixth or seventh SGA. As for the simplex method, figure 6 shows that solutions continue to be improved where the mGA was unable to offer better solutions.

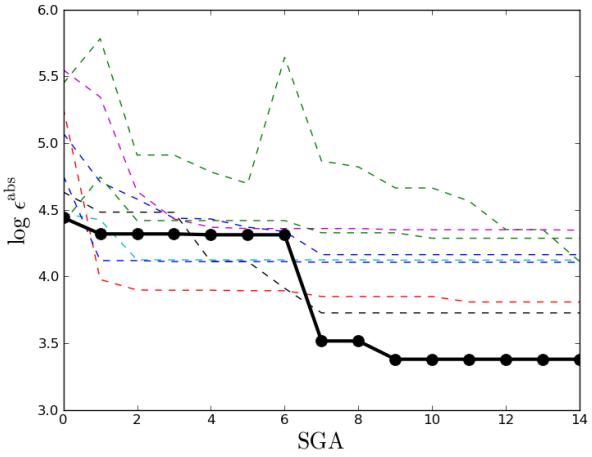

Figure 6 – Convergence of mGA: Nine mGA runs for the same set of downstream measurements as they change with each SGA. At the end of every SGA in the mGA, the error of the fittest member of the SGA population is recorded. Each dashed line repesents one mGA. The dots connected by a thick line denote the best solution in the group of nine solutions. For most mGA runs, error rapidly decreases and a solution is found within the first 6 or 7 runs .

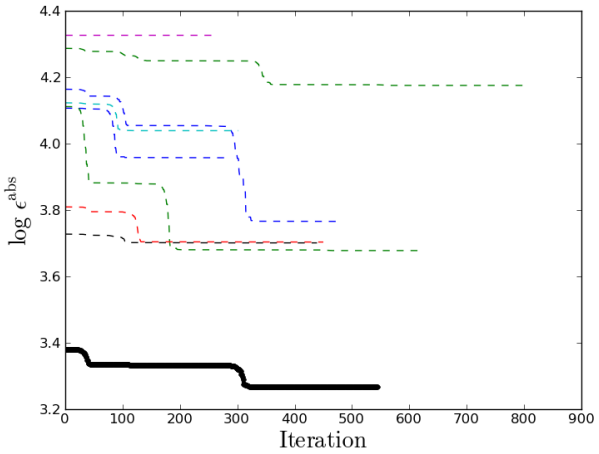

Figure 7 – Convergence of Simplex: Simplex improves mGA guesses in eight of nine selected cases. Each dashed line represents one simplex run. Except for the data shown as the uppermost horizontal line, the relative error from observed data decreases as simplex minimization runs. The solid black lines shows the best prediction obtained and corresponds to the solid black line in figure 6. The logarithm of absolute error between observed and predicted data is plotted for nine runs corresponding to same downstream data used for figure 6. These runs terminate when reaching a simplex size of 10^{-15}.

4 Conclusion

4.1 Summary

The mGA/simplex method is a viable approach for finding approximations to the one-dimensional transport equation. With the data set studied, DISCUS produced better model predictions as compared to traditional the central-difference spatial approximation. With either discretization, the error most often manifests near the peak of the concentration. Figure 2 and figure 3 show a result in downward facing triangles that exhibits this behavior. Better approximations, plotted in those figures as upward pointing triangles, get closer to the observed peak concentration. Figure 4 plots the values from figure 2 and figure 3 to show that both methods overestimate peak concentration. Qualitatively, the solutions obtained by all runs are similar to Figure 5 because the peak is often the greatest source of error.

Most runs found simulation parameters which did not accurately predict concentrations at peak values. Matching the peak concentration is typically a source of error in numerical simulations of transport phenomenon [3]. The treatment of diffusion and transient storage are the same in each method. For the results with the lowest norms, the traditional approach adopted by OTIS is not as successful as DISCUS at capturing the dynamics of the tracer experiment data used herein. The best results for each stream came from the DISCUS method when both methods were run 10 times for each set of measured concentrations.

As an alternative to a trial-and-error approach with simplex alone, the mGA/simplex approach is convenient. The simplex method works best when a reasonable guess is passed to it. If a local minimum in parameter space is nearby the n-dimensional simplex formed from a given parameter vector, the simplex method will converge to the values corresponding to that minimum. This is evidenced by the convergence graph in figure 6, where all but one solution continues to improve even after the mGA failed to find any better solution. Simplex alone may not be the best choice if determining a reasonable starting guess is not practical or straightforward.

However, while the need for a starting vector of parameter values is eliminated with the assistance of a preliminary mGA optimization, there is still information required by the approach that

usually requires manual adjustment. For example, one may not always know what maximum values to expect when given a large set of data. The mGA starts with random values in the range of 0 to 1, and does not use values outside this range. For the data used, a previous study with the same data showed that the highest value for U was found to be nearly 1, and all other values below 1 but above 0 [8]. All parameters in the genotype are initialized within these bounds. Adjusting other factors of the mGA, such as number of SGAs, population size, mutation rate, and convergence or selection criteria, presents additional concerns. These options determine the possible values of the parameters evaluated as well as how solutions are treated. An insufficient configuration may miss a good solution of the problem. In this study, results consistently had relative error lower than 0.12 in every run which is an indication that the range for parameters and the mGA options were defined appropriately for this minimization problem.

Although the mGA was able to find many good solutions no evidence is presented that it is any better at finding optimal solutions than trial-and-error, or whether it finds optimal solutions at all. Sometimes, a larger population size may increase the chances of finding a globally optimal solution with use of a genetic algorithm [2]. Preliminary investigations used population sizes of 200 or more, but it was later found that a size of 100 produced similar results. In fact, despite recommendations that mGA runs can succeed with very small populations numbering in tens in references 10 and 12, small populations of roughly 50 produced poor results. The benefit of small population size is that computation time is less. Unfortunately, a large population size is no guarantee that a solution will be found. The mGA did find a variety of candidate solutions, but there was no evidence that it tends towards a global minimum of the objective function. In contrast to the results shown in figure 6, we hoped to see most if not all twenty runs per data set converge to the same solution. This would haveindicated the possibility of a global minimum.

4.2 Next Steps

The approach presented can be improved. Computational efficiency of the methods is not compared here, but the genetic-algorithm parameter search in general lends itself to further optimization. Initial profiling of the mixed C,C++, and FORTRAN code revealed that most of the work is done in the objective function. The objective function relies on solving the PDE for hundreds of time-steps and this integration is expensive. In the genetic-algorithm model, populations sometimes in the hundreds all need to be evaluated by means of the objective function for tasks like sorting, mating selection, and convergence detection. Furthermore, each evaluation of the objective function is independent of other evaluations. Only when the genetic-algorithm or simplex search compare the set of evaluated objective scores is the result of more than one objective function evaluation necessary. The linear algebra routines used to evaluate such functions are expensive and therefore make the objective function the source of even more computation. These factors imply that evaluating a population simultaneously using parallel computing could be beneficial. Parallelization should result in speed up especially because the genetic algorithm relies on evaluating the entire population during each generation of the SGA runs.

The combined use of simplex minimization and genetic algorithms can be extended as well. The simplex method was shown to improve most solutions given by the mGA. If this is generally true, one option for future research could be to run a short simplex minimization routine on each member of the population. It would be computationally efficient to do this only on a subset of the fittest members. This may offer a greater chance of determining which solution in the population might be a global minimum because the relative error of candidate solutions would overall be less.

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