Interpreting the MT3D Mass Budget

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Last update: June 7, 2006

1. Introduction

One of the most subtle aspects of MT3D is its reporting of mass budget information. This note has been prepared to provide guidance on the interpretation of the mass budget. The note begins with a discussion of the significance of the mass budget. The individual terms in the budget are then defined, and the mass discrepancy calculation is explained. The concluding section includes suggestions for reducing the discrepancy.

2. The significance of mass balance

The governing equation for solute transport is a mathematical statement of mass conservation for a groundwater system. The equation states that the change in mass stored must be equal to the net mass flux, plus the difference between the mass contributed by sources and withdrawn by sinks:

change in mass stored = net mass flux + mass in from sources – mass out from sinks

The net mass flux represents the sum of advective and dispersive fluxes. The sources include injection wells, recharge, losing rivers and first-order production reactions. Sinks include extraction wells, drains, gaining rivers and decay reactions. In MT3D models, mass inflows and outflows from specified head and concentration cells are also treated as source and sinks.

Since the governing equation is a statement of mass balance, it seems basic to require that a solute transport code conserve mass during simulation, and be capable of demonstrating this conservation. Unfortunately, the calculation and evaluation of the mass balance error is not as obvious as it might seem. Each method of solving the governing equation approaches mass balance differently. For example, the finite difference method is based on an expression of mass balance for each cell in the model, whereas the finite element method minimizes the global mass balance error. The method-of-characteristics is based on an entirely different concept, an analogy between solute transport and moving particles, and departs from a strict adherence to mass conservation. It is also important to note that a small mass balance error is a necessary but insufficient condition for an accurate solution. That is, a small mass balance error is no guarantee that the solution is correct. For example, transport simulations that are too coarsely discretized may report perfect mass balance and yet be overwhelmed by numerical dispersion.

3. The units of mass in MT3D

The units of mass in MT3D are defined as the product of the units of concentration (mass per unit volume of water) and water volume. For example, if consistent units of length of *ft* are used, then for concentration units of lb/ft^3 the units of mass will be *lb*. Although consistent units may simplify interpretation of the mass budget, and are essential in other parts of the model (the MODFLOW flow model, for example), their use may sometimes require concentration values that are so low they are vulnerable to computer round-off errors. Consistent units may also be very awkward (labs do not report concentrations in units of lb/ft^3 or even kg/m^3). Inconsistent units can be specified for concentration units (for example, *mg/L* in model with length units of *ft*), as long as the user recognizes that the masses will be reported in unconventional units (in this case, $mg\text{-}ft^3/L$).

Example

Units of length in flow and transport models: feet
Units of concentration in transport model: µg/L

In this case, MT3D will report masses in the units of $ft^3\text{-}\mu g/L$. To convert to more readily understood units mass we apply the following calculations as postprocessing steps outside of MT3D.

$$M\left(kg\right) = M\left(ft^3\,\frac{\mu g}{L}\right)\left|\frac{28.32\,L}{ft^3}\right|\left|\frac{kg}{10^{-9}\,\mu g}\right| = M\left(ft^3\,\frac{\mu g}{L}\right)\cdot 2.832\times 10^{-8}$$

$$M\left(lb\right) = M\left(ft^3\,\frac{\mu g}{L}\right)\left|\frac{28.32\,L}{ft^3}\right|\left|\frac{kg}{10^{-9}\,\mu g}\right|\left|\frac{2.2046\,lb}{kg}\right| = M\left(ft^3\,\frac{\mu g}{L}\right)\cdot 6.243\times 10^{-8}$$

4. Terms in the MT3D mass budget summary

MT3D calculates a mass budget summary at the end of each transport step. The results of the mass budget calculation are reported in two places:

- The standard output file provides a detailed account of the cumulative mass terms at the NPRS values of TIMPRS specified in the basic transport package; and
- The budget summary file, `MT3D.MAS`, provides a continuous overall record that can be plotted directly.

The terms in the calculation of the cumulative mass budget are assembled on Table 1.

Table 1: Terms in the MT3D mass budget

Term	IN	OUT
Constant concentration cells	+	-
Constant head cells	+	-
Wells	+	-
Drains	NA	-
Rivers	+	-
Streams	+	-
General-head boundary cells	+	-
Recharge	+	NA
First-order transformations	+	-
Mass storage [Solute]	+	-
Mass storage [Adsorbed]	+	-
Total	IN	OUT
Net (In - Out)	IN - OUT	
Discrepancy (Percent)	100 * (IN-OUT) / 0.5 (IN+OUT)	

The interpretation of the mass additions and withdrawals from sources and sinks is straightforward. For sources, the cumulative mass is defined as the integral through time of the product of volumetric flow rate and injectate concentration. For sinks, the cumulative mass is the integral of the product of the flow rate and the concentration in the cell containing the sink. For *NW* injection/extraction wells, the cumulative masses added and withdrawn up to time *t* (after *NT* transport steps have elapsed) are calculated according to the following discrete forms:

$$\text{M wells [IN](t)} = \sum_{n=1}^{NT}\sum_{m=1}^{NW} Q_m^n C_m^n \Delta t^n$$

$$\text{M wells [OUT](t)} = \sum_{n=1}^{NT}\sum_{m=1}^{NW} Q_m^n C_{jik}^n \Delta t^n$$

The mass storage term in the budget accounts for the changes in dissolved and sorbed-phase concentrations, with the changes accumulated from one transport step to the next. The overall cumulative change in mass after NT transport steps is calculated from:

$$\Delta M \quad (t) = \sum_{n=1}^{NT}\sum_{k=1}^{NLAY}\sum_{i=1}^{NROW}\sum_{i=1}^{NCOL} \theta_{jik}\left(C_{jik}^n - C_{jik}^{n-1}\right)\Delta x_j \Delta y_i \Delta z_k$$
$$+ \sum_{n=1}^{NT}\sum_{k=1}^{NLAY}\sum_{i=1}^{NROW}\sum_{j=1}^{NCOL} \rho_{jik}\left(\bar{C}_{jik}^n - \bar{C}_{jik}^{n-1}\right)\Delta x_j \Delta y_i \Delta z_k$$

Where C and $\bar{C}$ denote the dissolved and sorbed-phase concentrations, and θ and ρ are the porosity and bulk density assigned to each cell.

Two separate "change in mass storage" terms are defined for the dissolved and sorbed phases: the **STORAGE[OUT]** term accumulates the mass in those cells in which the concentrations increase between two transport steps; and the **STORAGE[IN]** term accumulates the mass in those cells in which the concentrations decrease. The sign convention used in MT3D is identical to that used in MODFLOW. The mass in cells where concentrations increase is designated as a sink term, because the accumulation of mass storage in those cells removes mass that would otherwise be available to the rest of the system.

A key point to bear in mind when examining the storage terms is that they cannot be used to calculate either the total mass in the plume at a particular time, or the change in the total mass between transport steps. In order to reinforce this point, consider the simple case of the migration a non-reactive solute. The concentrations will decrease in upstream cells and increase in downstream cells as the plume moves through the system. These increases and decreases in concentrations will be recorded in the mass budget as ever-increasing outputs and inputs to mass storage, although the total mass in the system may remain constant through time.

5. Example mass budget

To illustrate the mass budget calculation, we will examine the results for test problem 7.2 from the MT3D manual. The solution was evaluated using the MOC solution option. The evolution of the mass budget terms is plotted on Figure 1. The volume units are m^3 of water and the concentration units are ppm (grams of solute/m^3 water); therefore, the units of solute mass are grams.

The only physical source in this problem is an injection well. Since the injection concentration and rate are constant, the exact cumulative mass input by the well can be calculated from their product. The values of injected mass plotted on Figure 1 are essentially identical to the mass reported under **WELLS[IN]** in the standard output file. The constant head cells along the outflow boundary are the only sinks, which draw mass out of the system once the plume reaches the boundary. The cumulative masses leaving the domain, reported as **CONSTANT HEAD [OUT],** remain small over the duration of the simulation, indicating that the duration of the problem (one year) is insufficient to observe significant mass transport across the boundary.

The **NET IN** and **NET OUT** terms are also plotted on Figure 1. Since mass is constantly added to the system, intuitively we would expect concentrations to increase everywhere and the **STORAGE[IN]** term to be negligible. However, the significant **STORAGE[IN]** and **STORAGE[OUT]** term indicates that there is a constant interchange of particles, due to the discreet nature of the MOC solution. These oscillations can be damped somewhat by using more particles.

Without sorption, the total mass in the plume at any time can be calculated by integrating the cell concentrations according to:

$$M(t) = \sum_{k=1}^{NLAY} \sum_{i=1}^{NROW} \sum_{j=1}^{NCOL} \theta_{jik} C_{jik}(t) \Delta X_j \Delta Y_i \Delta Z_k$$

Where ΔX_j and ΔY_i are the cell spacings along rows and columns, respectively, ΔZ_k is the layer thickness, and θ_{jik} is the porosity of each cell. The mass in the plume is plotted as the solid dots on Figure 1.

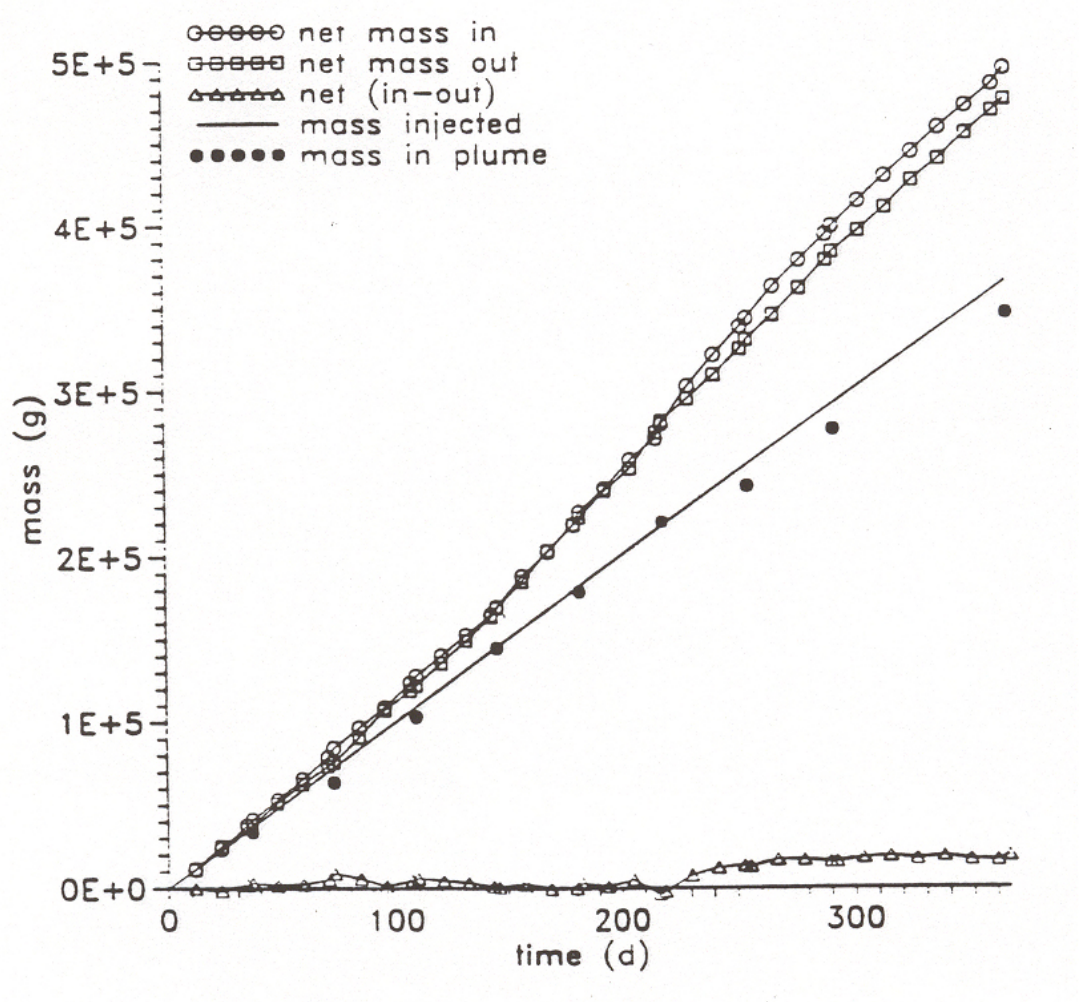

Figure 1. Cumulative mass accounts versus time

6. Definition of the mass budget discrepancy

There is no universal definition of mass balance error. This makes it difficult to compare codes. The mass balance can defined on a cell-by-cell basis, or for the model as a whole, and can be evaluated for each transport step or it can be cumulative.

The mass balance error, or discrepancy, reported in the MT3D Standard Output file is calculated using the total cumulative IN and OUT mass terms. Since both of these terms are approximate quantities, an absolute mass balance error cannot be quantified. Rather, a *relative mass discrepancy* is defined, calculated as a percentage according to:

$$ERROR(\%) = \frac{(IN - OUT)}{\frac{1}{2}(IN + OUT)} \times 100$$

This expression for the MT3D mass discrepancy serves as an indicator of the internal consistency of the simulation, but is not always a reliable indicator of the accuracy of the results. For example, the finite difference advection solution generally yields small mass discrepancies, even for simulations in which there is significant numerical dispersion.

The mass discrepancy for the simulation is plotted on Figure 2. The results indicate that a discrepancy in the range of about 5% is obtained with the MOC solution. For this example, since the exact rate of mass injection is known, and the mass leaving the domain is insignificant, it is straightforward to calculate an alternative, physically based mass balance error. The alternative expression for the mass balance error is written as:

$$M(t) = M_0 + M_{IN\ SOURCES} - M_{OUT\ SINKS}$$

Where $M(t)$ is the mass at any time t, M_0 is the mass in the domain at the start of the simulation, M_{IN} is the cumulative mass added to the system by sources, and M_{OUT} is the cumulative mass withdrawn from the system by sinks. Re-arranging these terms we can write:

$$M(t) + M_{OUT\ SINKS} = M_0 + M_{IN\ SOURCES}$$

Again, since both sides of this equation are approximations, an absolute mass balance error cannot be quantified. Rather, a *relative mass discrepancy* is defined, calculated as a percentage according to:

$$ERROR_2(\%) = \frac{\left(M_0 + M_{IN\ SOURCES}\right) - \left(M(t) + M_{OUT\ SINKS}\right)}{\frac{1}{2}\left[\left(M_0 + M_{IN\ SOURCES}\right) + \left(M(t) + M_{OUT\ SINKS}\right)\right]} \times 100$$

This alternative calculation of the mass discrepancy was added to the MT3D mass budget starting with MT3D[96] and has been carried over to all subsequent versions of the code.

This alternative calculation of the mass discrepancy is also plotted on Figure 2. We see that in this case there is not that great a difference between the two measures of mass discrepancy.

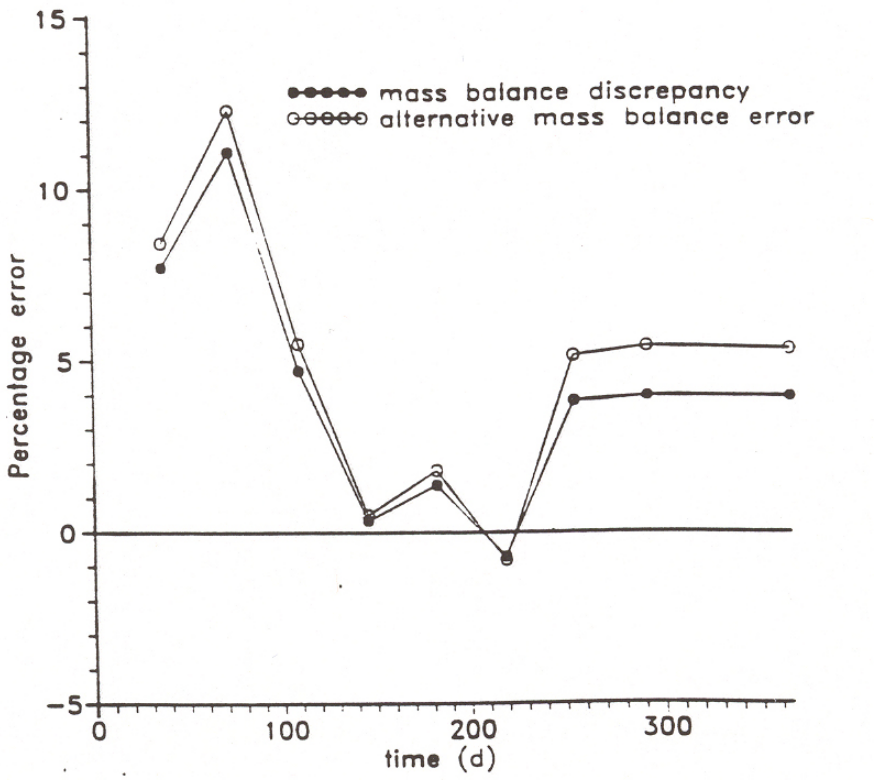

Figure 2. Mass balance errors versus time

As indicated previously, the alternative definition of the mass discrepancy has the benefit of being physically based compared with the original measure. The alternative measure of the mass discrepancy was added to the MT3D mass budget starting with MT3D[96] and has been carried over to all subsequent versions of the code.

7. Judging and improving the mass balance discrepancy

The magnitude of the mass balance discrepancy that can be accepted depends partly upon the method of solution. Some key points regarding the interpretation of the mass balance discrepancy are presented below.

1. For methods that solve the governing mass balance equation directly (e.g., finite element and finite difference methods), the global mass balance error is a direct measure of the internal consistency of the solution. Therefore, for these methods the global mass balance error must be small to ensure a correct solution (typically less than 1 percent). The recently added TVD solution scheme (3rd order ULTIMATE) is also by design mass conservative, so only a relatively small mass discrepancy should be accepted.

2. The mixed Eulerian-Lagrangian solutions (such as MOC, MMOC and HMOC implemented in MT3D) are not based explicitly on mass balance. In theory, for an infinite number of particles the analogy between moving particles and migrating solutes becomes exact. In practice, some trade-offs between the accuracy of the mass balance and the number of particles must be made, to deep the problem size manageable. The important point to keep in mind is that accurate concentrations can be calculated despite the fact that mass balance is not rigorously enforced. Unfortunately, there is no single criterion to judge whether the mass balance discrepancy for a particle-based solution is acceptable. Only some general guidelines can be used to assist in its evaluation. As noted in the MT3D manual, the mass discrepancy for particle methods at early times is particularly suspect, and the mass balance discrepancy should only be carefully examined after several transport steps have elapsed. The mass balance discrepancy will frequently oscillate. For this case, the results may be acceptable if the oscillation is about zero and the magnitude diminishes through time. A mass balance discrepancy that increases through time or that consistently exceeds 10-15% is usually indicative of an inaccurate solution.

3. There are several things that may be tried in order to reduce the mass balance discrepancy. It is important to bear in mind that mass balance errors may arise from both the flow and transport solutions. A severe mass balance discrepancy in the transport solution may be the first indicator of major problems in the flow solution. In addition, local errors in the flow solution can wreak havoc in the transport solution. The flow solution is second-order accurate in space for a grid with uniform spacings, but the accuracy drops to first-order for a variable grid spacing. In lieu of an extensive convergence analysis, it is good practice to follow the general guideline that the spacing between cells should not increase by a factor of more than about 1.5 to 2.

4. Abrupt changes in the cell sizes may give rise to errors in particle-based transport solutions. These errors are due to the average that must be made to calculate cell concentrations from particle concentrations. Early versions of the MT3D used simple arithmetic averaging, which is error-prone for highly irregular grids. Although the volume-weighted averaging scheme implemented in MT3D v. 1.8 is an improvement, there is still some error introduced. As a further precaution, we recommend using a uniformly spaced grid in the subregion of the flow model where accurate concentrations are critical.

5. If the grid-Péclet constraints can be satisfied, then the best option may be to switch from a particle-based method to a finite difference advection solution. The finite difference solution generally yields very small mass balance discrepancies and may sometimes be faster than the particle-based methods. However, for practical-sized problems with realistic dispersivities, the grid spacing may have to be excessively refined to contain numerical dispersion. A finite difference solution with explicit time-weighting may also require very small time steps to ensure stability. If the grid- Péclet constraints cannot be satisfied, then it is strongly recommended that the TVD solution option be tried.

6. If the method-of-characteristics must be used but large mass discrepancies persist, it may be necessary to experiment with the parameters in the advection package. For problems that are advection dominated, the concentration weighting factor, ω, should be increased towards 1.0. Sources and sinks often give rise to mass balance problems with MOC. Improvement may be obtained by specifying fourth-order Runge-Kutta particle tracking in their vicinity, by setting *ITRACK=3.* [Since the transport steps are generally quite small, it is rarely advantageous to use Runge-Kutta tracking for the entire model.] For complex flow fields, consider raising the initial number of particles placed in a cell, *NPH*, and the minimum number of particles allowed in a cell, *NPMIN*. Finally, increasing the maximum number of particles allowed in a cell, *NPMAX*, will reduce the amount of redistribution of particles, a procedure that sometimes leads to problems in strongly diverging and converging flow fields (such as between an injection-extraction doublet).