

MT3D Mass Balance: Checking the contents of the .MAS file

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1. Introduction

When it is stripped down to its basic elements, a numerical solute transport simulator is a “mass balance calculator”. A necessary condition for a valid solute transport solution is that all mass be accounted for over the duration of a simulation. MT3D provides sufficient output information to allow us to confirm for ourselves that this condition is indeed satisfied in our analyses.

MT3D provides an accounting of its mass budget in two places. A mass budget summary is printed in the Standard Output file at the end of each stress period. MT3D can also compile its internal mass calculations in the separate file MT3D00n.MAS (the n designates the species number).

The mass budget discrepancy printed in the Standard Output file provides a quick indication of the reliability of the simulation results. The particular quantity to look for in the Standard Output file is the overall mass budget discrepancy. This quantity is analogous to the MODFLOW budget discrepancy, and it should be regarded in the same way. In order for a solution to be valid the mass budget discrepancy must be relatively small (I sleep better if it is well below 1%). It is important to note, however, that the mass budget summary in the Standard Output file does not have much physical significance. As I have indicated elsewhere, the terms IN FROM MASS STORAGE and OUT TO MASS STORAGE are not particularly meaningful. Sometimes, these two terms can overwhelm other terms in the mass budget that are more significant, making it difficult to answer for ourselves the key question, “Has all of the mass been accounted for in my model?”. An additional limitation of the reporting of the mass budget summary in the Standard Output file is the difficulty in plotting it through time.

2. Mass budget summary in the MT3D00n.MAS file

To answer the question “Has all of the mass been accounted for in my model?”, you must examine the mass budget information reported in the file MT3D00n.MAS file, where n designates the species number. The .MAS file reports the same terms as are used to compute the mass budget discrepancy reported in the Standard Output file. However, it reports these values for every transport step. Furthermore, the .MAS file reports additional terms that provide direct measures of mass conservation in a simulation.

Let me explain what I mean by “direct measures” by writing a statement of mass conservation in its most basic form:

$$M(t) = M(t=0) + \sum M_{SOURCES} - \sum M_{SINKS}$$

Here $M(t)$ designates the mass in the aquifer (dissolved and sorbed) at any time t , $M(t=0)$ designates the mass in the aquifer (dissolved and sorbed) at the beginning of the simulation, and $M_{SOURCES}$ any M_{SINKS} denote the cumulative mass added and withdrawn by “physical” sources and sinks (for example, wells, drains, recharge, first-order transformation reactions). An alternative mass balance discrepancy is defined by rearranging the terms in the statement of mass conservation:

$$M(t=0) + \sum M_{SOURCES} = M(t) + \sum M_{SINKS}$$

If we designate:

$$LHS = M(t=0) + \sum M_{SOURCES}$$

$$RHS = M(t) + \sum M_{SINKS}$$

the relative error is calculated as:

$$ERROR_2(\%) = \frac{(LHS - RHS)}{\frac{1}{2}(LHS + RHS)} \times 100$$

This is the appropriate way to define a relative error when comparing two quantities that each may have some error.

3. Example mass budget calculations

To illustrate the interpretation of the mass budget terms, I have plotted some results from a project application on Figures 1 and 2. I have imported the contents of the file MT3D001.MAS into a spreadsheet and plotted selected results on Figure 1. Note that the sinks are plotted with a reversed sign from what appears in the .MAS file.

Let us check the results at an elapsed time of 1,500 days:

- Initial total mass, $M_0 = 9.51136E7$
- Current total mass: $M(t) = 1.84357E7$
- Cumulative mass in from sources = 0.0
- Cumulative mass out from sinks = 7.26981E7

One more term is needed to complete the mass budget, the “Cumulative Mass In from Changes in Fluid Storage” (M_{STRMS}). This term accounts for changes in solute mass associated with changes in the volume of fluid in the model. The example analysis included 6 stress periods, each of 1 year duration. The pumping rate from an extraction system varied from year to year. The effects of fluid transients are short-lived and insignificant relative to solute transport, so each stress period of the MODFLOW flow model was simulated as a sequence of steady-states which gives rise to jumps in the total mass in the model at the end of each year. These jumps are accounted for in the M_{STRMS} term.

MT3D considers the changes in fluid volume to be a solute source. In this example, by 1,500 days, the M_{STRMS} term in the example simulation was $-3.98014E6$, meaning that 3.98014E6 of mass units were actually withdrawn from the model (that is, M_{STRMS} was a negative source). Since M_{STRMS} is actually a loss term throughout this example, its absolute value is plotted on Figure 1 along with the designation “Mass out fluid-storage.”

Writing a mass balance at 1,500 days:

$$M(t) = M(t=0) + \sum M_{SOURCES} - \sum M_{SINKS}$$

$$LHS = 1.84357E7$$

$$RHS = 9.51136E7 + 0.0 + (-3.98014E6) - 7.26981E7 = 1.84354E7$$

Since the *LHS* matches the *RHS*, we can say that mass is indeed conserved.

We can also use the quantities indicated to calculate the alternative mass balance discrepancy. At 1,500 days we calculate:

$$ERROR_2(\%) = \frac{(LHS - RHS)}{\frac{1}{2}(LHS + RHS)} \times 100 = -3.73 \times 10^{-4} \%$$

This error is very small. The value differs slightly from that reported in the .MAS file. The value reported in the .MAS file is calculated with all of the internal numerical precision available to MT3D. As shown on Figure 2, the mass balance discrepancy calculated “manually” with the contents of .MAS file is a jagged approximation of the reported error that is on average correct.

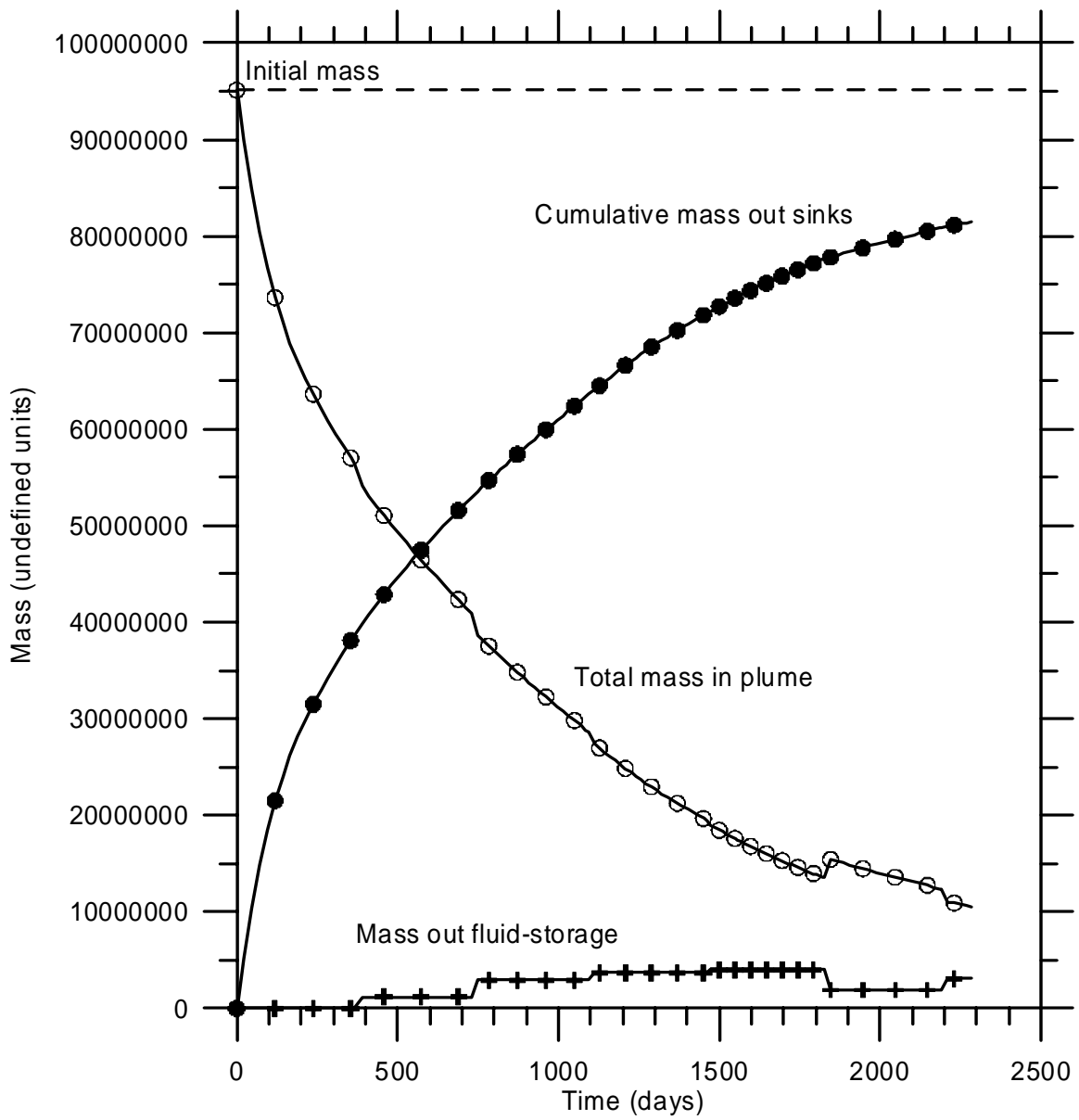


Figure 1. “Physically-motivated” plot of terms in the MT3D mass budget

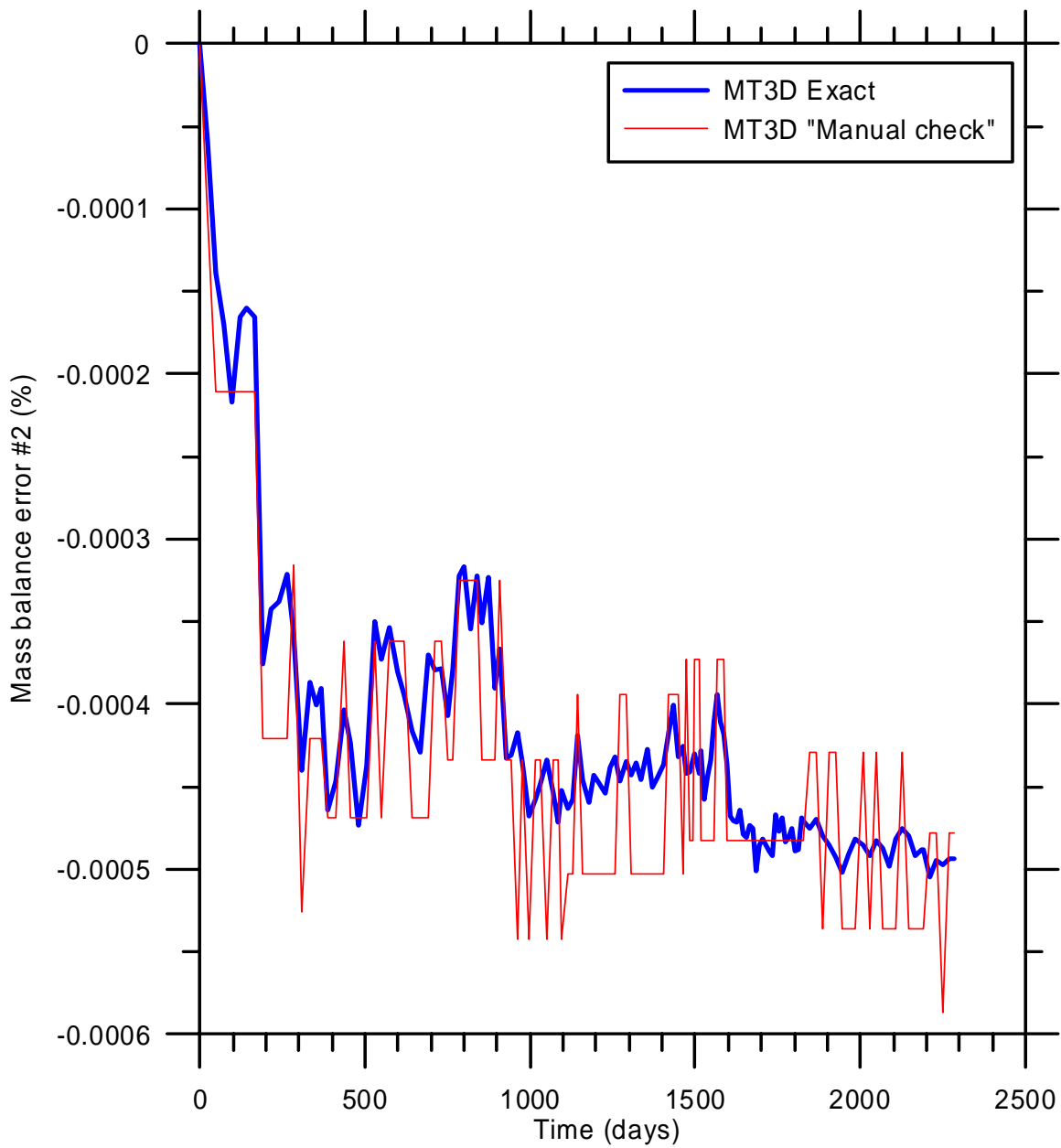


Figure 2. Alternative MT3D mass balance error