**Piecewise-Continuous Boundaries using the MODFLOW FHB and MT3DMS HSS Packages**

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**Abstract**

It is often necessary to simulate the influx to a groundwater model of water containing dissolved contaminants. Until fairly recently, users of MODFLOW and MT3DMS were restricted to varying the flux of water and contaminants on a stress-period basis: when a time-varying loading pattern required simulation, the modeler’s only recourse was to discretize the model into many stress periods. From a practical standpoint this is cumbersome, while from a technical standpoint it requires that the modeler define a-priori an appropriate time discretization that can accurately reproduce time-varying flow and mass loading. This is particularly undesirable when attempting to infer a time-varying flow or mass loading using inverse methods. The advent of the Flow and Head Boundary (FHB) package in the late 1990’s greatly mitigated these limitations from the flow perspective. The recent release of the Hydrocarbon Spill Source (HSS) package for MT3DMS has essentially removed the limitation from the contaminant mass perspective. This Methods Note verifies the FHB and HSS packages by comparison with more commonly-used boundary packages and highlights some benefits of their combined use, with reference to the reconstruction of historic flow and mass fluxes through inverse modeling. (NOTE: The Flow and Head Boundary and Hydrocarbon Spill Source packages are referred to throughout as “FHB” and “HSS”, respectively - i.e., omitting version number suffixes - since the discussion presented should apply to all releases of each package.)

**Introduction**

When undertaking transient simulations the groundwater flow simulator MODFLOW (Harbaugh and McDonald, 1996; Harbaugh et al, 2000) uses stress periods to discretize time and specify rate changes for boundary conditions. Although boundary conditions can only change on stress period intervals, calculated heads and flows can change during a stress period. As a result, stress periods are further divided into time steps, providing smaller time increments to improve the accuracy of the solution of the transient groundwater flow equation at intermediate times. When undertaking a subsequent transport simulation using MT3DMS (Zheng and Wang, 1999) time steps used in the flow simulation are further discretized into transport steps, during which heads and fluxes are considered constant, to provide for stable solution of the transport equation. As a result of this stress-period formulation it has been the case until fairly recently that when a modeler has desired to provide a time-varying influx of water containing dissolved contaminants to a MODFLOW / MT3DMS model, it has been necessary to discretize the flow model into sufficient stress periods to represent the time-varying water flux, and employ these same stress periods to provide the time-varying contaminant flux. This is undesirable from a practical standpoint since it is cumbersome to construct the large input files and produces large output files, and from a theoretical perspective since modelers rarely have the luxury of knowing a-priori the “true” time discretization of a flow or mass source term.

**The MODFLOW Flow-Head Boundary (FHB) Package**

The FHB package (Leake and Lilly, 1997) provides a mechanism within MODFLOW for specifying heads or flows that vary within a stress period. The FHB package processes input provided by the user that specifies flows (or heads) at certain times, and uses linear interpolation to obtain corresponding values at each flow time step. The times for which flow (or head) values are specified by the user need not coincide with the starting or ending times of flow time steps or stress periods: linear interpolation ensures that values are obtained for each flow time step. As a result, use of the FHB package enables the modeler to specify a fairly arbitrary time-varying water flux to/from a model. From a practical standpoint, this enables the user to change both the timing and the rates of this water flux *without modifying any other MODFLOW packages or inputs.* From the technical perspective, this goes some way toward unburdening the modeler from defining a-priori a flow model time discretization that accurately reflects the “true” time-varying flux. The FHB package can process fluxes to/from any number of model cells, enabling the user to provide one or a large number of locations at which time-varying loading occurs.

**The MT3DMS Hydrocarbon Spill Source (HSS) Package**

The HSS package (Zheng, Weaver and Tonkin, 2010) was developed to provide a mechanism within MT3DMS for specifying a mass flux that varies within a flow stress period. The package was conceived of as an alternative to the Source Sink Mixing (SSM) package, and originally implemented to accommodate mass-loading from the dissolution of a Light Non-Aqueous Phase Liquid (LNAPL). However, the HSS package can accommodate any arbitrary time-varying mass flux. The HSS package processes user input in a manner analogous to the FHB package, using interpolation to obtain values for the mass flux at each *transport* step. The times for which mass fluxes are specified by the user need not coincide with the times of flow stress periods, flow time steps, or transport steps: linear interpolation ensures that values are obtained for each transport step. Use of the HSS package enables the modeler to specify a fairly arbitrary time-varying mass flux to/from a model. As for the FHB package, the HSS package enables the user to change both the timing and the rates of this flux, *without modifying any other MODFLOW or MT3DMS packages or inputs*, thus largely absolving the modeler from a-priori time discretization decisions. The HSS package can also process fluxes to/from any number of model cells, enabling the user to provide one or a large number of locations at which time-varying loading occurs.

**Implications**

The implications of these two packages, used separately or together, are quite profound: the modeler is no longer restricted to specifying fluxes on a stress period basis. Faced with a detailed time-varying flow and mass flux, the modeler need no longer prepare boundary packages for a model that comprises tens or hundreds of stress periods (with ample opportunity for error), perhaps using baseless a-priori assumptions. Using the FHB and HSS package, the modeler can define a “base” model for which certain boundaries remain constant or vary on a stress period basis; provide an FHB package input file describing the time-varying water flux and an HSS package input file describing the time-varying mass flux; and ensure that sufficient time-steps are specified in the MODFLOW Discretization file, and sufficient transport steps in the MT3DMS Basic Transport file, so that the interpolation schema of each package can accurately reflect the specified fluxes.

These ostensibly practical advantages for input file preparation and data management are perhaps outweighed by the theoretical implications for the use of automated parameter estimation using codes such as PEST (Doherty, 2010) and UCODE (Poeter et al, 2005), to infer detailed time-varying fluxes on the basis of smoothly-varying functions described using fairly simple model input files.

**Summary**

The advent of the FHB and HSS packages provides the user with several alternative methods for specifying flow and mass fluxes to and from MODFLOW and MT3DMS models. These are summarized below together with the more common methods with which they are contrasted in the sections that follow:

Flow Options (MODFLOW)

* Well (WEL) = Specified flow on stress period intervals (effectively, L3T-1)
* Recharge (RCH) = Specified flow-per-unit-area on stress period intervals (effectively, LT-1)
* FHB = Specified flow interpolated to time step intervals (effectively, L3T-1)

Transport Options (MT3DMS)

* SSM Option 2 = Specified concentration each stress period (effectively, ML-3)
* SSM Option 15 = Specified mass flux each stress period (effectively, MT-1)
* HSS = Specified mass flux interpolated to transport step intervals (effectively, MT-1)

**Verification**

A synthetic example is used to verify that, when correctly implemented, use of the FHB and HSS packages reproduces the flow and mass flux loading that is obtained using the more commonly applied WEL and SSM packages; and, that correct construction of the FHB and HSS packages to describe sub-stress-period variability during long-duration stress periods gives identical results to the use of the WEL and SSM packages when short-duration stress periods are used to represent time-varying loading. The verification employs a single-layer, transient, groundwater model comprising 21 rows and 21 columns. The aquifer properties defined are (in equivalent units) hydraulic conductivity (100), specific yield (0.2), specific storage (10-4), and effective porosity (0.2). Time-invariant specified heads are ascribed to the upgradient and downgradient boundaries using the MODFLOW Basic (BAS) package, producing uniform flow across the domain. A single source of contaminated infiltration is located in the center of the model domain, for which the inflow rate and concentration vary through time. Results presented compare the time-varying inflow rate reported by MODFLOW and cumulative mass loading reported by MT3DMS throughout the simulation time of 200 units, as obtained using the following three combinations of flow and transport packages:

* Method 1: WEL + SSM Option 2 - Inflow rate and concentration specified each stress period. MT3DMS multiplies these to obtain mass loading. The system is simulated using 20 stress periods, one time step per stress period, with each stress period of 10 units duration.
* Method 2: WEL + SSM Option 15 - Inflow rate and mass loading specified each stress period. No multiplication is undertaken. MT3DMS loads the specified mass directly. The system is simulated using 20 stress periods, one time step per stress period, with each stress period of 10 units duration.
* Method 3: FHB + HSS - Inflow rate interpolated at each time step. Mass loading interpolated at each transport step. The system is simulated using one stress period, with 20 time steps.

Figure 1 illustrates the inflow rate reported in the MODFLOW List (LST) file at the conclusion of each flow simulation: the results are identical for each flow alternative. Figure 2 depicts the cumulative mass loading processed from the MT3DMS Output (OUT) file at the conclusion of each transport simulation: the results are identical for each transport alternative.

**An Illustrative Example of the Possible Pitfalls of a-Priori Time Discretization**

This example illustrates that the use of time-averaged flow/mass loading rates simulated using relatively long and arbitrarily-defined stress periods can prevent a flow-and-transport model from simulating hypothesized or known variation in a source term, with possible consequences for (a) predictions of peak concentrations and variability in breakthrough curves at receptors, and (b) the use of automated parameter estimation to reconstruct time-varying source terms on the basis of water levels and/or concentrations measured in wells (see, for example, Lui and Ball, 1999). The same basic model geometry is employed as for the verification example: however, the model simulates two long stress periods – the first comprising 200 units during which flow and mass are loaded at the source, the second comprising 800 units during which no flow or mass are loaded at the source. Results presented focus on time-varying water levels and concentrations calculated immediately downgradient of the infiltrating source throughout the total simulation time of 1000 units using the following combinations of flow and transport packages:

* Method 1: uses the WEL and SSM (option 15) packages to simulate two stress periods with one time step per stress period. During the first stress period, average flow and mass loading rates are used that produce total loads equivalent to that simulated under Method 1: however, since the WEL and SSM are used, the flow and mass loading rates are constant.
* Method 2: uses the FHB and HSS packages to simulate two stress periods, each discretized into 20 equal-length time steps. The first stress period is of duration 200 units during which the flow and mass loading vary each time step.

Figure 3 illustrates the water levels calculated downgradient of the source using each package combination: use of the FHB package results in a time-varying profile that reflects the time-varying inflow (not shown). Figure 4 depicts the concentrations calculated downgradient of the source using each package combination. Use of the FHB and HSS packages together results in a time-varying concentration such as would be expected to result from time-varying inflows and concentrations (not shown). It is noted that the concentration profile is “smoothed” as a result of numerical dispersion in the problem set up: nonetheless the patterns are evident. Although not shown, the cumulative inflows processed from the MODFLOW LST file, and the cumulative mass loading processed from the MT3DMS OUT file at the conclusion of each simulation are identical for each flow and transport package combination.

**Discussion**

Use of the FHB (flow) and HSS (transport) packages enables short-duration (high-frequency) variability to be included in MODFLOW and MT3DMS flow and transport models. One useful application for these combined packages would be the transfer of fluxes of water and contaminants from a vadose zone flow and transport model into a saturated groundwater flow and contaminant transport model. Use of the FHB and HSS packages has practical repercussions: discretization of the model into a large number of stress periods and intensive revisions to other boundary package input files may be avoided since revisions to the FHB and HSS packages can accomplish the same objective (Figure 5). Given this, the idea of “stress periods” as defining periods when boundary conditions do not change might appear to be in question.

The most significant advantage of the combined use of the FHB and HSS packages is the ability to simulate a time-varying source of water and contaminants without strict and perhaps erroneous a-priori definition of the model temporal discretization. A simple example illustrates that the use of time-averaged loading rates simulated using relatively long stress periods can disable a model from reproducing expected or known variation in a source term that is reflected in water levels and/or concentrations measured in wells. Though outside the scope of this Methods Note, this would become apparent when using automated parameter estimation - such as described by Lui and Ball (1999) – to reconstruct a time-varying source term. Under these circumstances, use of an erroneous time discretization may constitute structural error that will inhibit the use of inverse modeling to infer the time-varying source term (Doherty and Welter, 2010), and/or may lead the parameter estimation program to unwittingly infer spatial aquifer heterogeneity when the cause of head or concentration variability is actually temporal source term variation.

The HSS package specifies mass fluxes, and therefore is a natural alternative to the MT3DMS SSM package option 15. The HSS package can be used as an alternative to the MT3DMS SSM package option 2, but calculations external to the model will be required. As is often the case, there are subtleties to the preparation of input files to both the FHB and HSS packages, and the user is advised to read the manuals closely prior to using either package.

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**List of Figures**

Figure 1: Inflow rates processed from the MODFLOW List (LST) file

Figure 2: Cumulative mass loading processed from the MT3DMS output (OUT) file

Figure 3: Water Levels as processed from the MODFLOW Heads (HDS) file

Figure 4: Concentrations processed from the MT3DMS Unformatted Concentration (UCN) file

Figure 5: Schematic of the combined sub‐stress period flow and mass loading capabilities of the FHB and HSS packages







