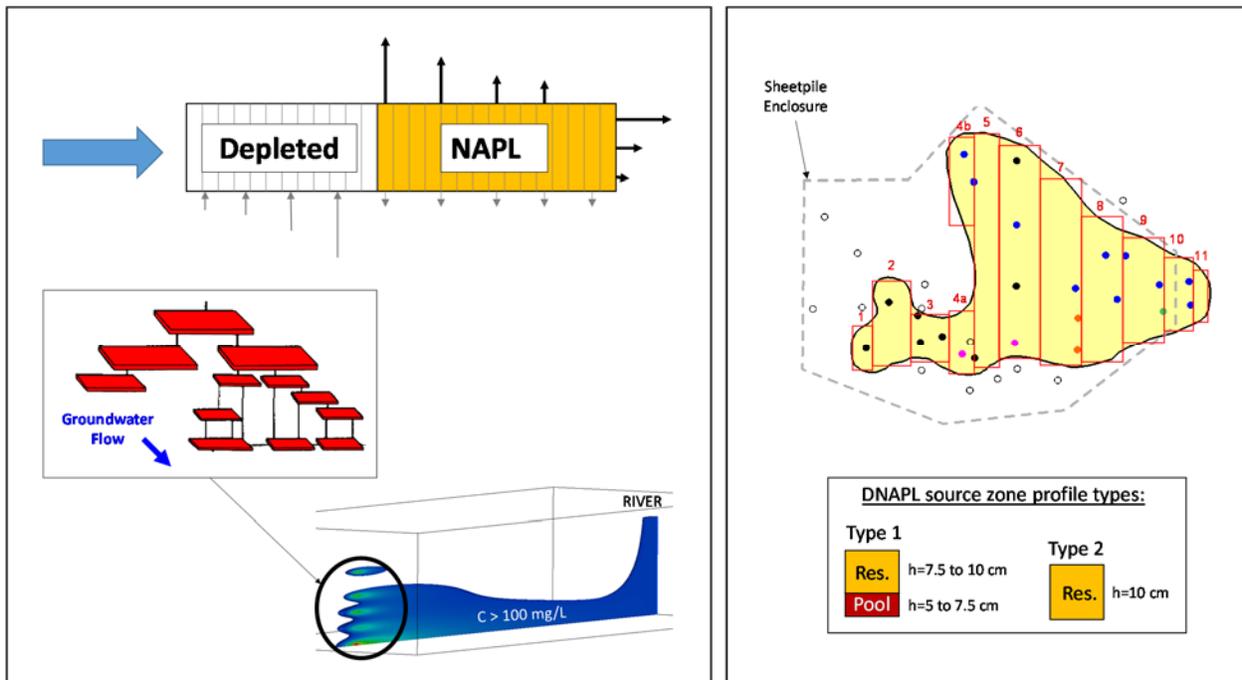




## NAPL Depletion Model (NDM) for Estimating Natural and Enhanced Attenuation Timeframes: Version 1.00 User's Guide

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## 1. NAPL Depletion Model (NDM) Development

### 1.1 Conceptual Model

The NAPL Depletion Model (NDM) is a semi-analytical screening model which may be used to estimate NAPL depletion under conditions of naturally-occurring or enhanced dissolution. NDM is a process-oriented model, which means that it explicitly represents various porous media and NAPL characteristics which influence the rate of dissolution for one or more NAPL sub-zones within an overall source zone. A sub-zone refers to a NAPL body (e.g. layer) which is relatively continuous, and may not be further discretized into smaller sub-zones on the basis of geometry, porous media characteristics, and/or NAPL characteristics (e.g. chemical composition, NAPL saturation, or density). A NAPL source zone in NDM is comprised of one or more individual sub-zones.

NDM is an alternative to the use of simpler up-scaled models, which typically represent domain-averaged dissolution rates or decline rates for a uniform source zone. NDM may be used for LNAPL or DNAPL, and was developed with the flexibility to simulate NAPL pools, residual sub-zones, and/or mixed zones of NAPL. NDM simulates three types of dissolution or discharge processes: (a) surface dissolution at the top or bottom of a sub-zone; (b) reduced groundwater flow through a sub-zone based on a user-specified or model-calculated relative water permeability; and (c) flux into or out of lower-permeability zones adjacent to one or more NAPL sub-zones.

The key output variables for NDM are the mass discharge and NAPL mass remaining for each individual sub-zone, and the total metrics for the combined source zone. NDM does not simulate changes in aqueous concentrations outside of the NAPL sub-zones, although it is possible to use simple multipliers to simulate or calibrate the ratios of daughter product formation for mass discharge calculations.

Uses of NDM may include:

- Interpretation of NAPL architecture based on calibration of a model to historical discharge trends;
- Estimation of future mass discharge decline rates and depletion timeframes for an existing alternative;
- Evaluation of the relative performance of various potential alternatives as part of feasibility study;
- Quantifying the relative sensitivity of predicted trends (e.g. depletion timeframe) to various site characteristics, in order to identify those characteristics which require further investigation.

NDM is a Fortran-based program which offers a number of options for representing NAPL pools, residual NAPL sub-zones, and/or mixed NAPL zones. A simple mass balance approach is

used within NDM to simulate the mass discharge, and mass remaining, in each NAPL sub-zone of a simulation at the end of each time step. The analytical governing equations for NDM are described in more detail below. General functionality in NDM includes:

- Use of a one-dimensional grid to represent each NAPL sub-zone, with user-defined length, width, thickness, and average NAPL saturation (or depth-specific NAPL saturation calculations performed by the model for NAPL pools with a capillary pressure of zero at the top surface).
- NDM simulates dissolution from the upgradient end of each sub-zone, and upgradient grid cells that become depleted in mass during a simulation are defined to be inactive for the remainder of the simulation. In this manner, the pool-scale declining NAPL-water interfacial area may be represented, as well as the corresponding influence on mass discharge associated with surface dissolution.
- Option to apply through-discharge to the upgradient-most, active cell in a NAPL sub-zone, or uniformly to all cells within a NAPL sub-zone.
- A user-defined multiplier which allows for simulation of surface discharge for none, one, or both the top and bottom surfaces of a NAPL sub-zone, or for simulating an accelerated specific discharge adjacent to the NAPL-water interface.
- Option to make the start of surface and/or through discharge for a NAPL sub-zone to be dependent on the depletion of another zone (e.g. an upgradient sub-zone, or an overlying or underlying layer of NAPL).
- Option for constant, exponential or linear decline models to represent the transient influence of intra-source bypassing and other rate-limited kinetics on the through-discharge with a NAPL sub-zone;
- Quasi-2D representation of discharge through the transition zone in the upper portion of NAPL pools where the relative water permeability is sufficiently large to allow for significant mass discharge, and the NAPL saturation is optionally calculated at specific depths within the pool;
- Enhanced dissolution corresponding to temporal changes in hydraulic gradient (e.g. at the start of pumping near a source zone), or an enhanced dissolution factor associated with in-situ remedies such as enhanced in-situ bioremediation (EISB) or in-situ chemical oxidation (ISCO).
- Automated non-linear calibration of the  $\beta$  term in  $Md/Md_o = (M/M_o)$  for each sub-zone;
- An adaptive time-stepping scheme to account for changing system dynamics when a sub-zone grid cell becomes inactive; and
- Option for through-discharge simulations for multicomponent NAPL (see Section A.6).
- Batch mode so that hundreds of simulations may be executed automatically. (A separate processor may be used to generate text input files and post-process output files for use with monte carlo or latin hypercube realizations.)

## 1.2 Sub-zone Mass Balance

As long as mass remains in NAPL sub-zone  $i$ , the total mass discharge related to NAPL dissolution to the aqueous phase is based on

$$Md_{i,diss}^t = Md_{i,thru}^t + Md_{i,surf}^t + Md_{i,diff}^t \quad (1)$$

where  $Md_{i,diss}^t$  = total mass discharge from dissolution of NAPL to the aqueous phase in sub-zone  $i$  at time step  $t$  [ML<sup>-1</sup>];

$Md_{i,thru}^t$  = mass discharge from dissolution of NAPL into groundwater flowing through sub-zone  $i$  at time step  $t$  [ML<sup>-1</sup>];

$Md_{i,surf}^t$  = mass discharge from dissolution of NAPL into groundwater flowing across the top and/or bottom of sub-zone  $i$  at time step  $t$  [ML<sup>-1</sup>]; and

$Md_{i,diff}^t$  = mass discharge from dissolution of NAPL and subsequent diffusion into a low-permeability unit above and/or below sub-zone  $i$  at time step  $t$  [ML<sup>-1</sup>].

The mass remaining in each grid cell  $j$  of NAPL sub-zone  $i$  at the end of the time step  $t$  is calculated using

$$M_{ij}^t = M_{ij}^{t-1} - (Md_{ij,thru}^t + Md_{ij,surf}^t + Md_{ij,diff}^t)\Delta t \quad (2)$$

Where  $M_{ij}^{t-1}$  refers to the mass remaining in NAPL sub-zone  $i$  cell  $j$  at the end of the previous time step [M], and  $\Delta t$  represents the length of the time step [T]. The total NAPL mass remaining in sub-zone  $i$  at the end of the time step is calculated by summing the NAPL mass remaining in each cell of the sub-zone grid. The total mass added to storage in low-permeability unit(s) adjacent to each NAPL source zone is also accounted for in the mass balance.

The equations and potential uses of each of the individual mass discharge terms in Eq. 1 are discussed further below.

Finally, the source strength contributing to the downgradient plume from NAPL dissolution is calculated as

$$Md_{i,source}^t = (Md_{i,thru}^t + Md_{i,surf}^t)f_{RXN1}^t \quad (3)$$

Where  $f_{RXN1}^t$  represents a multiplier for the reduction in source strength due to chemical transformations occurring in the source zone when NAPL is present. This term is useful for simple, quasi-representation of transformation reactions that may occur upon implementation of an active remedial technology such as EISB or ISCO.

When mass has been completely depleted in NAPL sub-zone  $i$ , mass discharge contributing to ongoing source strength via back-diffusion from adjacent diffusive source zones (if simulated) is then simulated for the time step using

$$Md_{i,source}^t = (Md_{b-diff}^t)f_{RXN2} \quad (4)$$

where  $f_{RXN2}$  represents a multiplier for the reduction in source strength due to chemical transformations occurring in the source zone once NAPL has been depleted. This term may be used to represent sustained transformation reactions which may occur after the cessation of EISB.

### 1.3 Sub-Zone Through-Discharge

#### Residual/Mixed Source Zones

For residual and mixed NAPL source zones, mass discharge due to dissolution of NAPL into groundwater flowing through sub-zone  $i$  is given by

$$Md_{i,thru}^t = (krw_i q_x^t C_{eff}^t w_i h_i) f_i^t f_{ed1}^t \quad (5)$$

where  $krw_i$  is the relative water permeability,  $q_x^t$  is the average specific discharge at time step  $t$ ,  $C_{eff}^t$  is the effective solubility (which is the same as solubility for a single component NAPL),  $w_i$  and  $h_i$  represent the width and height of source zone  $i$ ,  $f_i^t$  is a multiplier representing the proportion of the source zone cross-section which has streamtubes containing NAPL at time step  $t$ , and  $f_{ed1}^t$  is a multiplier for mass discharge through the zone representing potential enhanced dissolution at time step  $t$  as a result of active remediation. The current version of NDM does not consider transient  $krw_i$  during source depletion; further study is warranted to determine when transient representation of this parameter may be helpful.

As discussed above, NDM represents three types of decline models for the  $f_i^t$  term to provide a surrogate representation for the rate of decline in NAPL-water interfacial area (IA) in the source zone:

- Exponential decline,  $f_i^t = f_{io} e^{-\lambda_i^t t}$  where  $f_{io}$  represents the initial proportion of the source zone cross-section which has streamtubes containing NAPL, and  $\lambda_i^t$  represents the first-order rate of decline of the proportion of streamtubes containing NAPL at time step  $t$ ;
- Linear decline,  $f_i^t = f_{io} - f_{io} m_i^t t$  where  $m_i^t$  represents the linear decline slope at time step  $t$ ; and
- Constant  $f_i^t = f_{io}$ .

As an example, if a transect across the downgradient boundary of a source zone has 10% of the cross-sectional area with NAPL upgradient of the transect,  $f_{io}$  will be specified as 0.10. At field sites, it is expected that exponential decline models will typically be used to represent aged

sources and/or sources with a heterogeneous NAPL distribution, and the constant  $f_i^t$  model will be used to represent high-saturation portions of pools with relatively homogeneous distributions of NAPL.

For sites where an exponential decline model is applicable, the first-order rate ( $\lambda$ ) may be estimated based on historical monitoring data. Of note is the relationship summarized by Newell and Adamson (2005) such that  $\lambda = Md_o/M_o$ , where  $Md_o$  represents the source strength at the time of characterization and  $M_o$  represents an estimate of initial source mass contributing to the this source strength. If the first-order rate can be estimated from site monitoring data, then an estimate of  $M_o$  and the corresponding average NAPL saturation ( $Sn_o$ ) in a source zone can also be readily estimated. For residual and mixed source zones, the average NAPL saturation source zone ( $Sn_o$ ) is an input parameter for NDM to facilitate estimation of the initial NAPL mass in a source zone.

To represent the influence of changes in the specific discharge rate which may occur during active remediation, the time-dependent exponential and linear decline rates are calculated respectively based on:

$$\lambda_i^t = \lambda_{io} q_x^t / q_{xo} \quad (6)$$

$$m_i^t = m_{io} q_x^t / q_{xo} \quad (7)$$

### Pool Source Zones

Given the higher NAPL saturation in pools and the corresponding reduction in water permeability, as well as the occurrence of some pools that form in topographic depressions on the surface of a low-permeability layer, a relatively small flux of groundwater will occur through the body of the pool.

To facilitate a comparison of the mass discharge which may occur through pool sub-zones relative to the discharge arising from surface dissolution, NDM incorporates the flexibility of simulating the rate of reduced water flow at various depths within a NAPL pool. NDM also incorporates the option of specifying an average  $Sn_{io}$  and  $krw_i$  for use in estimating the initial mass discharge through the NAPL source zone based on Equation 5, or to specify a mass discharge of zero based on the assumption that the relative permeability in the pool layer is negligible relative to the mass discharge from the surface of the pool.

McWhorter and Kueper (1996) document the following equation for estimating the elevation in a pool corresponding to an effective saturation:

$$z = T - \frac{P_o}{\Delta\rho g} \left[ \left( \frac{S_w - S_{wr}}{S_m - S_{wr}} \right)^{-1/m} - 1 \right]^{1-m} \quad (8)$$

where  $z$  refers to an elevation in a pool layer with height  $T$ ,  $P_o$  is the reference capillary pressure defined as  $\rho_w g / \alpha$ , where  $\alpha$  [ $L^{-1}$ ] and  $m$  [dim.] are capillary pressure-saturation curve coefficients defined by Van Genuchten (1980),  $\rho_w$  is the density of water [ $ML^{-3}$ ],  $g$  is the gravitational acceleration constant [ $LT^{-2}$ ],  $\Delta\rho$  is the difference between NAPL and water density [ $ML^{-3}$ ],  $S_w$  is the water saturation,  $S_{wr}$  is the irreducible water saturation, and  $S_m$  is the maximum water saturation.

Re-arranging the above equation and solving for  $S_n=1-S_w$  at elevation  $z$  gives

$$S_n(z) = 1 - S_{wr} - (S_m - S_{wr}) \left[ 1 + \left( \frac{\alpha \Delta\rho (T-z)}{\rho_w} \right)^{\frac{1}{1-m}} \right]^{-m} \quad (9)$$

Van Genuchten (1980) defines the relative water permeability for a two-phase system as

$$krw = Se_{krw}^{1/2} \left[ 1 - (1 - Se_{krw}^{1/m})^m \right]^2 \quad (10)$$

where  $Se_{krw}$ , the effective saturation used to estimate relative water permeability, is given by

$$Se_{krw} = \frac{S_w - S_{wr}}{1 - S_{wr}} \quad (11)$$

To estimate the total mass discharge through a pool layer with variable  $S_n(z)$ , the pool layer is vertically discretized into  $m$  layers with uniform thickness  $\Delta z$ . The NAPL saturation in each layer ( $S_{nim}$ ) is calculated by substituting the pool height ( $h_i$ ) for  $T$  in Equation 8. The effective saturation  $Se_{krw}$  is calculated by substituting  $S_{wim}=1-S_{nim}$  for  $S_w$  in Equation 11, and the relative water permeability in layer  $m$  of the pool source zone  $i$  ( $krw_{im}$ ) is then calculated using Equation 10. The mass discharge arising from NAPL dissolution into groundwater flowing through source zone  $i$  at time step  $t$  is then calculated by summing the depth-specific discharges using

$$Md_{i,thru}^t = \left( \sum_{m=1}^{nlay} krw_{im} q_x^t C_{eff}^t w_i \Delta z \right) f_i^t f_{ed1}^t \quad (12)$$

Equation 12 includes a time-dependent enhanced dissolution multiplier, which may be used to represent enhanced dissolution periods within an overall model simulation (e.g. EISB or Strategic Pump-and-Treat). Note that NDM does not represent potential mobilization of NAPL that may occur with some in-situ remediation technologies. Care must be exercised during in-situ remediation to ensure that expansion of the source zone does not occur.

#### 1.4 Sub-Zone Surface Discharge

NAPL pools are typically characterized by a relatively limited NAPL-water interfacial area at the surface of pools where dissolution into flowing groundwater occurs. Solute transport at this surface interface is driven by transverse vertical dispersion. The solute transport equation is

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$$\theta \frac{\partial C}{\partial t} = \theta D_z \frac{\partial^2 C}{\partial z^2} - q_x \frac{\partial C}{\partial x} \quad (13)$$

where  $C$  is the solute concentration [ $\text{ML}^{-3}$ ],  $D_z$  is the hydrodynamic dispersion coefficient [ $\text{L}^2\text{T}^{-1}$ ], and  $q_x$  is specific discharge [ $\text{L}^3\text{L}^{-2}\text{T}^{-1}$ ]. In this form of the advection-dispersion equation, the hydrodynamic dispersion coefficient is calculated using

$$D_z = \alpha_{TV} v_x + D_e, \text{ and } D_e = \tau D_o \quad (14)$$

where  $\alpha_{TV}$  is the transverse vertical dispersivity [ $\text{L}$ ],  $v_x (=q_x/\theta)$  is the average linear groundwater velocity [ $\text{LT}^{-1}$ ],  $D_e$  is the effective diffusion coefficient [ $\text{L}^2\text{T}^{-1}$ ],  $\tau$  is the tortuosity coefficient, and  $D_o$  is the free-water molecular diffusion coefficient [ $\text{L}^2\text{T}^{-1}$ ].

In some cases, the above equation 13 is written as

$$\frac{\partial C}{\partial t} = D_z \frac{\partial^2 C}{\partial z^2} - v_x \frac{\partial C}{\partial x} \quad (15)$$

where the hydrodynamic dispersion coefficient and effective molecular diffusion coefficient are estimated based on Equation 14. In contrast, Hunt et al. (1988) expressed the advection dispersion equation based on an alternative form of the governing equation

$$\theta \frac{\partial C}{\partial t} = D_z^* \frac{\partial^2 C}{\partial z^2} - q_x \frac{\partial C}{\partial x} \quad (16)$$

where the adjusted hydrodynamic dispersion coefficient is calculated using

$$D_z^* = \alpha_{TV} q_x + D_e^*, \text{ and } D_e^* = \theta \tau D_o \quad (17)$$

In other words, when specific discharge is used in the advection term of the governing equation and for calculating mechanical dispersion, it is important to include a porosity term in the term representing the effective molecular diffusion coefficient.

### Analytical Solution for Mass Discharge from a Pool Surface

Based on the analytical solution cited by Johnson and Pankow (1992) for the steady-state form of Equation 15, mass discharge from dissolution along the surface of a pool with length  $L$  and width  $w$  is

$$Md = LwC_{eff}\theta \sqrt{\frac{4D_z v_x}{\pi L}} \quad (18)$$

Hunt et al. (1988) present the analytical solution based on Equation E-16 as

$$Md = LwC_{eff} \sqrt{\frac{4D_z^* q_x}{\pi L}} \quad (19)$$

Note that both Equations E-18 and E-19 yield the identical solution provided that  $\theta$  is used to estimate  $v_x$ . Equation E-19 can be further re-arranged to yield

$$Md = \left( 2LwC_{eff} \sqrt{\frac{q_x}{\pi L}} \right) \sqrt{\alpha_{TV} q_x + \theta \tau D_o} \quad (20)$$

It is not clear whether  $\theta$  should represent total or effective porosity, since both advection and diffusion contribute to solute transport to some degree during surface dissolution from a pool. From Equation 20 it is clear that under high specific discharge conditions, mechanical dispersion will dominate over the effective molecular diffusion term and porosity will have a negligible influence on the mass discharge calculation. In low specific discharge environments, molecular diffusion is likely to dominate the hydrodynamic dispersion term and it is appropriate then to assign  $\theta$  as total porosity. When considering the middle case where mechanical dispersion and effective molecular terms are equal in a fine sand, the total porosity may be twice as high as effective porosity (e.g. 0.40 vs. 0.20, respectively). In this case, mass discharge calculated using total porosity is approximately 20% higher than the discharge that would be calculated using effective porosity. There is a smaller range for total vs. effective porosity for a coarse sand (e.g. 0.35 to 0.275), resulting in a smaller difference for mass discharge calculated based on total versus effective porosity.

Given that these differences are relatively minor when compared to uncertainty in specific discharge or pool dimensions, and that total porosity is more directly measured at the site and more applicable under conditions of low specific discharge, it is recommended that the total porosity be used when estimating mass discharge on the basis of Equation 20.

It is also recommended that the solution in Equation in 20 be used for estimating mass discharge instead of Equation 18, since  $v_x$  is typically calculating using effective porosity which is not the appropriate porosity to use in Equation 18 for sites where transport is diffusion-dominated.

Based on the analytical solution presented in Equation 20, NDM estimates the mass discharge from the surface of source zone  $i$  discretized in  $j=1$  to grid cells using the equations

$$Md_{i,surf}^t = \left[ \sum_{j=1}^{n_{col}} (Md_{i,surf,j}^t - Md_{i,surf,j-1}^t) \right] \quad (21)$$

$$Md_{i,surf,j}^t = \left[ x_{ij} w_i C_{eff}^t \sqrt{\frac{4D_z^* q_x^t}{\pi x_{ij}}} \right] f_{ed2}^t f_{surf} \quad (22)$$

where  $x_{ij}$  is the length from the upgradient edge of the pool to the downgradient end of column  $j$ ,  $f_{ed2}^t \geq 1$  is a multiplier that is used during the portion of the simulation where a dissolution enhancement technology has been implemented, and  $f_{surf}$  is a multiplier that is equal to 0, 1, or 2 to represent the number of source zone surfaces where dissolution is occurring into overlying

and/or underlying groundwater.  $f_{surf}$  may also be assigned a real number to represent a multiplier for accelerated specific discharge adjacent to the boundary surface of the NAPL sub-zone. For a pool source zone, typically  $f_{surf}=1$  (e.g. when the pool is underlain by a low-permeability silt or clay). For a residual NAPL layer that has transmissive layers both above and below it,  $f_{surf}=2$ .

### 1.5 Diffusive Mass Discharge Into and Out of Low-Permeability Units

Seyedabbasi et al. (2012) present the analytical equations used to estimate mass discharge associated with both forward diffusion into the low-permeability unit (which is based on work presented in Parker et al., 1994), as well as for back-diffusion into the more transmissive unit.

Mass discharge from a single component NAPL source zone  $i$  to a low-permeability unit is estimated based on

$$Md_{i,diff}^t = \phi L_i w_i C_s \sqrt{\frac{R\tau D_o}{\pi t}} \quad ; \quad t < t_{depletion} \quad (23)$$

where  $\phi$  is total porosity in the low-permeability unit [ $L^3L^{-3}$ ],  $C_s$  is solubility [ $ML^{-3}$ ],  $R$  is the retardation coefficient in the low-permeability unit,  $\tau$  is the tortuosity coefficient for the low-permeability unit, and  $t_{depletion}$  is the simulation time at which all NAPL in the source zone has been depleted. This equation is based on the assumption that the low-permeability unit is a semi-infinite domain; therefore, this equation is only valid when the low-permeability unit is sufficiently thick that significant mass does not diffuse through the exit boundary of the low-permeability unit. This equation also assumes a constant solubility in time in the source zone and therefore is not applicable for multicomponent NAPLs when effective solubility changes significantly over time.

The analytical solution for estimating the time-varying mass discharge associated with back-diffusion from the low-permeability unit into the depleted source zone is presented in Seyedabbasi et al. (2012) as

$$Md_{i,b-diff}^t = \phi L_i w_i C_s \left( \sqrt{\frac{R\tau D_o}{\pi t}} - \sqrt{\frac{R\tau D_o}{\pi(t-t')}} \right) \quad ; \quad t > t_{depletion} \quad (24)$$

The reader is referred to Seyedabbasi et al. (2012) for an evaluation of the relative longevity of plumes sustained by back-diffusion relative to the initial NAPL dissolution period. These analytical models may be used to compare the magnitude of the diffusive discharge from a NAPL pool, to surface and/or through-discharge. Generally, the diffusive discharge is much lower in magnitude, on average, relative to the other two types of mass discharge from a NAPL pool.

## 1.6 Multicomponent NAPL Dissolution

A version of NDM has been prepared to simulate multicomponent NAPL dissolution (NDM-MC). The present version of NDM-MC is limited in that surface discharge is not simulated; only through-discharge may be simulated for a multicomponent NAPL, and the maximum number of species in this current version is limited to three.

The model equations are similar to those described above for NDM, with the main difference being that the effective solubility for each species is calculated in each sub-zone grid cell at the end of each time step, based on an automated re-calculation of the species molar fraction in each cell. If an upgradient cell has a smaller effective solubility for a species than a downgradient cell, then mass will be dissolved from the downgradient cell to ensure that local equilibrium is achieved at the NAPL-water interface. Similarly, if an upgradient cell has a larger effective solubility than a downgradient cell, then mass will be re-dissolved into the NAPL in the downgradient cell to maintain equilibrium. The influence of intra-source by-passing may be simulated using one of the transient dilution factor equations (see Section A.3).

For further information regarding the availability of NDM-MC, please contact Grant Carey at Porewater Solutions (*email: [gcarey@porewater.com](mailto:gcarey@porewater.com); telephone: 613-270-9458*).

## 2. INPUT FILE FORMAT

The input files for NDM are free format, which means that any number of spaces may be entered between variables on the same line of the text input file. The sequence and list of variables for each record (i.e. line) in the text input file are listed below. Units must be entered as specified in the record descriptions.

### 2.1 General Scenario Data

R01 Record: IPFLUX

- IPFLUX is a flag indicating the through-discharge model to be utilized for all sub-zones.
  - IPFLUX = 0: Through-discharge is not simulated for any sub-zones.
  - IPFLUX = 1: Through-discharge is simulated based on the model-calculated  $S_n$  and  $k_{rw}$  profiles over the thickness of each NAPL sub-zone; through-discharge mass is removed only from the first active segment in the upgradient end of the NAPL sub-zone.
  - IPFLUX = 2: Through-discharge is simulated based on the model-calculated  $S_n$  and  $k_{rw}$  profiles over the thickness of each NAPL sub-zone; through-discharge mass is removed equally from all active segments in the 1-D sub-zone grid.
  - IPFLUX = 3: Through-discharge is simulated based on the user-specified average  $S_n$  and  $k_{rw}$  for each sub-zone (see Record R##).

(Enter R02 through R08 if IPFLUX = 1 or 2.)

R02 Record:  $S_{wr}, S_m$

- $S_{wr}$  is the irreducible water saturation.
- $S_m$  is the maximum water saturation after invasion of NAPL, and is equal to 1 – residual saturation threshold.

R03 Record:  $\sigma_{mw}, \sigma_{aw}$

- $\sigma_{mw}$  is the NAPL-water interfacial tension (dynes/cm).
- $\sigma_{aw}$  is the air-water interfacial tension (dynes/cm).

R04 Record:  $\alpha_{aw}$

- $\alpha_{aw}$  is the Van Genuchten permeability model parameter defined by the inverse of the entry pressure head ( $\text{m}^{-1}$ ).

R05 Record:  $n$

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- $n$  is the Van Genuchten permeability model parameter related to the pore size distribution.

R06 Record:  $\rho_w$

- $\rho_w$  is the density of groundwater (kg/m<sup>3</sup>).

R07 Record:  $\Delta z$

- $\Delta z$  is the vertical spacing for layers in the NAPL sub-zone over which  $S_n$  and  $k_{rw}$  are to be estimated.

R08 Record:  $F_{eff}$

- $F_{eff}$  is a factor between 0 and 1 which is used to adjust the through-discharge. For example,  $F_{eff} < 1$  when geologic factors reduce the magnitude of through-discharge relative to the calculated value under ideal conditions.

R09 Record:  $nzone$

- $nzone$  is the number of sub-zones to be simulated within the source zone. There is a limit of 20 sub-zones that may be simulated.

## 2.2 NAPL Sub-Zone Data

(Enter R10 through R14  $nzone$  times i.e. for each sub-zone.)

R10 Record:  $IDsz, IDsz-upgradient$

- $IDsz$  is the ID number of the current sub-zone (between 1 and  $nzone$ ).
- $IDsz-upgradient$  is the ID number of a sub-zone which is upgradient of the current sub-zone. Dissolution of the current sub-zone may be restricted until the upgradient source zone has been completely depleted (see Records R12 and R13 below). If  $IDsz-upgradient$  is zero, then there is no upgradient sub-zone which restricts dissolution of the current sub-zone.

R11 Record:  $X_1, X_2, Y_1, Y_2, Z_1, Z_2$

- $X_1$  and  $X_2$  are the absolute coordinates of the upgradient and downgradient ends of the NAPL sub-zone, respectively. The length of the subzone (parallel to groundwater flow) is  $X_2 - X_1$ .
- $Y_1$  and  $Y_2$  are the absolute coordinates of the cross-gradient ends of the NAPL sub-zone. The width of the subzone (cross-gradient to groundwater flow) is  $Y_2 - Y_1$ .

- $Z1$  and  $Z2$  are the absolute bottom and top elevations of the NAPL sub-zone, respectively. The thickness of the subzone is  $Z_2 - Z_1$ .

R12 Record:  $f_{surf}, f_{surfdep}$

- $f_{surf}$  is a real number multiplicative factor which is multiplied by the calculated  $Md_{surf}$  based on the analytical solution (see Eq. 20).  $f_{surf} = 1.0$  is specified when surface discharge occurs only at one of the top or bottom surfaces of the sub-zone.  $f_{surf} = 2.0$  implies that dissolution occurs at both the top and bottom surfaces of the sub-zone.
- $f_{surfdep}$  is the multiplicative factor to use when the upgradient sub-zone  $ID_{sz-upgradient}$  (see Record R10) becomes depleted.

(Enter R13 if IPFLUX > 0)

R13 Record:  $f_{effo}, jfeffmdl, f_{effm}, f_{effodep}$

- $f_{effo}$  is a real number multiplicative factor which is multiplied by the calculated  $Md_{thru}$  to represent the ratio of initial  $Md_{thru}$ , to the  $Md_{thru}$  that would be calculated based on the assumption of solubility concentration in the sub-zone effluent. For example, if the average concentration at the downgradient sub-zone boundary is 50% of solubility, then  $f_{effo}$  is specified to be 0.50.
- $jfeffmdl$  is a flag indicating the type of decline model to be used for  $Md_{thru}$ . (0=constant, 1=linear, and 2=exponential.)
- $f_{effm}$  is the rate of decline for  $Md_{thru}$  (used when  $jfeffmdl$  is 1 or 2).
- $f_{effodep}$  is the replacement value of  $f_{effo}$  to use when the upgradient sub-zone  $ID_{sz-upgradient}$  has become depleted (see Record R10).

R14 Record:  $SZfname$

- $SZfname$  is the root name of the output file to be created for the current sub-zone, with extensions \*.5 and \*.6.  $SZfname$  has a limit of 20 characters.

### 2.3 Remaining Simulation Input Parameters

R15 Record:  $\rho_{NAPL}$

- $\rho_{NAPL}$  is the NAPL density (kg/m<sup>3</sup>).

R16 Record:  $C_{sol}$

- $C_{sol}$  is the pure component solubility (mg/L).

R17 Record:  $D_o$

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- $D_o$  is the free-water diffusion coefficient ( $m^2/s$ ).

R18 Record:  $K$

- $K$  is the hydraulic conductivity ( $m/s$ ).

R19 Record:  $i$

- $i$  is the horizontal hydraulic gradient in the aquifer ( $m/m$ ).

R20 Record:  $\theta$

- $\theta$  is total porosity ( $m^3/m^3$ ).

R21 Record:  $\alpha_{TV}$

- $\alpha_{TV}$  is the transverse dispersivity ( $m$ ).

R22 Record:  $\tau$

- $\tau$  is the tortuosity coefficient (dimensionless).

R23 Record:  $SimTime$

- $SimTime$  is the simulation time (days).

R24 Record:  $\Delta t$

- $\Delta t$  is the simulation time step (days).

R25 Record:  $\Delta t_{min}$

- $\Delta t_{min}$  is the minimum time step to be used during dynamic time step calculation (days).

R26 Record:  $\Delta x$

- $\Delta x$  is the horizontal 1-D grid cell (i.e. segment) spacing for the sub-zone ( $m$ ).

R27 Record:  $nPERed$

- $nPERed$  is the number of periods with enhanced dissolution.

(Enter R28 if nPERed > 0, and repeat R28 nPERed times i.e. one line for each period with enhanced dissolution.)

R28 Record:  $t1\_ed, t2\_ed, fed, fedRateMult$

- $t1\_ed$  is the start of the current period with enhanced dissolution (days).  $t1\_ed$  is greater than or equal to zero.
- $t2\_ed$  is the end of the current period with enhanced dissolution (days). The last R28 record (if nPERed>0) must have  $t2\_ed = SimTime$  specified in Record R23 above. That is, the last enhanced dissolution period must have  $t2\_ed$  equal to the length of the simulation.
- $fed$  is a multiplicative factor ( $\geq 1$ ) representing the magnitude of enhanced dissolution. For example,  $fed=2$  indicates a 100% increase in both  $Md_{surf}$  and  $Md_{thru}$  due to enhanced dissolution.  $fed=3$  indicates a 200% increase.  $fed=1$  implies that there is no enhanced dissolution for the specified time period.
- $fedRateMult$  is a multiplicative factor for adjusting the through-discharge decline rate ( $\lambda_{thru}$ ) from the previous time step if the exponential decline model is used ( $jfeffmdl=2$ ). For example, if  $fedRateMult$  is 2 or 0.25, then the decline rate from the previous time step is multiplied by 2 or 0.25 when  $t=t1\_ed$ .

R29 Record:  $fgrad, igradrate$

- $fgrad$  is a multiplicative factor representing a change in horizontal hydraulic gradient relative to the value specified in Record R19 above.  $fgrad$  is used by the model to adjust the specific discharge used for the calculation of  $Md_{surf}$  and  $Md_{thru}$ , for the time period specified in Record R30 below. For example,  $fgrad = 2$  implies that the hydraulic gradient, specific discharge, and groundwater velocity increase by a factor of two relative to the gradient specified in Record R19. Note that  $fgrad$  applies at most to only one time period (specified in Record R30 below); this is in contrast to the  $fed$  multiplicative factor which may be applied in multiple time periods (see Record R28 above).
- $igradrate$  is a flag indicating whether the through-discharge decline rate ( $\lambda_{thru}$ ) should be adjusted by the same magnitude as  $fgrad$ .  $igradrate=0$  means that  $\lambda_{thru}$  will not be changed, and  $igradrate=1$  means that  $\lambda_{thru}$  from the previous time step will be multiplied by  $fgrad$ .

R30 Record:  $t1\_fgrad, t2\_fgrad$

- $t1\_fgrad$  is the start of the time period where  $fgrad$  is to be applied. May be any value greater than or equal to zero. If  $t1\_fgrad$  is greater than the simulation period, then  $fgrad$  will not be applied during the simulation.
- $t2\_fgrad$  is the end of the time period where  $fgrad$  is to be applied. May be any value greater than or equal to zero. If  $t2\_fgrad$  is greater than the simulation period, then  $fgrad$  will be applied for all times greater than  $t1\_fgrad$ .

R31 Record:  $itimeunit$

- $itimeunit$  is an integer flag indicating whether the times reported in NDM output files are in units of years ( $itimeunit=1$ ) or days ( $itimeunit=2$ ).

(Enter R32 if  $IPFLUX=0$ , and repeat R32  $nzone$  times i.e. one line for each sub-zone.)

R32 Record:  $S_{n\_avg}$

- $S_{n\_avg}$  is the initial average NAPL saturation for the corresponding NAPL sub-zone. This parameter is used to estimate the initial mass of NAPL in each sub-zone.

(Enter R33 if  $IPFLUX=3$ , and repeat R32  $nzone$  times i.e. one line for each sub-zone.)

R32 Record:  $S_{n\_avg}, k_{rw\_avg}$

- $S_{n\_avg}$  is the initial average NAPL saturation for the corresponding NAPL sub-zone. This parameter is used to estimate the initial mass of NAPL in each sub-zone.
- $k_{rw\_avg}$  is the initial average relative water permeability through the corresponding NAPL sub-zone. This parameter is used to estimate the average through-discharge ( $Md_{surf}$ ) for the sub-zone.

## 2.4 Example Input File

An image of an example input file is shown below. This example considers the case where NDM is used to estimate depth-varying NAPL saturation and relative water permeability ( $IPFLUX=1$ ), and there are four NAPL sub-zones with thicknesses ranging from 0.02 to 0.2 m. The length and width of all four sub-zones are equal (3 m by 3 m).

The example input file includes text comments at the right of each record, including the Record ID numbers starting with Record R01.

```

Example.IN - Notepad
File Edit Format View Help
1 'R01-ipflux (0=no, 1=yes, flux from first seg only, 2=yes, flux uniform from
0.04 0.85 'R02-Swr, Sm (ipflux=1 or 2)
34.0 72.0 'R03-IFT-nw, IFT-aw (dyne/cm) (ipflux=1 or 2)
4.26 'R04-alpha-aw (1/m) (ipflux=1 or 2)
4.23 'R05-n (ipflux=1 or 2)
1000. 'R06-water density (kg/m^3)(ipflux=1 or 2)
0.0025 'R07-delta-z for calculating Krw and qavg (ipflux=1 or 2)
1 'R08-Feff for flux through pool (ipflux=1 or 2)
4 'R09-number of NAPL sub-zones
1 0 'R10.1-source zone ID, ID of src affecting depletion rate
0.0 3.0 0.0 3.0 0.0 0.02 'R11.1-(x1,x2,y1,y2,z1,z2 in units of m)
1.0 1. 'R12.1-fsurf,fsurfdep
1.0 0 1. 1. 'R13.1-fio,jfeffmdl(0=constant; 1=linear; 2=exponential),feffm:
R04-H02
2 0 'R10.2-source zone ID, ID of src affecting depletion rate
0.0 3.0 0.0 3.0 0.0 0.05 'R11.2-(x1,x2,y1,y2,z1,z2 in units of m)
1.0 1. 'R12.2-fsurf,fsurfdep
1.0 0 1. 1. 'R13.2-fio,jfeffmdl(0=constant; 1=linear; 2=exponential),feffm:
R04-H05
3 0 'R10.3-source zone ID, ID of src affecting depletion rate
0.0 3.0 0.0 3.0 0.0 0.10 'R11.3-(x1,x2,y1,y2,z1,z2 in units of m)
1.0 1. 'R12.3-fsurf,fsurfdep
1.0 0 1. 1. 'R13.3-fio,jfeffmdl(0=constant; 1=linear; 2=exponential),feffm:
R04-H10
4 0 'R10.4-source zone ID, ID of src affecting depletion rate
0.0 3.0 0.0 3.0 0.0 0.20 'R11.4-(x1,x2,y1,y2,z1,z2 in units of m)
1.0 1. 'R12.4-fsurf,fsurfdep
1.0 0 1. 1. 'R13.4-fio,jfeffmdl(0=constant; 1=linear; 2=exponential),feffm:
R04-H20
1460.0 'R15-density (kg/m^3)
1400.0 'R16-solubility (mg/L)
7.0e-10 'R17-free-water diffusion coefficient (m^2/s)
1.00e-4 'R18-hydraulic conductivity (m/s)
0.0100 'R19-hydraulic gradient (m/m)
0.38 'R20-total porosity
0.00035 'R21-transverse dispersivity (m)
0.46 'R22-tortuosity
36500.0 'R23-simulation time (d)
10.0000 'R24-delta-t (d)
1.0000 'R25-minimum delta-t (d)
0.2 'R26-pool length discretization (m)
0 'R27-nperiods for enhanced dissolution
1.000 0 'R29-Fgrad, and flag to optionally re-calculate feffm (Md-thru decline rate) for
0.00000 36500.0 'R30-Fgrad time period
1 'R31-itimeunit=2 (1=years, 2=days) - for output times (all time input in units of

```

### 3. RUNNING NDM

Because the NAPL Depletion Model (NDM) is typically used to run sensitivity analyses, it has been set up to run in “batch” mode, meaning that multiple simulations may be conducted sequentially when running the model only once.

In addition to the individual simulation input file(s) that are needed to run NDM (refer to Section 2), there is also a more simple run input file which NDM reads to determine how many simulations are to be executed, the names of folders containing NDM simulation input and output files, and the names of each individual simulation file that is to be run. The name of this run input file must be: “NDM\_Batch\_Runs.IN”.

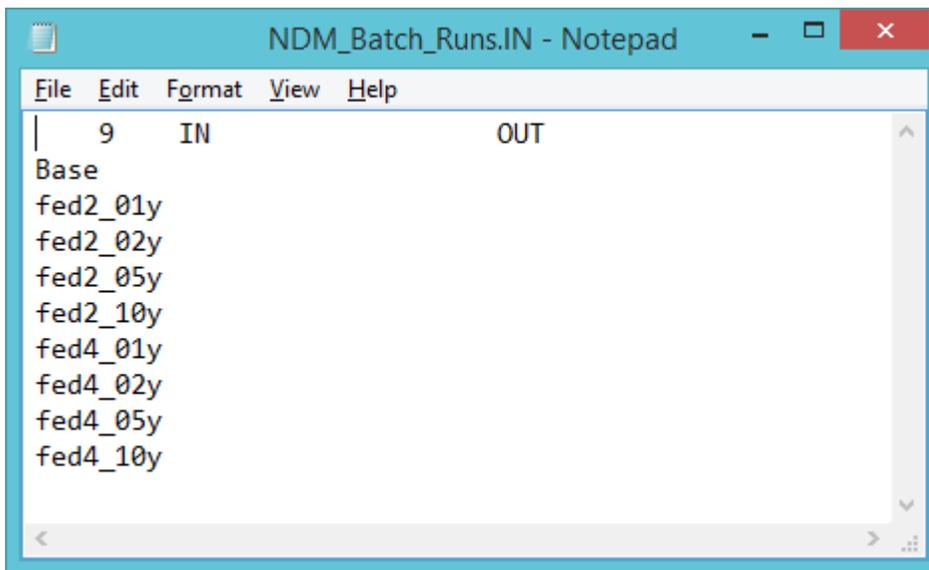
This run input file is free format, and individual records are defined below, followed by an image with an example of a RUN INPUT file.

Record 1: Names of folders containing input and output files. (maximum of 20 characters in each folder name.)

Record 2: *nrun* - Number of individual simulations to be run (minimum of 1).

(Repeat Record 3 *nrun* times i.e. one line for each individual simulation to be run.)

Record 3: Simulation input filename contained in the input file folder. (maximum of 45 characters in each input filename.)



#### 4. OUTPUT FORMAT

There are six types of output files associated with each individual NDM simulation, with file extensions from \*.1 through \*.6, inclusive. The first four output files contain data pertaining to the overall simulation (\*.1 through \*.4, inclusive). The last two output files (\*.5 and \*.6) are specific to each source zone. If a simulation includes multiple NAPL sub-zones, then one set of files (\*.5 and \*.6) will be output for each individual sub-zone. The contents of each type of output file are described below, followed by example images of the contents of each type of output file.

**Output File \*.1** – includes the specific discharge calculated for the overall source zone where permeability is not reduced due to NAPL presence, as well as specific calculations or input parameters for each sub-zone such as average  $S_n$  and  $k_{rw}$ , and the initial  $Md_{thru}$ . If IPFLUX=1 or 2, this file also contains the sub-zone calculations of depth-specific  $S_n$  and  $k_{rw}$ .

**Output File \*.2** – includes the following for each NAPL sub-zone: output filename for \*.5 and \*.6 output files, average  $S_n$ , coordinate extents and length, width, thickness; and the initial NAPL volume and mass.

**Output File \*.3** – simulated overall source zone output for each time step. The source zone data represents the combined mass and mass discharge for all sub-zones included in the simulation. Parameters output to the \*.3 text file include:

- Time (years or days, depending on the value of *itimeunit* input in Record R31 (see Section 2));
- Msrc (kg) – NAPL mass remaining in source zone;
- Md (kg/y) – mass discharge from source zone;
- MR – ratio of Msrc / Mo;
- MdR – ratio of Md / Md<sub>o</sub>;
- Msurf (kg) – total mass dissolved from NAPL sub-zone surface(s) during time step (not counting mass dissolved from enhanced dissolution based on  $f_{ed}$ );
- Mbio – not used in current version of NDM;
- Mthru (kg) – mass dissolved from through-discharge within NAPL sub-zones (not counting mass dissolved from enhanced dissolution based on  $f_{ed}$ , but including the effects of  $f_{grad}$ );
- Med (kg) – additional mass dissolved at surface or through NAPL sub-zones due to enhanced dissolution (when  $f_{ed} > 1$ );
- Mout (kg) – total mass dissolved from NAPL during time step.

$$Mout = Msurf + Mthru + Med$$

**Output File \*.4** – includes initial parameters for the overall source zone (i.e. combined NAPL sub-zone(s)), such as total length, width, height (based on global coordinate extents), average  $S_n$

and  $k_{rw}$  (geometric mean), total initial mass and mass discharge components for surface and through-discharge. The simulated remediation timeframe is output for each NAPL sub-zone (i.e. time to reach mass depletion in each sub-zone). The “Estimated RTF” is also calculated, based on a constant-length model. (This calculation is not relevant when using a box model, and only applies when a 1-D grid is used to represent a NAPL sub-zone where the length of the active portion of the sub-zone declines over time.) The number of time steps and calibrated  $\beta$  are also presented. ( $\beta$  is calibrated by using a least squared residual approach, and is not applicable when higher than 4.99 which is the maximum assumed  $\beta$  used by NDM during the calibration process.)

**Output File \*.5** – This file presents detailed data pertaining to a single NAPL sub-zone, and is output to facilitate checking of the mass and mass discharge data pertaining to each segment of a 1-D sub-zone grid, or a single segment if a box model approach is used for the sub-zone. The types of variables output in this sub-zone file are consistent with those listed above for the \*.3 output file.

**Output File \*.6** – a summary of output for each time step for a specific NAPL sub-zone, including the step number, simulated time (y), length of the sub-zone (m), NAPL mass remaining (kg), total mass discharge during the current time step (kg/y), and the ratio of mass remaining ( $MR = M/M_0$ ) and mass discharge reduction ( $MdR = Md/M_{d0}$ ).

Example of NDM Output File Type \*.1

```

R04.1 - Notepad
File Edit Format View Help
| NAPL SATURATION AND RELATIVE Krw IN POOLS
-----

Darcy velocity (m^3/m^2/d):    0.086
  ALPHA-aw (1/m):              4.260
  ALPHA-nw (1/m):              9.021
  Van Genuchten n:              4.230
  Van Genuchten m:              0.764
  Water density (kg/m^3):      1000.000
  Delta-rho (kg/m^3):          460.000
  Flow efficiency factor:       1.000

Sub-Zone ID:  1
-----

Initial dilution factor:      1.000
Dilution factor model:      Constant
  Z      Se      Sw      Sn      SeKrw      Krw      qw      Md
  (m)
0.0013  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15245E+00
0.0037  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15245E+00
0.0063  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15245E+00
0.0088  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15245E+00
0.0112  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15245E+00
0.0138  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15246E+00
0.0163  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15246E+00
0.0187  1.000    0.850    0.150    0.844    0.46E+00  0.398E-01  0.15246E+00

Average Sn in pool:           0.1500
Average Krw:                   0.4604E+00
Average Darcy Velocity (m/d):  0.3978E-01
Discharge through zone (kg/y): 0.12196E+01

Sub-Zone ID:  2
-----

```

### Example of NDM Output File Type \*.2

```
File Edit Format View Help
| Number of pools: 4

Sub-zone ID: 1
-----
                Output file:  R04-H02
Average NAPL saturation in pool:  0.1500
Md Multiplier for surface diss.:  1.00
                X1,X2,Lp (m):  0.00    3.00    3.00
                Y1,Y2,Width (m): 0.00    3.00    3.00
                Z1,Z2,Height (m): 0.000   0.020   0.020
NAPL volume in zone (L):          10.26021
NAPL mass in zone (kg):           14.97991

Sub-zone ID: 2
-----
                Output file:  R04-H05
Average NAPL saturation in pool:  0.1502
Md Multiplier for surface diss.:  1.00
                X1,X2,Lp (m):  0.00    3.00    3.00
                Y1,Y2,Width (m): 0.00    3.00    3.00
                Z1,Z2,Height (m): 0.000   0.050   0.050
NAPL volume in zone (L):          25.67603
NAPL mass in zone (kg):           37.48700

Sub-zone ID: 3
-----
                Output file:  R04-H10
Average NAPL saturation in pool:  0.1528
Md Multiplier for surface diss.:  1.00
                X1,X2,Lp (m):  0.00    3.00    3.00
                Y1,Y2,Width (m): 0.00    3.00    3.00
                Z1,Z2,Height (m): 0.000   0.100   0.100
NAPL volume in zone (L):          52.26778
NAPL mass in zone (kg):           76.31096

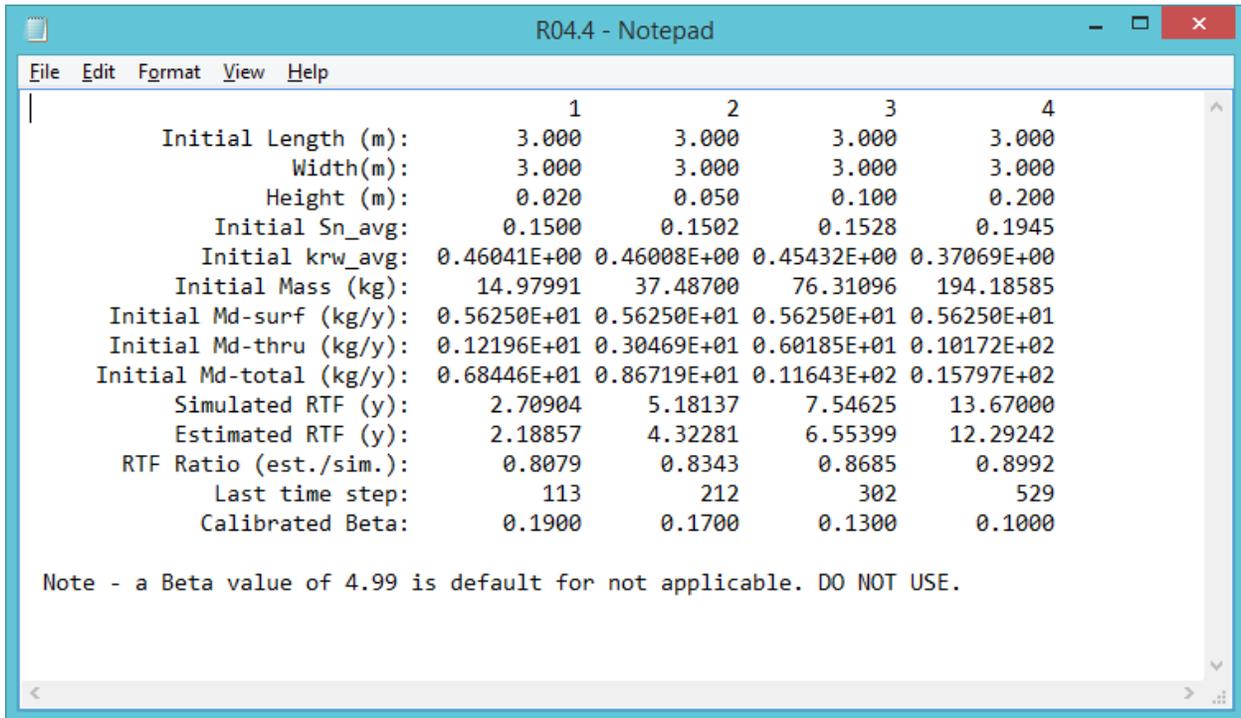
Sub-zone ID: 4
-----
                Output file:  R04-H20
```

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### Example of NDM Output File Type \*.3

Time (y)	Msrc (kg)	Md (Kg/y)	MR (%)	MdR (%)	Msurf (kg)	Mbio (kg)	Mthru (kg)	Med (kg)	Mout (kg)	Md/Msrc (1/y)
0.000E+00	0.323E+03	0.000E+00	0.100E+03	0.100E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.274E-01	0.322E+03	0.430E+02	0.996E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.133E+00
0.548E-01	0.321E+03	0.430E+02	0.993E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.134E+00
0.822E-01	0.319E+03	0.430E+02	0.989E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.134E+00
0.110E+00	0.318E+03	0.430E+02	0.985E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.135E+00
0.137E+00	0.317E+03	0.430E+02	0.982E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.135E+00
0.164E+00	0.316E+03	0.430E+02	0.978E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.136E+00
0.192E+00	0.315E+03	0.430E+02	0.974E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.136E+00
0.219E+00	0.314E+03	0.430E+02	0.971E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.137E+00
0.247E+00	0.312E+03	0.430E+02	0.967E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.138E+00
0.274E+00	0.311E+03	0.430E+02	0.964E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.138E+00
0.301E+00	0.310E+03	0.430E+02	0.960E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.139E+00
0.329E+00	0.309E+03	0.430E+02	0.956E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.139E+00
0.356E+00	0.308E+03	0.430E+02	0.953E+02	0.100E+03	0.616E+00	0.000E+00	0.560E+00	0.000E+00	0.118E+01	0.140E+00
0.374E+00	0.307E+03	0.430E+02	0.950E+02	0.100E+03	0.396E+00	0.000E+00	0.360E+00	0.000E+00	0.756E+00	0.140E+00
0.401E+00	0.306E+03	0.428E+02	0.947E+02	0.996E+02	0.611E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.140E+00
0.429E+00	0.305E+03	0.428E+02	0.943E+02	0.996E+02	0.611E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.140E+00
0.456E+00	0.303E+03	0.428E+02	0.939E+02	0.996E+02	0.611E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.141E+00
0.483E+00	0.302E+03	0.428E+02	0.936E+02	0.996E+02	0.611E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.142E+00
0.511E+00	0.301E+03	0.428E+02	0.932E+02	0.996E+02	0.611E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.142E+00
0.538E+00	0.300E+03	0.428E+02	0.929E+02	0.996E+02	0.611E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.143E+00
0.555E+00	0.299E+03	0.428E+02	0.926E+02	0.996E+02	0.386E+00	0.000E+00	0.354E+00	0.000E+00	0.741E+00	0.143E+00
0.583E+00	0.298E+03	0.426E+02	0.923E+02	0.991E+02	0.606E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.143E+00
0.610E+00	0.297E+03	0.426E+02	0.919E+02	0.991E+02	0.606E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.143E+00
0.638E+00	0.296E+03	0.426E+02	0.915E+02	0.991E+02	0.606E+00	0.000E+00	0.560E+00	0.000E+00	0.117E+01	0.144E+00
0.663E+00	0.295E+03	0.426E+02	0.912E+02	0.991E+02	0.569E+00	0.000E+00	0.526E+00	0.000E+00	0.109E+01	0.145E+00
0.681E+00	0.294E+03	0.424E+02	0.910E+02	0.987E+02	0.386E+00	0.000E+00	0.360E+00	0.000E+00	0.746E+00	0.144E+00
0.708E+00	0.293E+03	0.422E+02	0.906E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.144E+00
0.736E+00	0.291E+03	0.422E+02	0.903E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.145E+00
0.763E+00	0.290E+03	0.422E+02	0.899E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.145E+00
0.791E+00	0.289E+03	0.422E+02	0.895E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.146E+00
0.818E+00	0.288E+03	0.422E+02	0.892E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.146E+00
0.845E+00	0.287E+03	0.422E+02	0.888E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.147E+00
0.873E+00	0.286E+03	0.422E+02	0.885E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.148E+00
0.900E+00	0.285E+03	0.422E+02	0.881E+02	0.982E+02	0.595E+00	0.000E+00	0.560E+00	0.000E+00	0.116E+01	0.148E+00
0.907E+00	0.284E+03	0.422E+02	0.880E+02	0.982E+02	0.156E+00	0.000E+00	0.147E+00	0.000E+00	0.303E+00	0.148E+00
0.935E+00	0.283E+03	0.420E+02	0.877E+02	0.977E+02	0.590E+00	0.000E+00	0.560E+00	0.000E+00	0.115E+01	0.148E+00
0.962E+00	0.282E+03	0.420E+02	0.873E+02	0.977E+02	0.590E+00	0.000E+00	0.560E+00	0.000E+00	0.115E+01	0.149E+00
0.990E+00	0.281E+03	0.420E+02	0.869E+02	0.977E+02	0.590E+00	0.000E+00	0.560E+00	0.000E+00	0.115E+01	0.150E+00

### Example of NDM Output File Type \*.4



	1	2	3	4
Initial Length (m):	3.000	3.000	3.000	3.000
Width(m):	3.000	3.000	3.000	3.000
Height (m):	0.020	0.050	0.100	0.200
Initial Sn_avg:	0.1500	0.1502	0.1528	0.1945
Initial krw_avg:	0.46041E+00	0.46008E+00	0.45432E+00	0.37069E+00
Initial Mass (kg):	14.97991	37.48700	76.31096	194.18585
Initial Md-surf (kg/y):	0.56250E+01	0.56250E+01	0.56250E+01	0.56250E+01
Initial Md-thru (kg/y):	0.12196E+01	0.30469E+01	0.60185E+01	0.10172E+02
Initial Md-total (kg/y):	0.68446E+01	0.86719E+01	0.11643E+02	0.15797E+02
Simulated RTF (y):	2.70904	5.18137	7.54625	13.67000
Estimated RTF (y):	2.18857	4.32281	6.55399	12.29242
RTF Ratio (est./sim.):	0.8079	0.8343	0.8685	0.8992
Last time step:	113	212	302	529
Calibrated Beta:	0.1900	0.1700	0.1300	0.1000

Note - a Beta value of 4.99 is default for not applicable. DO NOT USE.

**Example of NDM Output File Type \*.5**

Feff	Step	Time (y)	Lp (m)	Description	1	2	3	4	
1.0000	1	0.027397	3.000	Starting_Mass_(kg)	0.999E+00	0.999E+00	0.999E+00	0.999E+00	
				M_surf_totLp (kg)	0.398E-01	0.563E-01	0.689E-01	0.796E-01	0.890E-01
				Msurf_at_seg_(kg)	0.398E-01	0.165E-01	0.126E-01	0.107E-01	0.939E-01
				Mbio_(kg)	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
				Mthru_(kg)	0.334E-01	0.000E+00	0.000E+00	0.000E+00	0.000E+00
				Med_at_seg_(kg)	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
				Mout_(kg)	0.732E-01	0.165E-01	0.126E-01	0.107E-01	0.939E-01
				Ending_Mass_(kg)	0.925E+00	0.982E+00	0.986E+00	0.988E+00	0.989E+00
				Md(kg/y)	0.267E+01	0.602E+00	0.462E+00	0.389E+00	0.343E+00
				1.0000	2	0.054795	3.000	Starting_Mass_(kg)	0.925E+00
M_surf_totLp (kg)	0.398E-01	0.563E-01	0.689E-01					0.796E-01	0.890E-01
Msurf_at_seg_(kg)	0.398E-01	0.165E-01	0.126E-01					0.107E-01	0.939E-01
Mbio_(kg)	0.000E+00	0.000E+00	0.000E+00					0.000E+00	0.000E+00
Mthru_(kg)	0.334E-01	0.000E+00	0.000E+00					0.000E+00	0.000E+00
Med_at_seg_(kg)	0.000E+00	0.000E+00	0.000E+00					0.000E+00	0.000E+00
Mout_(kg)	0.732E-01	0.165E-01	0.126E-01					0.107E-01	0.939E-01
Ending_Mass_(kg)	0.852E+00	0.966E+00	0.973E+00					0.977E+00	0.980E+00
Md(kg/y)	0.267E+01	0.602E+00	0.462E+00					0.389E+00	0.343E+00
1.0000	3	0.082192	3.000					Starting_Mass_(kg)	0.852E+00
				M_surf_totLp (kg)	0.398E-01	0.563E-01	0.689E-01	0.796E-01	0.890E-01
				Msurf_at_seg_(kg)	0.398E-01	0.165E-01	0.126E-01	0.107E-01	0.939E-01
				Mbio_(kg)	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
				Mthru_(kg)	0.334E-01	0.000E+00	0.000E+00	0.000E+00	0.000E+00
				Med_at_seg_(kg)	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
				Mout_(kg)	0.732E-01	0.165E-01	0.126E-01	0.107E-01	0.939E-01
				Ending_Mass_(kg)	0.779E+00	0.949E+00	0.961E+00	0.967E+00	0.970E+00
				Md(kg/y)	0.267E+01	0.602E+00	0.462E+00	0.389E+00	0.343E+00
				1.0000	4	0.109589	3.000	Starting_Mass_(kg)	0.779E+00
M_surf_totLp (kg)	0.398E-01	0.563E-01	0.689E-01					0.796E-01	0.890E-01
Msurf_at_seg_(kg)	0.398E-01	0.165E-01	0.126E-01					0.107E-01	0.939E-01
Mbio_(kg)	0.000E+00	0.000E+00	0.000E+00					0.000E+00	0.000E+00
Mthru_(kg)	0.334E-01	0.000E+00	0.000E+00					0.000E+00	0.000E+00
Med_at_seg_(kg)	0.000E+00	0.000E+00	0.000E+00					0.000E+00	0.000E+00
Mout_(kg)	0.732E-01	0.165E-01	0.126E-01					0.107E-01	0.939E-01
Ending_Mass_(kg)	0.706E+00	0.933E+00	0.948E+00					0.956E+00	0.961E+00
Md(kg/y)	0.267E+01	0.602E+00	0.462E+00					0.389E+00	0.343E+00

**Example of NDM Output File Type \*.6**

Step	T (y)	L (m)	M (kg)	Md (kg/y)	MR	MdR
1	0.02740	3.000	14.79239	0.68446E+01	0.987482	1.000000
2	0.05479	3.000	14.60486	0.68446E+01	0.974963	1.000000
3	0.08219	3.000	14.41734	0.68446E+01	0.962445	1.000000
4	0.10959	3.000	14.22982	0.68446E+01	0.949927	1.000000
5	0.13699	3.000	14.04229	0.68446E+01	0.937408	1.000000
6	0.16438	3.000	13.85477	0.68446E+01	0.924890	1.000000
7	0.19178	3.000	13.66725	0.68446E+01	0.912372	1.000000
8	0.21918	3.000	13.47972	0.68446E+01	0.899853	1.000000
9	0.24658	3.000	13.29220	0.68446E+01	0.887335	1.000000
10	0.27397	3.000	13.10468	0.68446E+01	0.874817	1.000000
11	0.30137	3.000	12.91715	0.68446E+01	0.862298	1.000000
12	0.32877	3.000	12.72963	0.68446E+01	0.849780	1.000000
13	0.35616	3.000	12.54211	0.68446E+01	0.837262	1.000000
14	0.37375	3.000	12.42173	0.68446E+01	0.829226	1.000000
15	0.40115	2.800	12.23943	0.66539E+01	0.817056	0.972134
16	0.42855	2.800	12.05713	0.66539E+01	0.804887	0.972134
17	0.45594	2.800	11.87483	0.66539E+01	0.792717	0.972134
18	0.48334	2.800	11.69254	0.66539E+01	0.780548	0.972134
19	0.51074	2.800	11.51024	0.66539E+01	0.768378	0.972134
20	0.53814	2.800	11.32794	0.66539E+01	0.756209	0.972134
21	0.55545	2.800	11.21273	0.66539E+01	0.748518	0.972134
22	0.58285	2.800	11.03043	0.66539E+01	0.736348	0.972134
23	0.61025	2.800	10.84813	0.66539E+01	0.724179	0.972134
24	0.63764	2.800	10.66583	0.66539E+01	0.712009	0.972134
25	0.66336	2.800	10.49475	0.66539E+01	0.700588	0.972134
26	0.68097	2.600	10.38103	0.64562E+01	0.692997	0.943253
27	0.70837	2.600	10.20415	0.64562E+01	0.681189	0.943253
28	0.73576	2.600	10.02727	0.64562E+01	0.669381	0.943253
29	0.76316	2.600	9.85039	0.64562E+01	0.657573	0.943253
30	0.79056	2.600	9.67350	0.64562E+01	0.645765	0.943253
31	0.81795	2.600	9.49662	0.64562E+01	0.633957	0.943253
32	0.84535	2.600	9.31974	0.64562E+01	0.622149	0.943253
33	0.87275	2.600	9.14286	0.64562E+01	0.610341	0.943253
34	0.90015	2.600	8.96598	0.64562E+01	0.598533	0.943253
35	0.90733	2.600	8.91957	0.64562E+01	0.595435	0.943253
36	0.93473	2.400	8.74832	0.62508E+01	0.584003	0.913239
37	0.96213	2.400	8.57706	0.62508E+01	0.572571	0.913239
38	0.98953	2.400	8.40581	0.62508E+01	0.561139	0.913239
39	1.01692	2.400	8.23456	0.62508E+01	0.549707	0.913239
40	1.03663	2.400	8.11135	0.62508E+01	0.541482	0.913239
41	1.06403	2.400	7.94010	0.62508E+01	0.530050	0.913239