

**Guidance for Using the SESOIL and AT123D Models  
to Develop Site Specific Impact to Ground Water  
Soil Remediation Standards**

June 2, 2008

## **Introduction**

The person responsible for conducting the remediation may use the SESOIL vadose zone model coupled with the Analytical Transient, One, Two, and Three-Dimensional ground water flow model (AT123D) to develop a site-specific Impact to Ground Water Soil Remediation Standard. SESOIL is used to model vadose zone soil contamination and the source of ground water contamination. SESOIL must be run as outlined in the Department's SESOIL modeling guidance. The proposed soil contaminant mass distribution entered in SESOIL will be used to establish the contaminant load to be entered in the AT123D ground water model.

AT123D is used to model ground water concentrations at two compliance points; the downgradient edge of the vadose zone contaminant source area, and a downgradient compliance point located at the edge of the delineated ground water contaminant plume. Ground water monitoring is required to confirm the predictions of the AT123D model.

The original AT123D code is available free of charge but it lacks a user interface. Commercially available software packages contain both the source code and interfaces to assist users in the selection and preparation of input data and for viewing and presenting model output.

The vadose zone contaminant mass distribution and concentration modeled in SESOIL will be an acceptable impact to ground water soil remediation standard provided the AT123D modeled results meet the requirements outlined below.

## **AT123D Modeling Prerequisites**

The coupled SESOIL/AT123D model simulates impacts to ground water and contaminant fate and transport in ground water from specified vadose zone soil contamination conditions. To develop a site-specific impact to ground water soil remediation standard the models are used in a trial and error fashion to calculate an acceptable soil concentration for certain acceptable ground water contaminant plume conditions. This method of calculating a Site Specific Impact to Ground Water Soil Remediation Standard may be used only when the following conditions have been met:

1. Ground water quality is currently degraded by contamination migrating from soil at the area of concern;
2. Ground water contaminated above the applicable ground water remediation standard will not reach the nearest downgradient receptor, as estimated by an appropriate ground water flow/contaminant transport model selected pursuant to N.J.A.C. 7:26E-4.4(h)3iv;
3. Contaminant concentrations in ground water do not present a vapor intrusion risk to any receptors. This determination must be made on a site-by-site basis;
4. Predicted impacts to potential receptors are consistent with the current and potential ground water uses based on a 25-year planning horizon as projected by local and county land use documents. This must include, without limitation, information pertaining to the existence of

water lines, proposed future installation of water lines, local and/or county ordinances restricting installation of potable wells;

### **AT123D Input Parameter Limitations**

The Department has assigned default input parameter values for several model variables while the remainder of the model input parameters must be measured at the site. Input parameters are established as follows:

1. The following AT123D input parameters must be measured or estimated using site specific data:
  - hydraulic conductivity;
  - hydraulic gradient;
  - Organic carbon content must be measured using the Lloyd Khan method, “Determination of Total Organic Carbon in Sediment”. U.S. Environmental Protection Agency, Region II, Edison, New Jersey (1998). This method is available at <http://www.epa.gov/region2/qa/documents.htm>;
  - Longitudinal dispersivity must be estimated based on the measured plume length using the following equation (Xu and Eckstein 1995):

$$\alpha_L = 0.83(\log_{10} L)^{2.414}$$

where:

$\alpha_L$  = longitudinal dispersivity

L = length of contaminant plume

Transverse dispersivity must be calculated as 1/10th the longitudinal dispersivity (Gelhar et al. 1992)

Vertical dispersivity must be calculated as 1/100th the longitudinal dispersivity (Gelhar et al. 1992)

- Aquifer thickness must be measured in the field by logging continuous core in accordance with the Department’s Field Sampling Procedures Manual or must be determined using available data from the New Jersey Geological Survey or the United States Geological Survey where available.
2. The following AT123D input parameters must be estimated based on aquifer material texture:
    - Bulk density must be determined based on aquifer material texture. Typical values for bulk density relative to soil texture are given in Table I of the AT123D documentation (Yeh 1981). They are:

<b>Texture</b>	<b>Bulk Density (g/cm<sup>3</sup>)</b>
Sand	1.18~1.58
Silt	1.29~1.8
Clay	1.4~2.2

- Effective porosity must be measured or determined based on aquifer material texture. Typical values for effective porosity relative to soil texture are given in Table I of the AT123D documentation (Yeh 1981). They are:

<b>Texture</b>	<b>Effective Porosity</b>
Sand	0.1~0.3
Silt	0.05~0.1
Clay	0.03~0.05

3. The following input parameters must be fixed as follows:
  - First-Order decay coefficient must be set to zero
  - Aquifer width must be set to “infinite”
  - Eigen values must be set between 500 and 1,000 and may be used to calibrate the model
  - Error tolerance must be set to 0.001
  
4. The SESOIL model must set the following AT123D input parameters.
  - AT123D release coordinates must be identical to SESOIL source configuration.
  - AT123D load parameters must be set in the SESOIL model
  - The SESOIL contaminant source must be modeled as a horizontal area (planar) source located at the top of the water table in AT123D.
  
5. The following chemical properties must be copied from the Departments list of chemical properties (see the Department’s Basis and Background Document for the Inhalation Soil Remediation Standards pathway for Chemical Properties):
  - K<sub>oc</sub> value
  - K<sub>d</sub> value
  - Water diffusion coefficient

### **AT123D Ground Water Model Compliance Points**

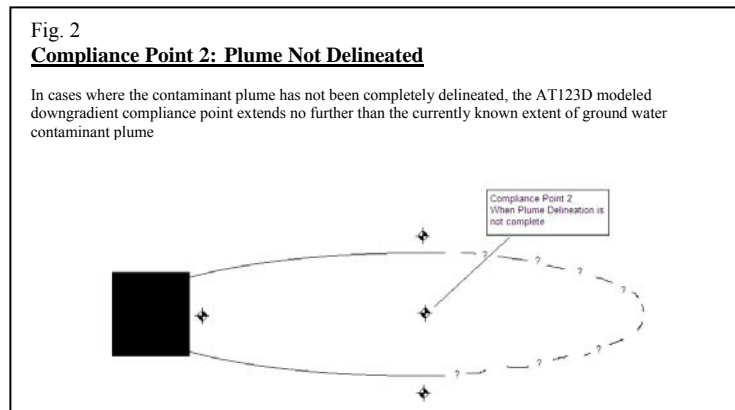
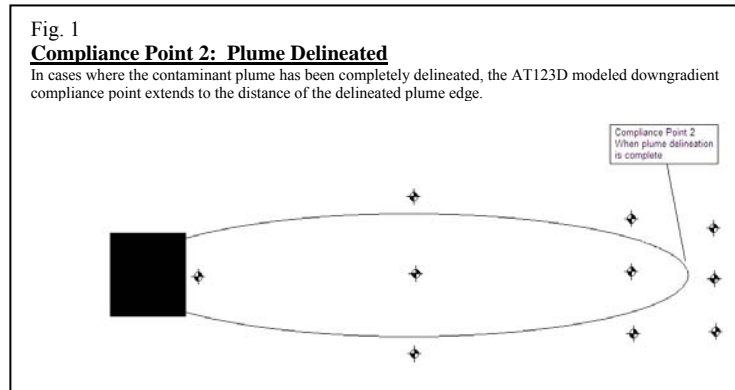
Two compliance points must be established in the AT123D model. They are:

- **Compliance Point 1:** One modeled compliance point must be located at the downgradient edge of the SESOIL modeled contaminated soil. This compliance point must be at the plume centerline at the top of the water table.

The AT123D predicted ground water contaminant concentration resulting from the SESOIL modeled soil contamination must meet the health based ground water quality criterion at Compliance Point 1 within five years.

- **Compliance Point 2:** The second AT123D modeled compliance point must be located; at the downgradient edge of the delineated ground water contaminant plume in cases where ground water contamination has been delineated (fig. 1), or at the currently known extent of the contaminant plume in cases where ground water contamination has not been completely delineated.

The AT123D predicted ground water contaminant concentration resulting from the SESOIL modeled soil contamination must never exceed the health based ground water quality criterion at Compliance Point 2.



### **Establishing the Site Specific Impact to Ground Water Soil Remediation Standard**

The SESOIL/AT123D models must be run to determine if the vadose zone contaminant mass distribution/concentration results in acceptable ground water conditions for both compliance points outlined above. If both compliance points are NOT met, the SESOIL/AT123D models must be re-run with a lower vadose zone contaminant mass distribution until both AT123D modeled ground water compliance points are met.

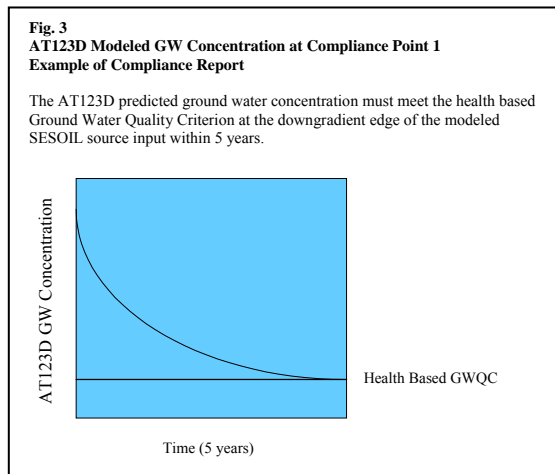
When both compliance points are met, calculate the site-specific impact to ground water soil remediation standard using the SESOIL input parameter POLIN ( $\mu\text{g}/\text{cm}^2$ ) input parameter in the following equation:

$$X \text{ ug/g (ppm)} = \text{POLIN (ug/cm}^2\text{)} / \{\text{SESOL layer thickness (cm)} * \text{soil bulk density (g/cm}^3\text{)}\}$$

### SESOL/AT123D Model Reporting Requirements

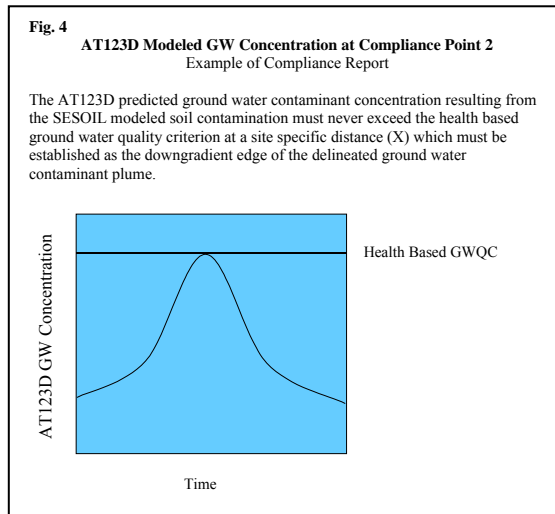
AT123D modeling results must be submitted to the Department. A SESOIL/AT123D modeling report must be submitted to the Department that includes:

1. Two AT123D modeled compliance point graphs as follows:
  - One graph at Compliance Point One. This graph must show that the AT123D predicted



ground water contaminant concentration meets the health based ground water quality criterion at Compliance Point 1 within five years (see fig. 3).

- One graph at Compliance Point 2. This graph must show that the AT123D predicted



ground water contaminant concentration never exceeds the health based ground water quality criterion at Compliance Point 2 (see fig. 4). AT123D must be run, at a minimum, until the peak ground water concentration is achieved at Compliance Point 2.

2. An AT123D conceptual model form. See Attachment 1 of this guidance.
3. An AT123D model documentation form. See Attachment 1 of this guidance.

### **Ground Water Monitoring Requirements**

- A Department approved ground water monitoring program designed to monitor the predictions of the AT123D model must be implemented.
- Additional remediation is required when ground monitoring does not agree with AT123D predictions at either the source area or downgradient compliance point.

### **References**

Gelhar, L.W., Welty, C. and Rehfeldt, K.R. (1992). A Critical Review of Data on Field-Scale Dispersion in Aquifers. *Water Resources Res.* 28(7): 1955-1974.

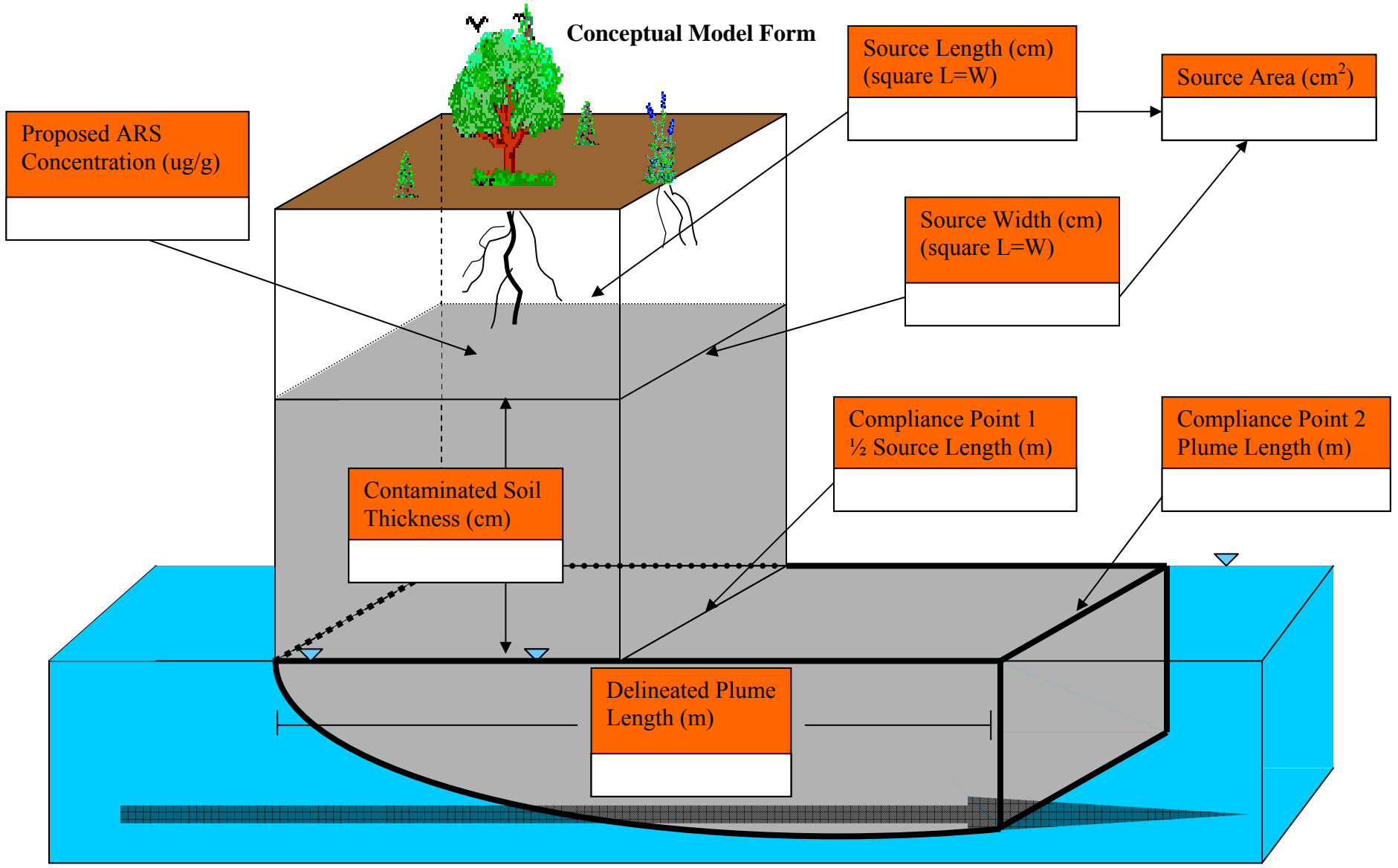
Xu, M. and Eckstein, Y. (1995). Use of Weighted Least-Squares Method in Evaluation of the Relationship Between Dispersivity and Field Scale. *Ground Water* 33(6):905-908.

Yeh, G.T. (1981). AT123D: Analytical Transient One-, Two-, and Three-Dimensional Simulation of Waste Transport in the Aquifer System. Publication No. 1439, Environmental Sciences Division, Oak Ridge National Laboratory: Oak Ridge, TN, ORNL-5602.



# Attachment 1

## Conceptual Model Form



## Aquifer Data Form

	Source of Value	Value Used in Model
Hydraulic Conductivity (m/hr) <sup>a</sup>		
Hydraulic Gradient <sup>b</sup>		
Effective Porosity <sup>c</sup>		
Soil Bulk Density (kg/m <sup>3</sup> ) <sup>d</sup>	Yeh AT123D Model	
Length of Delineated Plume <sup>e</sup>		
Longitudinal Dispersivity(m) <sup>f</sup>		
Transverse Dispersivity(m) <sup>g</sup>		
Vertical Dispersivity(m) <sup>h</sup>		
Aquifer Width (m) <sup>i</sup>	FIXED	Infinite
Aquifer Depth (m) <sup>j</sup>		
Number of Eigen values <sup>k</sup>	500-1000	
Steady State Error Tolerance <sup>l</sup>	FIXED	0.001

- a Determine site specific hydraulic conductivity, pursuant to N.J.A.C. 7:26E-4.4(h)3iii. Submit results of slug tests and or pumping tests as an attachment to this documentation.
- b Determine hydraulic gradient, pursuant to N.J.A.C. 7:26E-4.4(h)3iii. Submit site map with ground water contours as an attachment to this documentation.
- c Use the effective porosity for the soil type as indicated by the model documentation or site specific measurement.
- d Bulk density must be determined based on aquifer material texture. Typical values for bulk density are given in Table I of the AT123D documentation (Yeh 1981).
- e The length of the delineated ground water plume based on site ground water quality data.
- f Longitudinal dispersivity must be estimated based on the measured plume length using the following equation (Xu et al. 1995):

$$\alpha_L = 0.83(\log_{10} L)^{2.414}$$

where:

$\alpha_L$  = longitudinal dispersivity

L = length of contaminant plume

- g Transverse dispersivity must be calculated as 1/10<sup>th</sup> the longitudinal dispersivity (Gelhar et al. 1992)
- h Vertical dispersivity must be calculated as 1/100<sup>th</sup> the longitudinal dispersivity (Gelhar et al. 1992)
- i Aquifer width must be set to "infinite".
- j Aquifer thickness must be measured in the field by logging continuous core in accordance with the Department's Field Sampling Procedures Manual or must be determined using available data from the New Jersey Geological Survey or the United States Geological Survey where available.
- k Eigen values must be set between 500 and 1,000.
- l Error tolerance must be set to 0.001.

### Source Dimensions, Soil and Chemical Properties Form

Release Coordinates	Source	Value Used in Model
X (meters) <sup>a</sup>	Use SESOIL Values	
Y (meters) <sup>a</sup>	Use SESOIL Values	
Z (meters) <sup>a</sup>	Horizontal Plane Source Required	
Soil Organic Carbon <sup>b</sup>		
K <sub>oc</sub> (mL/g) <sup>c</sup>	NJDEP Inhalation Soil Remediation Standards	
K <sub>d</sub> (mL/g) <sup>c</sup>	NJDEP Inhalation Soil Remediation Standards	
Water Diffusion Coefficient (m <sup>2</sup> /hr) <sup>c</sup>	NJDEP Inhalation Soil Remediation Standards	
First Order Decay <sup>d</sup>	FIXED	0

<sup>a</sup> AT123D release coordinates must be identical to SESOIL source configuration.

<sup>b</sup> Organic carbon content must be determined using the Lloyd Kahn Method. A default value of 0.2 percent (0.002) may also be used. Submit the results of the organic carbon content analysis as an attachment to this documentation.

<sup>c</sup> NJDEP Inhalation Pathway Soil Remediation Standards Basis and Background

<sup>d</sup> First-Order decay coefficient must be set to zero