Notes on the GoldSim Plume Function

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	Printed Name	Signature	Date
Title: Notes on the GoldSim Plume Function			
Description: This documents calculation details of the GoldSim plume function, as interpreted from the source code: PlumeFuncNode.cpp			
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Remarks:

24 Sep 08 – Corrected a typo in the in-line equations in Section 2.0, and added the image source illustration in Figure 2. – JT

28 Sep 08 – Added Figure 1, and made clarifying edits to text. – IM

13 Sep 10 – Corrected the text in sections 3.2.3 and 3.3.3 to clarify the lack of dilution in cases where the observations point is within the plume.

22 Aug 2014 – Revised for release as a Neptune NAC document. - JT

CONTENTS

FIGURES

1.0   Introduction

The plume() function in GoldSim produces a value between 0 and 1, which is to be used as a multiplier applied to the concentration at the end of a Pipe Pathway element in order to account for lateral and vertical dispersion when the Pipe is intended to represent an aquifer, for example. These are not allowed in the Pipe calculation, which has a specified cross-sectional area and circumference around impermeable walls—more like a straw than an aquifer. A point of observation is identified in three dimensions, X_L, X_T, and X_V, corresponding to longitudinal, transverse (lateral), and vertical locations in a coordinate system based on the center of the upstream edge of the source zone and aligned with the flow of water in the Pipe. The longitudinal location X_L corresponds to the end of the Pipe. Figure 1 indicates the geometry that is assumed.
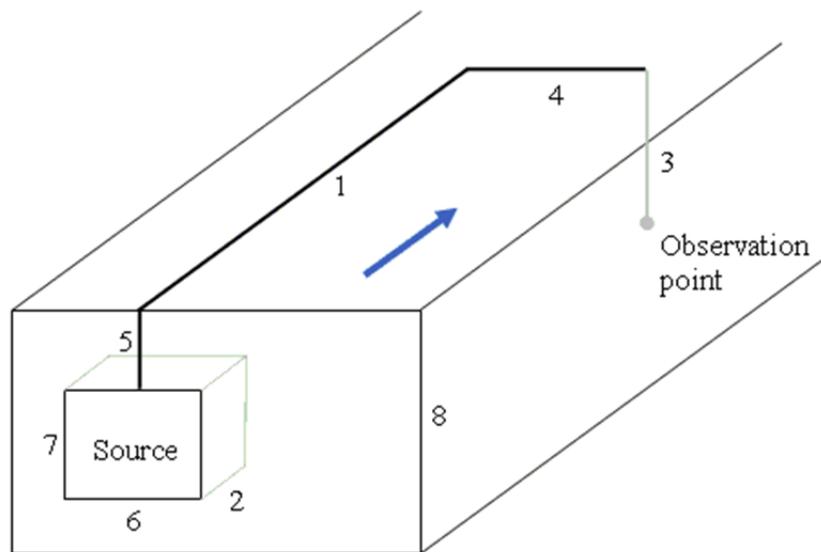

Figure 1. Plume function geometry (courtesy of GoldSim Technology Group).

It should be noted that as of GoldSim version 10, the plume() function was upgraded to handle inputs that are GoldSim vectors and matrices. These calculations are simply term-by-term calculations, as if the plume() function had been applied to each term independently. This is useful in GoldSim programming, since a single use of the function can be used to determine plume corrections at a large number of independent locations.

GoldSim contaminant transport (CT) models developed in support of Performance Assessments (PAs) at the Savannah River Site (SRS) have applied this plume "correction" to concentrations at the end of a "column" of Cell Pathway elements, also used to represent an aquifer. This technique offers several advantages to the Pipe, the discussion of which is beyond the scope of this document. For simplicity, references to "Pipe" in the remainder of this document could be replaced with "column of Cells," except where noted.

The plume() function has eleven arguments, in the following order. The corresponding items in Figure 1 are shown in brackets:

X_L length of the Pipe, or, in a Cell column, the longitudinal position of the observation point, which should be made coincident with the center of the Cell nearest the desired column length [1]

A cross-sectional area of the Pipe

L_s length of the source parallel to the flow direction [2]

X_V vertical position of the observation point [3]

X_T transverse position of the observation point [4]

D_s vertical depth to the top of the source from the top of the aquifer [5]

W_s width of the source, transverse to the aquifer flow [6]

b_s thickness of the source [7]

b thickness of the aquifer [8]

α_T dispersivity in the transverse direction

α_V dispersivity in the vertical direction

All these inputs except the area have dimensions of L (length), with the area A in L^2. GoldSim evaluates all arguments to ensure consistent dimensions and units, so this need not be addressed further in this discussion.

The dispersivity in the longitudinal direction does not enter this equation directly, since it is included in the Pipe solution of concentration. For the column of Cells, longitudinal dispersion is handled numerically. Other time- and chemical-related parameters are also handled in the contaminant transport (CT) calculations, as discussed in the following section.

2.0   Assumptions and Boundary Conditions

A clever aspect of the plume() function is that it does not include a full-blown plume calculation, which would necessarily involve transport-relevant parameters like retardation, decay and ingrowth, and such. These are all handled by the transport Pathways (Pipe or Cell column), so all the plume() function needs to do is modify the spatial distribution of contamination. It does so by providing the scalar by which the end-of-the-Pipe concentration is modified, effectively dispersing the straw-like Pipe calculation in space.

Boundary conditions include the assumption of zero concentration at infinite distance, and a special handling of the output of the GoldSim Pipe element. The Pipe element provides a contaminant concentration (in dimensions of M/L^3) at the end of the Pipe expressed as a mass flux discharge per flow rate, that is, $\dfrac{\text{mass flux discharge}(M/T)}{\text{Pipe flow rate }(L^3/T)}$. As discussed below (in Section 3.1.1) the factor calculated by the plume function includes the cross-sectional area of the Pipe, A, so that the calculated Pipe concentration is thereby a mass per volume (M/L^3):

$\dfrac{\text{areal mass flux}(M/TL^2)}{\text{Darcy velocity }(L/T)}$.

3.0   Functionality of PlumeFuncNode.cpp

PlumeFuncNode.cpp is the C++ source code for the plume() function, kindly provided by GoldSim Technology Group for the purposes of this documentation.

3.1   Setting Up

After running all arguments through the GoldSim Eval() function, which assures that they all have proper numeric and dimensionally consistent values, and after determining whether the arguments are scalars, or vectors or matrices of scalar values, the plume() function begins constructing the answer that it will return—the value (or vector or matrix of such values) between 0 and 1 that is to be multiplied by the end-of-the-Pipe concentration to arrive at a concentration at the designated observation location(s). This result is called dilute within the function.

3.1.1 Initial Value

The value of dilute is calculated in parts, with all parts multiplied in the end, as described in Section 3.4. Initially, we set dilute$_{init}$ to the cross-sectional area of the Pipe, A. As the value of dilute is modified for dispersion effects in the subsequent calculations, it is twice divided by a length, leaving it dimensionless. In effect, this counteracts the use of cross-sectional area in the Pipe calculation. In the development of this calculation, we shall keep track of the various parts of the equation for dilute that are proffered. So far, we have

$$dilute_{init} = A, \tag{1}$$

where A is the cross-sectional area of the Pipe or column of Cell Pathway elements. Equation (1) converts the end-of-the-Pipe concentration to the total mass flux leaving the Pipe divided by the total flow in the pipe, as shown in Section 2.0. In order to convert that to a concentration at an observation point, it needs to be converted to the mass flux rate across a (small) unit area at the monitored location, divided by the Darcy velocity. This is done by multiplying by the 2-D spatial density at the observation point, for the density function in the plane perpendicular to the flow, of a unit mass input uniformly distributed over the source region, as dispersed after traveling the specified advective transport distance.

3.1.2 Relative Length Adjustment

The length X_L of the Pipe is assumed to be measured from the upstream end of the source. It is then modified in order to center the source at the longitudinal "origin." The following cases are considered:

Case: if $X_L <= 0$, then the point of observation is upstream of the source, and

$$dilute_{init} = 0 \tag{2}$$

At this point, X_L is also set to $X_L = 1$ (with units of m implied), to preclude divide-by-zero errors.

Case: if $X_L > L_s$, then the point of observation is downstream of the source, and X_L is adjusted thus

$$X_L^* = X_L - \frac{L_s}{2} \qquad (3)$$

so that the "source" end of the Pipe is moved to the center of the source. This adjusted length is denoted X_L^*.

Case: if neither of the above cases is true, then $X_L <= L_s$, meaning that the Pipe is shorter than the source. In this case, X_L is halved:

$$X_L^* = \frac{X_L}{2} \qquad (4)$$

This, in effect, truncates the source to be the length of the Pipe, and the upstream end is moved to the center of the source. In the latter two cases, the value of dilute$_{init}$ remains set equal to A.

3.2   Transverse Dispersion

In accounting for transverse dispersion, various cases are considered: a narrow (point) source, a wide source, and the case where the observation point is too far afield to be considered part of the plume. The cases are presented as follows:

3.2.1 Narrow (Point) Source

A narrow source triggers the point-source solution for transverse dispersion. In comparing the source width W_s to the transverse standard deviation of the plume $\sqrt{2\alpha_T X_L^*}$, a narrow source solution is used if

$$W_s < \frac{\sqrt{2\alpha_T X_L^*}}{100}, \qquad (5)$$

where the value of 100 is "hard coded" into the function, based on the judgment of the developer.

In this case, the point-source solution is used, and the transverse portion of dilute, hereafter called dilute$_T$, assumes the form of the normal distribution density function:

$$dilute_T = \frac{\exp\left[-\frac{\left(\frac{X_T}{\sqrt{2\alpha_T X_L^*}}\right)^2}{2}\right]}{\sqrt{2\pi}\sqrt{2\alpha_T X_L^*}} = \frac{\exp\left(-\frac{X_T^2}{4\alpha_T X_L^*}\right)}{\sqrt{4\pi\alpha_T X_L^*}} \qquad (6)$$

Keep in mind that dilute$_T$ is to be multiplied by dilute$_{init}$ as defined in Section 3.1 in order to arrive at the final answer.

3.2.2 Wide (General) Source

A "wide" source, the general full solution, is indicated if the following is true:

$$W_s < 1,000,000 \times \sqrt{2\alpha_T X_L^*} \tag{7}$$

This applies in the case where a source is not negligibly wide, and dispersion cannot be ignored. In this case, the point-source solution is integrated over the width of the source, and dilute$_T$ is

$$dilute_T = \frac{\mathrm{erf}\left(\dfrac{X_T + \dfrac{W_s}{2}}{\sqrt{4\alpha_T X_L^*}}\right) - \mathrm{erf}\left(\dfrac{X_T - \dfrac{W_s}{2}}{\sqrt{4\alpha_T X_L^*}}\right)}{2W_s} \tag{8}$$

3.2.3 Negligible Transverse Dispersion

If neither of the previous two situations occurs, then the transverse dispersion is negligible (i.e. the plume does not spread at all), and the observation point is tested to see if it is inside or outside of the plume. The test for being outside the plume is if the transverse location of the observation point is greater than half the source width from the plume centerline:

$$|X_T| > \frac{W_s}{2} \tag{9}$$

In effect, if the observation location is further from the centerline than the edge of the source, then it is out of the plume. If equation (9) holds true, then the point is outside the plume, and dilute$_T$ (and therefore dilute, as described in Section 3.4) is set to zero. Otherwise dilute$_T$ is set equal to the inverse of the source width, W_s.

3.3   Vertical Dispersion

In the case of dispersion in the vertical direction, again perpendicular to flow, five cases are considered: a fully mixed aquifer, a thin source, a thick source, no source geometry adjustment, and the case where the observation point is too shallow or deep to be considered part of the plume. Since the flow field is assumed to have natural boundaries on the top and bottom, but not on the sides, the calculation of concentrations at vertical locations within the aquifer takes advantage of superposed image source mathematics. Note that, unlike the transverse case, where the source is always centered horizontally, the vertical position of the source may be anywhere within the flow field. Similar to the transverse case, however, the vertical aspect of the source may be relatively thin or thick compared to vertical dispersion. The cases are presented as follows:

3.3.1 Fully Mixed Aquifer

If an aquifer (or, more generically, the flow field) is sufficiently thin in comparison to dispersion in the vertical direction, then the flow field can be assumed to be fully mixed in the vertical direction, and no image sources are used. That is, if we compare the aquifer thickness *b* to the vertical standard deviation of the plume $\sqrt{2\alpha_V X_L^*}$, and

$$b < \frac{\sqrt{2\alpha_V X_L^*}}{3} \tag{10}$$

(where again the value of 3 is chosen by the developer) then dilute is merely divided by that thickness, so that the vertical term dilute$_V$ becomes

$$dilute_V = \frac{1}{b} \tag{11}$$

3.3.2 Use of Image Sources

If the aquifer is not sufficiently thin to be considered fully mixed, it is examined for suitability in using nine image sources to refine the vertical distribution of contaminants, as illustrated in Figure 2. In effect, the plume from each image source, identical to the original source, is offset and its contribution to the concentrations in the aquifer is superimposed. This has the same effect as "bouncing" the original plume off the top and bottom of the aquifer.

Image sources are invoked if, analogous to equation (7),

$$b < 1{,}000{,}000 \times \sqrt{2\alpha_V X_L^*} \tag{12}$$

where the value of 1,000,000 is selected by the developer. If this inequality is not true, then no image sources are used, and no further changes are made to dilute for vertical dispersion (and the following sections testing for a thin or thick source are also precluded). Like the transverse case presented in equation (7), equation (12) is true only for very small dispersivities.
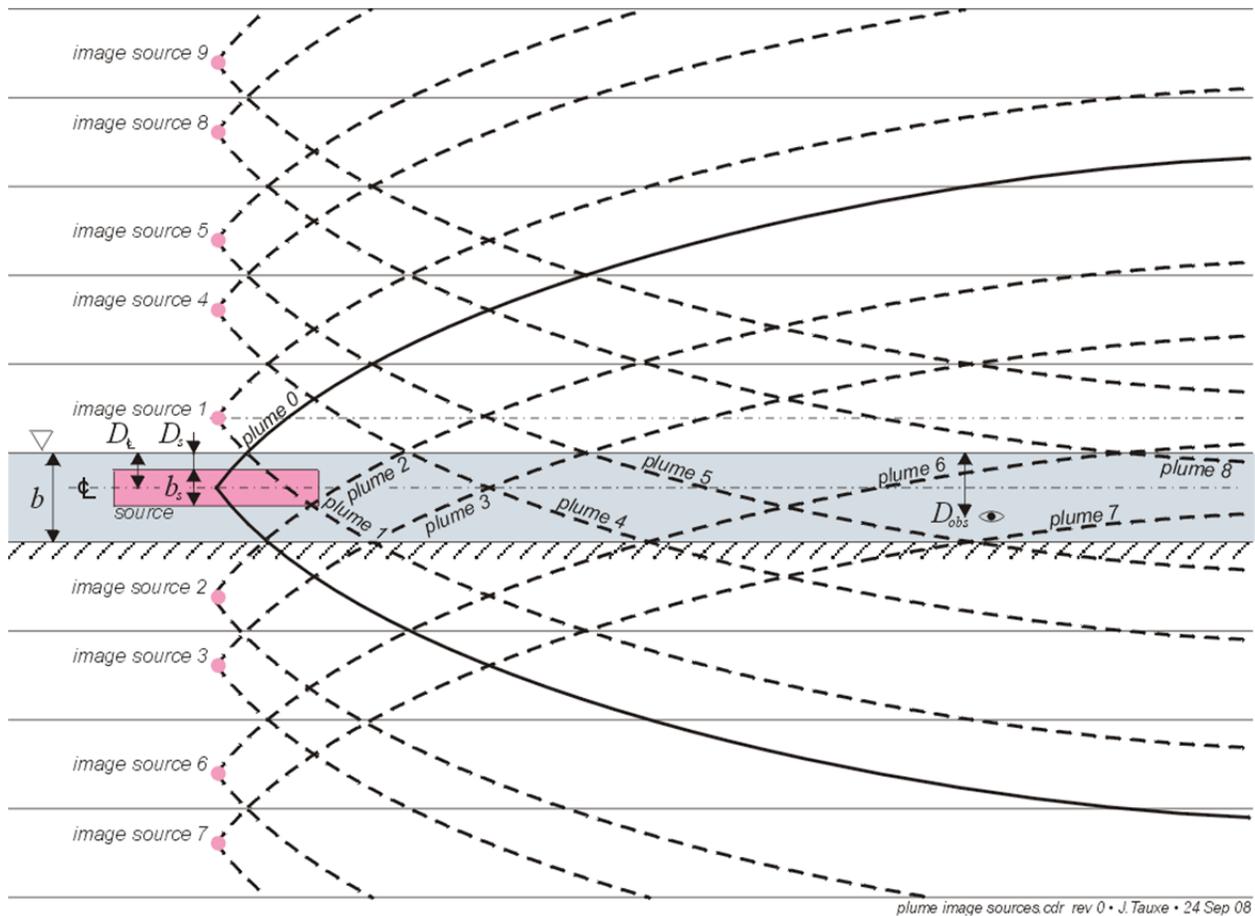
plume image sources.cdr rev 0 • J. Tauxe • 24 Sep 08

Figure 2. Placement of image sources relative to the aquifer and actual source.

3.3.2.1 Thin Source

A thin source triggers the point-source solution for vertical dispersion, expanded to include the additional image sources (the development of which is not covered here). In comparing the aquifer thickness b to the vertical standard deviation of the plume $\sqrt{2\alpha_V X_L^*}$, a thin source solution is used if

$$b < \frac{\sqrt{2\alpha_V X_L^*}}{100} \tag{13}$$

In this case, the point-source solution is used with i images at vertical locations X_{Vi} relative to the source's vertical centerline, and dilute$_V$ is the summation of a number of normal distribution density terms:

$$dilute_V = \frac{\sum_i \exp\left(-\frac{X_{V_i}^2}{4\alpha_V X_L^*}\right)}{\sqrt{4\pi\alpha_V X_L^*}} \tag{14}$$

Here $dilute_V$ is to be multiplied by $dilute_{init}$ as defined in Section 3.1 and $dilute_T$ from Section 3.2 in order to arrive at the final answer.

If the criterion for using images is met, that is, equation (12) is true, and that for a thin source is not met, that is, equation (13) is false, then the source is assumed to be relatively thick.

3.3.2.2 Thick Source

In the case of a source that is relatively thick in comparison to vertical dispersion, the point-source solution is integrated over the thickness of the source b_s and is summed over i image sources, so that $dilute_V$ is

$$dilute_V = \frac{\sum_i \left[\mathrm{erf}\left(\frac{X_{V_i} + \frac{b_s}{2}}{\sqrt{4\alpha_V X_L^*}}\right) - \mathrm{erf}\left(\frac{X_{V_i} - \frac{b_s}{2}}{\sqrt{4\alpha_V X_L^*}}\right) \right]}{2b_s} \tag{15}$$

3.3.3 Negligible Vertical Dispersion

In the case where we still do not assume vertical mixing and also do not invoke the use of image sources, that is equations (10) and (12) are false, then a final test is made to determine whether the observation point is vertically outside the plume. If the vertical location of the observation point relative to the vertical centerline of the source is greater than half the source thickness, expressed as

$$|X_V| > \frac{b_s}{2} \tag{16}$$

then the observation point is considered to be out of the plume and $dilute_V$ (and therefore dilute, as described in Section 3.4) is set to zero. Otherwise $dilute_V$ is set equal to the inverse of the source thickness.

3.4 Final Assembly

Having completed the various multiplicative factors involved in the calculation of dilute, we assemble the final calculation as the product

$$dilute = dilute_{init} \times dilute_T \times dilute_V . \tag{17}$$

In some cases, one or more of these terms may be equal to unity, in effect removing its influence, or zero, in effect making the entire calculation equal to zero.

The entire process is repeated for each item in the vector or matrix, if the plume() function is fed them rather than a collection of scalar arguments.

4.0   Implications for Use of the plume() Function at SRS

At the SRS, GoldSim PA models use the plume() function in the calculation of saturated zone contaminant transport from beneath the various sources (trenches in E-Area, high-level waste tanks in F- and H-Areas, and Saltstone vaults in Z-Area) to a number of potential locations for receptors' groundwater wells, generally located 100 m from the collection of sources. Each plume is modeled with a single horizontal "column" of Cell Pathway elements, and the plume() function is used to derive a PlumeCorrectionFactor for each source. Each well location is transposed into coordinates relative to each source, and the plume() function is applied to that longitudinal and transverse X_L and X_T. The aquifer is assumed to be fully mixed vertically, resulting from the assumption of a fully penetrating water well. The concentration at each well is the superposition of the contributions from each source. Since each source originates in the unsaturated zone above the aquifer, contamination is introduced at the top of the aquifer, using the same areal footprint as the source (i.e. trench, tank, or vault).

So, the assumptions in invoking the plume() function in the SRS PA models are that there is no explicit vertical dispersion (since complete vertical mixing is assumed), and that horizontal transverse dispersion is controlled only by the supplied dispersivity α_T. Parameters supplied to the plume() function are therefore

X_L length of the Cell column from the upstream end of the source to the receptor's well
A cross-sectional area of the Cell column (source width × Cell column thickness)
L_s length of the source parallel to the flow direction
X_V vertical position of the observation point (set to 0 m)
X_T transverse position of the observation point, perpendicular to the flow centerline for a given source, at X_L
D_s vertical depth to the top of the source from the top of the aquifer (set to 0 m)
W_s width of the source, transverse to the aquifer flow
b_s thickness of the source (set to 0 m)
b thickness of the aquifer
α_T dispersivity in the transverse direction
α_V dispersivity in the vertical direction (set to an arbitrarily large value)

For this specific set of input arguments, the plume() function will perform the following calculation:

First, dilute$_{init}$ is set to the cross-sectional area in equation (1):

$$dilute_{init} = A. \tag{18}$$

In all cases, the receptor wells are at least 100 m from the downstream edge of the source, so $X_L > L_s$ and equation (3) adjusts the assumed length of the column to be

$$X_L^* = X_L - \frac{L_s}{2}. \tag{19}$$

The value of L_s varies with the disposal facility, and can be as large as 200 m, reducing the column length X_L from, for an extreme example, 300 m to $X_L^* = (300 - 200/2)$ m $= 200$ m, a reduction of 33%. At the other extreme, the tanks are circular with a diameter of about 23 m, and the distance to the well may be as large as 310 m, so the column length X_L would be reduced from 333 m to $X_L^* = (333 - 23/2)$ m $= 312.5$ m, a reduction of only about 6%.

In considering transverse dispersion, we consider the width of the source (again ranging from about 23 m to 200 m), and the transverse dispersivity. Currently, the transverse dispersivity α_T is expressed as about 1/3 of the longitudinal dispersivity α_L, which in turn is a ratio of the column length, about $X_L / 27.5$, or $\alpha_T \approx X_L / 82.5$.

To test the possibility of a narrow source, examine the narrowest source and the longest path length, or 23 m and 310 m, respectively. In this case, plume() would be supplied the arguments $X_L = 310$ m, $W_s = 23$ m, and $\alpha_T \approx 3.8$ m.

Since the value for X_L is adjusted internally by plume() (in this case to about 300 m), the standard deviation of the transverse dispersion in the plume is about $\sqrt{2\alpha_T X_L^*} = \sqrt{2 \cdot 3.8\,\text{m} \cdot 300\,\text{m}} = 48\,\text{m}$. The test for a narrow source comes from equation (5):

$$W_s < \frac{\sqrt{2\alpha_T X_L^*}}{100} \quad \text{or} \quad 23\,\text{m} \overset{?}{<} \frac{48\,\text{m}}{100} \tag{20}$$

Clearly, 23 m > 0.48 m, so the narrow source test fails. Even when the SRS models are modified to accommodate contaminant transport to groundwater seeps a mile or more away, the narrow source test will fail. We may also reconsider the estimation of dispersivities, basing them on groundwater model calibrations rather than rough literature reviews. For now, however, suffice it to say that the sources are not classified as narrow.

Neither would they be expected to be particularly wide, though the "widest" aspect ratio of source to receptor locations could be at the Saltstone facility, where the Type I and IV vaults are 200 m "wide," and may be as close as 100 m from the receptor's well. In this case, $\sqrt{2\alpha_T X_L^*} = \sqrt{2 \cdot 1.2\,\text{m} \cdot 100\,\text{m}} = 16\,\text{m}$.

However, if we consider the definition of a "wide" source using equation (7), we see that

$$W_s < 1{,}000{,}000 \times \sqrt{2\alpha_T X_L^*} \quad \text{or} \quad 200\,\text{m} \overset{?}{<} 16 \times 10^6\,\text{m}. \tag{21}$$

Certainly, this is true, and would be for all cases. It seems that, for the purposes of calculations, the plume() function considers all the sources as wide sources. If that is the case, then equation (8) would be used to calculate the transverse dispersion, dilute$_T$.

The vertical dispersivity α_V in the SRS models is supplied to plume() as an arbitrarily large number. Therefore the standard deviation of the vertical dispersivity, $\sqrt{2\alpha_V X_L^*}$ is also very large. The test for a fully mixed aquifer in equation (10) therefore passes, and equation (11) is invoked:

$$dilute_V = \frac{1}{b}.$$

In the SRS application, therefore, as long as the arguments X_V, D_s, and b_s are all 0 m and the vertical dispersivity α_V is very large, the final expression for dilute (used as the PlumeCorrectionFactor in the SRS models) is based on equation (8), including the column cross-sectional area A and dividing by the aquifer thickness b, and with the substitution of the modified $X_L - \dfrac{L_s}{2}$ for column length X_L, just to keep the equation in terms of the original inputs

$$A \times \frac{\mathrm{erf}\left[\dfrac{X_T + \dfrac{W_s}{2}}{\sqrt{4\alpha_T\left(X_L - \dfrac{L_s}{2}\right)}}\right] - \mathrm{erf}\left[\dfrac{X_T - \dfrac{W_s}{2}}{\sqrt{4\alpha_T\left(X_L - \dfrac{L_s}{2}\right)}}\right]}{2bW_s} \tag{22}$$

Since through careful definition of the Cell column, the area A normal to flow equals the source width W_s times the aquifer thickness b, the equation for PlumeCorrectionFactor simplifies to

$$\frac{\mathrm{erf}\left[\dfrac{X_T + \dfrac{W_s}{2}}{\sqrt{4\alpha_T\left(X_L - \dfrac{L_s}{2}\right)}}\right] - \mathrm{erf}\left[\dfrac{X_T - \dfrac{W_s}{2}}{\sqrt{4\alpha_T\left(X_L - \dfrac{L_s}{2}\right)}}\right]}{2}. \tag{23}$$