On the Use of Hermite Polynomials
to Test Integration Techniques for
Mass Recovery in Groundwater Tracer Experiments

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Introduction

The Hermite polynomials satisfy several differential equations, two of which are given below:

$$\frac{d^2y}{dx^2} + 2x\frac{dy}{dx} + 2ny = 0 \quad y = \sum CnHn(x) \tag{1}$$

$$\frac{d^2y}{dx^2} + \left(2n + 1 - x^2\right)y = 0 \quad y = \sum CnHn(x)e^{\frac{-x^2}{2}} \tag{2}$$

The Hermite polynomials are orthogonal with respect to the weighting function exp(-x^2/2) over the doubly infinite range (viz. -∞to +∞) as indicated by the following integral:

$$\int_{-\infty}^{+\infty} Hn(x)Hm(x)e^{-x^2}dx \quad = \begin{cases} \sqrt{\pi 2^n n!} & if\left(n = m\right) \\ 0 & if\left(n \neq m\right) \end{cases} \tag{3}$$

Figure 1 shows the first 6 Hermite polynomials with the associated weight and normalized to unity.

Hermite Approximation

Figure 2 shows the successive orders of the Hermite series approximation for a test data set. This is similar to the successive order of the Fourier expansion for a function in the time domain. The terms in the series are computed from the orthogonality conditions as follows:

$$Cn = \frac{\int_{-\infty}^{+\infty} F(x)Hn(x)e^{-x^2}dx}{\int_{-\infty}^{+\infty} H_n^2(x)e^{-x^2}dx} \tag{4}$$

Test of Integration the Techniques

A test of the integration methods follows by applying the technique to the orthogonality condition (Equation 3). If you generate a sequence of data sets, which are the various products of the Hermite functions, the accuracy of the integration technique can be determined by checking the residual matrix whose elements are defined as follows:

$$Rn = \frac{\int_{-\infty}^{+\infty} Hn(x)Hm(x)e^{-x^2}\,dx}{\int_{-\infty}^{+\infty} H_n^2(x)e^{-x^2}\,dx} \tag{5}$$

The diagonal elements will be one and the off-diagonal elements should be much smaller than one.

<u>Extension to 2 and 3 Dimensions</u>

In order to extend this method to 2 or 3 dimensions it is only necessary to define the series of products of the one-dimensional Hermite polynomials as indicated below:

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} Hn(x)Hm(x)e^{\left(-x^2-y^2-z^2\right)}dxdydz \quad = \begin{cases} \neq 0 \;if\left(n=m\right) \\ = 0 \;if\left(n \neq m\right) \end{cases} \tag{6}$$

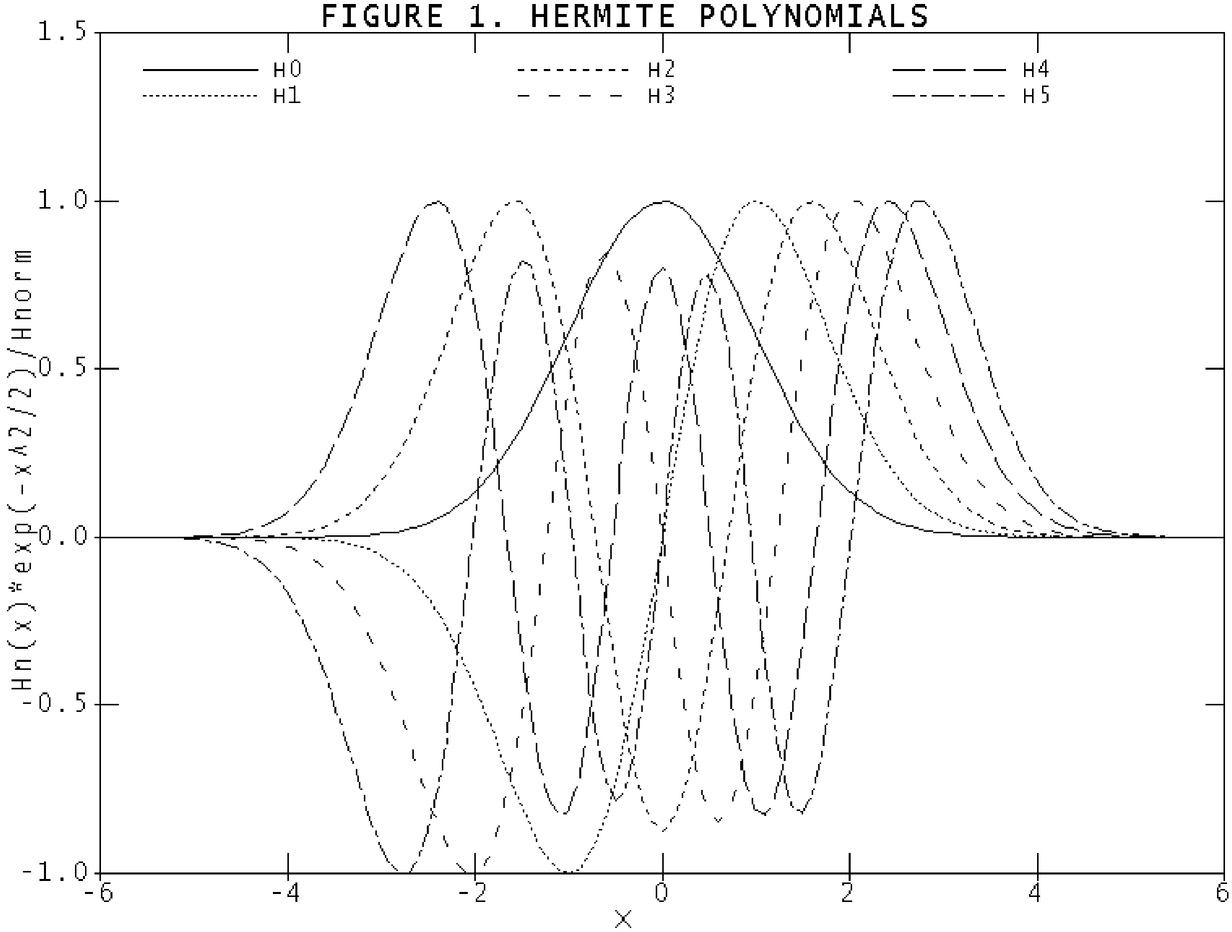

FIGURE 1. HERMITE POLYNOMIALS

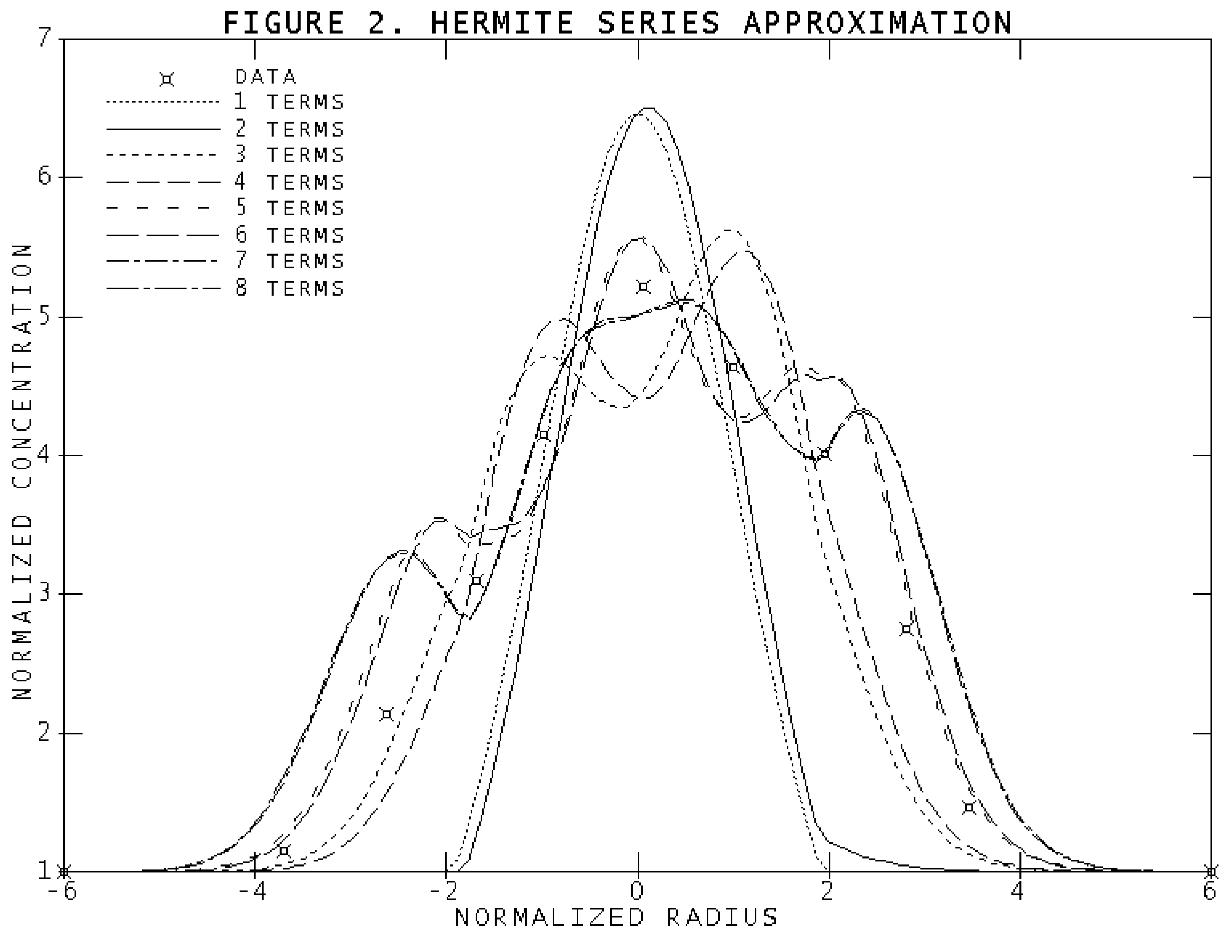
FIGURE 2. HERMITE SERIES APPROXIMATION
DATA
1 TERMS
2 TERMS
3 TERMS
4 TERMS
5 TERMS
6 TERMS
7 TERMS
8 TERMS
NORMALIZED CONCENTRATION
NORMALIZED RADIUS
1
2
3
4
5
6
7
-6
-4
-2
0
2
4
6

Examples

Figure 3 shows the successive orders of the Hermite series approximation for asymmetrical concentration data of contaminants in groundwater.

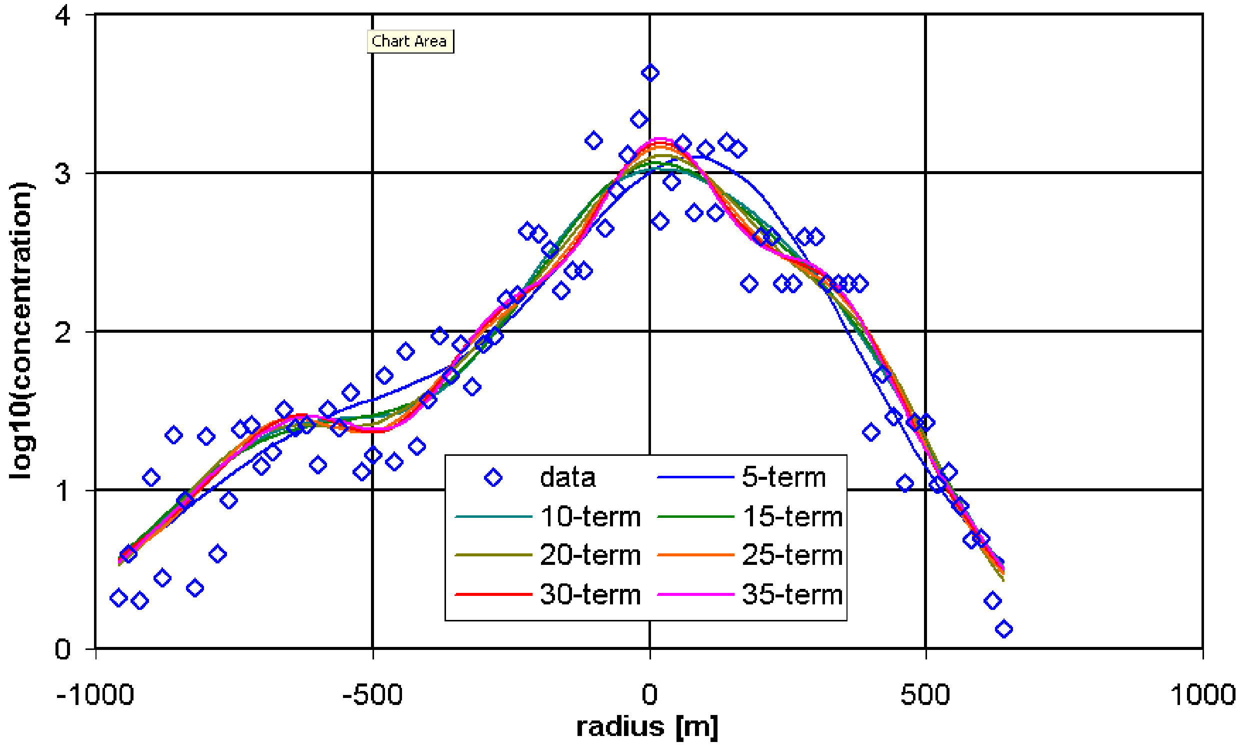

Figure 3. Approximate Concentrations

Figure 4 shows spatially and temporally variant ozone data across a region of the Southeastern US for which Hermite approximation is used to naturally fill in data gaps.

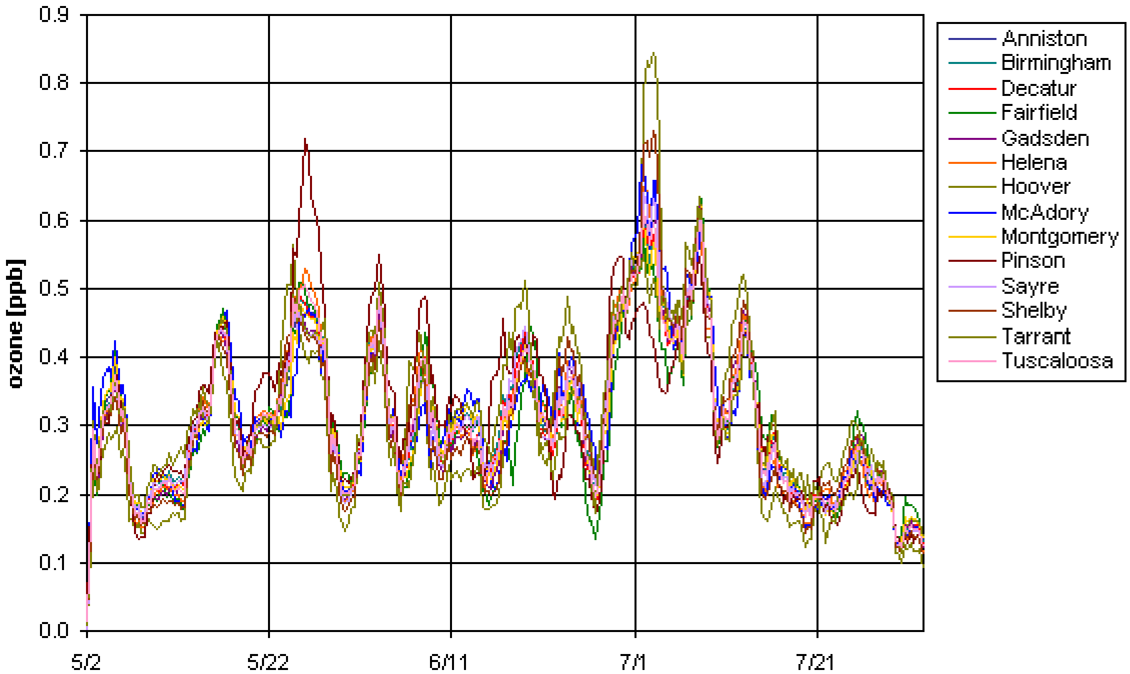

Figure 4. Ozone Data and Approximation