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VERIFICATION TESTS FOR CONTAMINANT TRANSPORT CODES


ABSTRACT: The importance of verifying contaminant transport codes and the techniques that may be used in this verification process are discussed. Commonly used contaminant transport codes are characterized as belonging to one of several types or classes of solution, such as analytic, finite layer, boundary element, finite difference and finite element. Both the level of approximation and the solution methodology should be verified for each contaminant transport code. One powerful method that may be used in contaminant transport code verification is cross-checking (benchmarking) with other codes. This technique is used to check the results of codes from one solution class with the results of codes from another solution class. In this paper cross-checking is performed for three classes of solution; these are, analytic, finite layer, and finite element.

KEYWORDS: transport modeling, model verification, analytic and numerical models, landfill design

There are two key aspects to a verification of computer models used to simulate contaminant transport in the subsurface. The first is to compare model

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predictions with observed field performance. When dealing with long term performance of modern disposal facilities this will often be controlled by largely diffusive transport of contaminant through the barrier system followed by advective-dispersive transport in any underlying aquifer. Because of the time frame involved and the relatively recent nature of these facilities, experimental validation of models is usually restricted to short periods of migration through clayey barriers—up to about 20 years; see Rowe et al. 1995 for two examples—or long term natural profiles developed over 10,000 - 15,000 years since the last glaciation—see Rowe et al. 1995 for three examples. While these cases provide a means of validating the basic transport mechanism and the mathematical idealization, they also tend to be problems that are essentially one-dimensional in nature and provide a limited opportunity to check the numerical and dimensional limitation of the models with respect to many practical applications.

In addition to field validations, there is a need for verifications of more sophisticated numerical models (and related codes) by cross-checking (benchmarking) against simple models and, conversely, using the more sophisticated models to establish the dimensional limits of simpler models. This is the second aspect of verification and the focus of the present paper. It is particularly important for models which are to be used to predict contaminant migration from modern facilities such as municipal solid waste and hazardous waste landfills and nuclear waste disposal facilities where the time for predicting potential impact ranges from many decades to thousands of years and hence the potential for field verification is limited to the short term (less than 20 years) and long term cases (greater than 10,000 years) as noted above. For these problems there will always be sufficient uncertainties regarding key parameters that it will not be practical to make precise prediction of impact (Frind 1987) irrespective of the model used. Rather it is usually necessary to perform parametric or statistical analyses to assess the sensitivity of the prediction to a reasonable uncertainty and hence establish likely bounds or potential impact (Rowe and Fraser 1993). It is generally desirable to use the simplest model that captures the essential features of the problem since this tends to reduce both computer time and the potential for numerical errors affecting the final results.

There are a growing number of models and related computer codes that may be used to simulate contaminant transport in the subsurface. The models can be subdivided into five broad categories; namely, analytic, finite layer, boundary element, finite element and finite difference models. These models employ a wide variety levels of idealization and solution techniques. Some may require extensive experience in numerical analyses to achieve accurate results. The precision of the results from a contaminant transport model will depend on the validity of the model implementation (i.e., mathematical approximations and computer algorithms used) and the appropriateness of the model and the solution technique to the specific problem being addressed (e.g., conceptualization including choice of dimensionality (1-D, 2-D or 3-D) and boundary conditions).
This paper considers three types of models: analytic, finite layer and finite element. The analytic solutions are ideal for making quick calculations and useful in checking the results of numerical analyses. The finite layer technique is applicable to situations where the hydrostratigraphy can be idealized as being layered, with the soil properties being the same at any location within a particular layer. This technique is particular well-suited for parametric and Monte Carlo studies. The finite element techniques can be used to model problems with complex geometries, complicated flow patterns, heterogeneity and nonlinearity. However, this technique requires a high level of sophistication in the user if accurate results are to be consistently achieved.

It is important that computer codes be verified to ensure their correct implementation of the relevant theory (the model) and to determine the benefits and limitations involved with each conceptualization and solution technique. The objective of this paper is to compare results from three different classes of model and to discuss the problem domains that each solution technique is capable of accurately and efficiently solving. The implication of using simple models that only consider one dimensional uniform stepwise steady-state flow is also examined.

VERIFICATION OF FINITE LAYER TECHNIQUES WITH ANALYTICAL SOLUTION

Analytic solutions are ideal for making quick preliminary calculations and are useful in checking the results of more sophisticated analyses. In this section, the 1-D and 2-D implementations of the finite layer technique (see Rowe and Booker 1985a, 1985b) are cross-checked against the analytic solutions for both a 1-D and 2-D plane advection-dispersion problem in an infinitely deep porous medium. All codes provide a solution to the advection-dispersion equation. The finite layer technique involves firstly taking the Laplace transform of the governing equation, boundary conditions and initial conditions. An analytic solution to the governing equations is obtained subject to the boundary and initial conditions in transform space. This is a similar approach to that adopted in developing most analytic solutions, however the finite layer technique allows consideration of multiple layers each with different material properties as well as a wider range of boundary conditions than can be accommodated by analytic solutions. The price for this greater generality is that the Laplace transform cannot be inverted analytically and hence is inverted numerically.

The solution to the 1-D advection-dispersion equation (with sorption and a first order sink term) for a layered system and a range of boundary conditions (i.e. 1-D FLT) as implemented in program POLLUTE (Rowe and Booker, 1994) involves the numerical inversion of the Laplace transform. The 2-D finite layer technique (2-D FLT) involves the introduction of both a Laplace and Fourier transform which allows the development of an analytic solution to the 2-D advection-dispersion equation. The Fourier transform and Laplace transform are
then both inverted numerically in the computer program MIGRATE (Rowe and Booker, 1995). The analytic solutions can only consider an infinitely deep layer however the finite layer can deal with this situation as a limiting case. More complete details regarding the finite layer technique are given by Rowe et al. (1995).

To allow comparison with the results from analytic solutions, a problem involving a constant contaminant source on an infinitely deep layer was examined for a vertical groundwater velocity \( v = 1 \text{ m/a} \). Results were obtained at 4 years for the values of the dispersion coefficient \( D \) (assumed to be isotropic for 2-D analyses) which bound the likely practical range allowing for diffusion control as a lower bound (0.01 \( \text{m}^2/\text{a} \)) and a very high dispersivity as the upper bound (\( D=10 \ \text{m}^2/\text{a} \)). Most practical applications would be closer to the lower end of this range.

Comparison of the 1-D FLT results with the 1-D analytic solution (Ogata and Banks 1961), gave identical results and demonstrates that the numerical inversion of the Laplace transform that is required to evaluate the finite layer solution is accurate and that the finite layer technique can give accurate solutions even for problems where advection dominates and the Peclet number is large. For the 2-D comparison, the width of the contaminated source, \( B \), was specified (\( B=1 \text{ m} \)) and results were evaluated along the centreline of the contaminated source. Both the 2-D analytic solution as coded in program TDAST (Javandel et al., 1984) and 2-D finite layer solution (2-D FLT) gave the same results to plotting accuracy (e.g. see Figure 1 which shows both the 1-D and 2-D results for \( D=10 \ \text{m}^2/\text{a} \)).

![Comparison of solution obtained by 1-D and 2-D FLTs and analytical technique.](image-url)

Fig. 1 Comparison of solution obtained by 1-D and 2-D FLTs and analytical technique.
Since the 2-D finite layer analysis requires the numerical inversion of both Laplace and Fourier transforms this comparison showed that the errors associated with numerical integration are small in the domain examined and that the 2-D finite layer technique can accurately capture the effect of 2-D migration predicted by the analytic solution.

**VERIFICATION OF FINITE ELEMENT IMPLEMENTATION USING THE FINITE LAYER TECHNIQUE**

Due to the analytic basis of the finite layer technique (FLT) there is no discretization error and hence the FLT can be useful for both verifying finite element codes and finite element meshes. The implementation of the two-dimensional hybrid finite element approach called Laplace Transform Galerkin (LTG) method (implemented in the computer program RECTRAN, Sudicky 1989) is assessed by comparing the results with the one-dimensional finite layer model. We begin by comparing results for a problem of identical dimensionality whereby the boundary conditions and material properties used in the LTG model are selected to match the 1-D conditions modelled by the 1-D finite layer technique. This LTG model is referred to as LTG1. The more general comparison of LTG and FLT will be given in the following section.

To check the implementation and application of the equivalent LTG code (LTG1), the variation of concentration in the aquitard with depth (for various times) and the variation of concentration in the aquifer with time are examined for a 200-m long hypothetical landfill shown schematically in Fig. 2a. The initial concentration, \( C_0 \), of the contaminant of interest in the landfills was taken as 1500 mg/L. Both a constant source concentration \( (C_0 = \text{constant}) \), which corresponds to infinite mass, and a finite mass source boundary condition were considered. With the finite mass boundary, the source concentration begins at an initial value \( C_0 \) but decreases with time as contaminant mass is removed from the source. This is described in detail by Rowe et al. (1995). In this example, the mass of contaminant available for transport into the soil, \( m_a \), was taken to be 1.5 kg/m² and hence for the initial source concentration \( C_0 = 1500 \text{ mg/L} = 1.5 \text{ kg/m}^2 \) this gives a ratio \( H_r = m_a/C_0 = 1 \text{ m} \).

Figures 2a and 2b show the variation of concentration with time, obtained from both 1-D FLT and LTG1 models, for infinite and finite mass conditions, respectively. It is evident that both models produce identical results. It can, therefore, be concluded that the LTG model can provide an adequate representation of the concentration history for at least simple essentially one-dimensional problems. We now extend this to look at a more complicated problem.
Fig. 2a Comparison of 1-D FLT and LTG1 models (infinite mass, \( H_r = \infty \), \( C_0 = \text{constant} \); uniform flow field).

VERIFICATION OF FINITE LAYER TECHNIQUE WITH FINITE ELEMENT METHOD

Uniform flow field

The 1-D finite layer technique (1-D FLT) assumes that the landfill is built on a liner or in an aquitard which is underlain by one or more aquifer(s). The 1-D FLT program models one dimensional vertical transport in the aquitard layer but considers lateral (horizontal) contaminant removal in the underlying aquifer. The leachate removal from the drainage layer can be approximated by a first order sink term (Rowe et al. 1995). This involves a number of approximations and raises the question as to how well this simplified approach can model the actual situation. For comparison purposes, consideration will be given to the results from the 2-D LTG program.
Consider a 200-m long landfill (see Fig. 3) built on a 2-m thick aquitard which is underlain by a 1-m thick aquifer. The landfill is engineered with a 1.2-m thick liner and a 0.3-m thick hydraulic control layer. The uniform velocity field below the landfill shown in Fig. 3 is for the situation after the failure of the primary leachate collection system, resulting in leachate mounding in the landfill to a maximum height of 6.9 m above the liner.

The purpose of this example is to examine how well the one-dimensional finite layer analysis (1-D FLT) predicts the concentration in the aquifer (directly beneath the edge of the landfill) in comparison to the equivalent two dimensional LTG model. A range of coefficient of hydrodynamic dispersion values, $D_h$ (i.e., 0.1, 10 and 100 $m^2/a$) in the aquifer is considered for the LTG (2-D) analysis. The results of the LTG (2-D) analysis are shown in Fig. 4 and it is evident that the 1-D FLT and LTG (2-D) are in good agreement for the most practical cases where $D_h$ is likely to be of the order of 0.1 $m^2/a$ (or lower) and indeed is good
1.0 LTG (2-D)

Fig. 3 Landfill configuration and transport parameters (uniform flow field).

(a) Infinite mass

(b) Finite mass

Fig. 4 Comparison of 1-D FLT with 2-D LTG calculated concentrations in the aquifer below the edge of the landfill (uniform flow field).
for $D_b \leq 10 \text{ m}^2/\text{a}$. For very high values of lateral dispersion $D_b$, the 1-D finite layer analysis over predicts the maximum concentration in the aquifer by about 15% however dispersion of this magnitude is not very likely in practice.

**Non-uniform flow field**

Non-uniform flows beneath landfills are very often encountered in the design of landfills. For example, the flow beneath a landfill built in a groundwater discharge zone would be initially upward; when leachate mounding occurs in the landfill, perhaps due to the failure of the primary leachate collection system, the direction of flow in the central portion of the landfill may reverse, resulting in a non-uniform flow condition (i.e., the flow would be downward in the central portion and upward near the edges of the landfill). Since the finite layer technique is developed for uniform flow conditions, it is of interest to examine the ways by which 1-D FLT can be used to model such non-uniform flow conditions.

Figure 5a shows the configuration of the landfill which is about 550 m long and built in an aquitard of 16 to 19 m thick with an average thickness of 17 m. The aquitard is underlain by an aquifer with an average thickness of 2 m. The elevation of the aquifer varies beneath the landfill as shown in Fig. 5a.

As the landfill has been designed to induce upward flow (i.e., a "hydraulic trap") from the aquifer during the normal operating life of the landfill, the flow condition is expected to become non-uniform due to leachate mounding, after the failure of the primary leachate collection system and subsequent failure to operate the hydraulic control layer. The estimated velocity field obtained using a groundwater flow model is shown in Fig. 5b. The flow is downward in the central

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**Fig. 5a** Hypothetical landfill examined for transport modelling.
part of the landfill (from 713 to 1049 m) and it is upward at the edges (from 620 to 713 m; and 1049 to 1150 m). A groundwater divide develops at 908 m due to the leachate mound.

The objective here is to model impact on the aquifer at the edge of the landfill base (e.g., at 660 m). This can be achieved by considering the landfill between the point of interest (660 m) and the groundwater divide (908 m). However, an inspection of Fig. 5b indicates that there is only downward flow over a 195 m distance from 713 m to 908 m and upward flow from 660 m to 713 m. As an engineering approximation, we consider only the portion of the landfill where the downward flow occurs. The predictions obtained using 1-D FLT are verified using the 2-D LTG model. A range of hydrodynamic dispersion values (${D_b =0.1,10 and 100 m^2/a}$) was examined for the full 2-D LTG modelling.

The results are shown in Fig. 5c for finite mass ($H_r$=10 m) and infinite mass ($H_r = \infty$, $C_r$= constant) conditions. The maximum concentration predicted by the 1-D FLT is in very good agreement with the 2-D LTG model. This demonstrates that with appropriate engineering judgement a very simple model can be used for this type of problem and that the agreement with the more rigorous analysis is good.

Transient flow conditions

For contaminant transport modelling it is common to use the steady-state velocities on the basis of the argument that the short-term transients, such as seasonal fluctuations of flow, can often be averaged out and the flow system can
be considered effectively at steady-state (Frind 1987). Although the steady-state assumptions are often justified, there are situations where changes in the flow field with time do warrant consideration. For example, the contaminant transport beneath a landfill may be affected by the time varying flows created under the following conditions:

- During leachate mounding in the landfill due to progressive failure of the primary leachate collection system (PLCS).
- During clogging of the secondary leachate collection system (SLCS) or following termination of its operation.
- When the head in the aquifer fluctuates so that the "hydraulic trap", if any, become ineffective during a portion of the fluctuating cycle.

For transient flows the changes in velocity field beneath the landfill with time (i.e., the transient changes) can be incorporated in the "time marching" scheme.

Fig. 5c  Comparison of concentration in the aquifer below the downgradient edge of landfill as calculated from the 1-D FLT with 2-D LTG codes (non-uniform flow field).
used in a finite element transport model by changing the flow field with time. Finite layer models can also be used to follow a defined time history as a sequence of flow fields each for a specified time interval. This allows for modelling the build-up of a leachate mound in a series of steady-state velocity increments (Rowe et al. 1995). To test the validity of this approximate approach, Rowe and Nadarajah (1995) made comparisons between the results of a full 2-D LTG finite element analysis performed using a transient velocity field generated by a transient flow program and those obtained from a 1-D finite layer analysis using a time history that involved a sequence of steady state flow fields. It was shown that for the range of situations examined, the simplified finite layer analysis provided quite adequate agreement with the more rigorous analysis. The interested reader is referred to that paper for more details.

SUMMARY AND CONCLUSIONS

A number of solution techniques have been used in contaminant transport modelling. Each solution technique works very well in the problem domain to which it was originally developed. The precision of the results of such a model will depend on the validity of the model implementation and the appropriateness of the solution technique to the specific problem domain being addressed. Both the solution methodology and its implementation should be verified for each model. In this paper a cross-checking approach is used to verify the results of one code and model type with another. Three types of models, analytical, finite layer and finite element, were examined.

Analytical models are well suited to preliminary analyses and for checking more sophisticated models. However they are limited by the simplified nature of the boundary conditions and the fact that they usually assume a uniform deposit. The finite layer technique provides greater flexibility than analytical solutions while minimizing computational requirements and the potential for numerical errors. The comparison of results obtained using 1-D finite layer technique with results from a 2-D finite element analysis indicated that the 1-D finite layer technique provided good results for problems involving a large source (e.g., a landfill) separated from an underlying aquifer by a relatively thin aquitard. It was also shown that with appropriate engineering judgement in the conceptualization of the problem, the impact due to a highly non-uniform flow field could be quite well modelled.

The 1-D finite layer technique has advantages over 2-D finite layer or finite element methods in terms of the very small amount of computation required to model even quite complex time histories and the relatively small potential for numerical problems and numerical errors although as with all models, the user must understand the approximations involved and the consequent limitations of the model.
The 2-D finite layer approach gave essentially (to plotting accuracy) the same results as the 2-D analytical solution showing that accurate results can be obtained. The 2-D finite layer technique involves more computation than the 1-D finite layer technique since it requires the numerical inversion of a Fourier transform. Thus greater care is required with the numerical aspect of the problem but at the same time it is also possible to consider more complex problems (e.g., the expansion of a landfill or the combined impact of two adjacent landfills).

While the 2-D finite layer technique can consider layered deposits and each layer may have different properties, it can not deal with significant change in properties in the horizontal plane. It does require that the hydrostratigraphy be approximated by essentially parallel layers. More complex problems can be modelled using the finite element method. However, the power of this technique is offset by the potential for numerical errors. Often an approximate solution can also be obtained using the 2-D finite layer technique and in these cases a comparison of the results can be used to "verify" the finite element analysis for idealized cases where a direct comparison can be made. It can also be used to provide bounds on the likely impact for more complex condition which can not be directly modelled by the finite layer technique but where impact can be calculated by adoption of reasonable limiting idealizations of the problem. This will improve confidence in the finite element results.

It is concluded that while verification of transport codes against field data is highly desirable, the availability of suitable data often limits the level of this type of verification that can be achieved. Under these circumstances, cross-comparison of different models can provide a very powerful tool to assist in the verification of the computer code for a given model.

REFERENCES


