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# CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

## TRIP REPORT

**SUBJECT:** Paper Presentation at the Fifth International Conference on Solving Ground Water Problems with Models (Account No. 20-3704-115)

**DATE AND PLACE:** February 11-13, 1992 - Dallas, Texas

**AUTHOR:** Amvrossios C. Bagtzoglou

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### TRIP REPORT

**SUBJECT:** Paper Presentation at the Fifth International Conference on Solving Ground Water Problems with Models (Account No. 20-3704-115)

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**BACKGROUND AND PURPOSE OF TRIP:**

The author attended the fifth International Conference on Solving Ground Water Problems with Models, and presented a paper entitled "Are Particle Methods only Suited for Modeling Advective Transport? Some Counter-Examples" (attached). The objective of the conference, as stated in the proceedings, was to disseminate state-of-the-art knowledge on the use of models to analyze and find working solutions to ground water problems. Based on this premise the organizers accepted an approximately equal number of papers discussing theoretical and practical, site-specific, results.

**SUMMARY OF PERTINENT POINTS:**

The meeting was co-sponsored by the International Ground Water Modeling Center (IGWMC) and the Association of Ground Water Scientists and Engineers, a division of the National Ground Water Association (NGWA). A total of 65 papers were accepted and presented at the meeting, including 15 papers presented in a special poster/computer demonstration session presentation. Sessions were devoted to the following topics:

- Session I : Mathematical Techniques in Ground Water Modeling
- Session II : Modeling Regional Ground Water Flow Systems
- Session III : Calibration and Parameter Estimation
- Session IV : Remedial Action Modeling
- Session V : Optimization in Ground Water Quality Management
- Session VI : Modeling Solute and Vapor Transport in Soils
- Session VII : Geostatistics and Stochastic Ground Water Modeling
- Session VIII : Bioremediation Modeling
- Session IX : Movement of Dense Fluids in Aquifers
- Session X : Modeling for Ground Water Quality Protection

Three key-note presentations were made:

1) "Recent Developments in Two-Dimensional Analytical Solute Transport Models", by V. Batu

2) "Compilation of Ground Water Models: An Ongoing IGWMC Core Activity", by P. K.M. van der Heijde (IGWMC Director)

3) "Standards for Ground Water Models: A Progress Report", by J. Ritchey (ASTM Task Force Coordinator)

A brief description of the most important papers is presented below on a paper by paper basis. The term "important" reflects the author's interest in specific topics, and should not be related to the quality of the papers being omitted.

## Session I

1) "A Performance Comparison of Different Analytical and Numerical Saturated Zone Contaminant Transport Models", by F. Arnold.

Various numerical and analytical models were used to simulate a contamination site in Minnesota. Predicted ground water contamination at a distant receptor point 4,000 feet from a constant source of contamination was found to vary over two orders of magnitude from 0.1% to 15% of the source concentration. These findings emphasize the vast variability of results obtained through the use of different numerical models and stress the need of model standardization within a regulatory analyses context.

2) "Dynamic Coupling - A New Tool for Three-Dimensional Flow and Transport Simulations", by A. Haug, G.E. Grisak, and F.G. Wolf.

The ground water flow and transport code SWIFT II was enhanced to include a dynamic coupling option. Using this technique, aquifer-aquitard systems are discretized into a couple of distinctly different grids. The aquifers are discretized into normal finite differences and the aquitards into columns of one-dimensional vertical subgrids. By implementing this approach, memory and computer time requirements were decreased by an approximate factor of 150 and 600, respectively.

3) "Local Adaptive Grid Refinement (LAGR) for Contaminant Transport Modeling", by A.V. Wolfsberg, and D.L. Freyberg.

In order to solve accurately and efficiently the mathematical equations representing reactive, multicomponent transport in two or more dimensions, a system of local adaptive grid refinement (LAGR) is implemented. LAGR is based on automatic generation of multiple, high resolution patch finite difference grids. These grids are placed at locations in the domain of interest, where uniform solution accuracy is imperative to be achieved. Accurate solutions to nonreactive single component as well as to reactive, multicomponent (competitive sorption) problems are provided using LAGR at computational requirements approximately 20% of what a fine-grid solution would take.

## Session III

1) "Interpretation of Two-Dimensional Characteristics of Stochastic, Fractal Heterogeneous, Porous Media Models from One-Dimensional Sampling", by P.A. Zlatev, and E.P. Poeter.

Two-dimensional stochastic fractal models of heterogeneous porous media were developed. This way, complex representations of porous media which yield velocity distributions similar to the ones observed in the field can be obtained. Lacunarity was found to be a far better tool, compared to the fractal dimension, for differentiating two-dimensional hydraulic conductivity fields. Integration of hydraulic conductivity and velocity fields is an imperative step for generating representative realizations of porous media models from sparse data samples.

2) "Selecting Calibration Values and Formulating Calibration Targets for Ground Water Flow Simulations", by W.W. Woessner, and M.P. Anderson.

A systematic method to organize the model calibration process is presented. This approach involves the a priori selection of calibration values (heads, fluxes, or mass balance), setting ranges of aquifer parameter estimates, fitting of simulated results to calibration targets, and evaluation/documentation of the calibration process. The paper concludes with the presentation of a case study where more than 90% of the calibration targets were matched at acceptable levels.

3) "Application of the Adjoint-Sensitivity Technique for the Guidance of Efficient Ground Water Model Calibration"*, by A.M. La Venue, and J.F. Pickens.

A new approach for model calibration, combining an adjoint-sensitivity algorithm with kriging, is presented. The method makes use of the novel concept of "pilot" points where changes of the transmissivity field would most improve the fit. The case study discussed is the calibration of a two-dimensional flow model for the Culebra formation at the Waste Isolation Pilot Plant (WIPP) site.

### Session IV

1) "Remediation of Ground Water Contamination at the Rocky Mountain Arsenal: Numerical and Geostatistical Analysis", by J. Warner, A. Abdel-Rachman, C. Tamayo-Lara, and J. May.

A remediation effort at the Rocky Mountain Arsenal is evaluated based on the Colorado State University Finite Element Groundwater Modeling Package. Co-kriging of hydraulic conductivity fields and saturated thickness was used to account for aquifer heterogeneities. An experimentally (field data) derived cross-semivariogram was used and various variogram models were tested for their fit.

### Session V

1) "Design of Optimal, Reliable Plume Capture Schemes: Application to the Glouchester Landfill Ground Water Contamination Problem"[1*], by R.M. Gailey, and S.M. Gorelick.

Paper emphasized the ill-poseness of the calibration process being based only on head measurements. The authors developed an approach that makes use of concentration data for hydraulic conductivity parameter estimation. The methodology presented in this work is applied under a deterministic as well as stochastic optimization formulation.

2) " A Coupled Simulation-Optimization Technique for Protecting Municipal Ground Water Supplies from Contamination", by M.D. Varljen, and J.M. Shafer.

A technique based on conventional finite difference ground water flow modeling and numerical flowpath/travel time calculation is developed. These numerical tools are coupled with nonlinear

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[1*] Manuscripts not available at the time of proceedings print.

mathematical programming. The objective is to specify pumping rates for wells in such a way that the configuration of capture zones in relation to existing potential sources minimizes the risk of contamination while maximizing the total water output from the wellfield.

### Session VI

1) "Simulation of Two-Phase Carbon-14 Transport at Yucca Mountain, Nevada", by M.D. White, M.D. Freshley, and P.W. Eslinger.

Transport of $C^{14}$ in the unsaturated zone was numerically modeled with the Multiphase Subsurface Transport Simulator (MSTS). MSTS solves the nonlinear partial differential equations with an implicit finite difference scheme. Nonlinearities are dealt with the Newton-Raphson iterative scheme. Transport results of $C^{14}$ distributions, surrounding the proposed nuclear waste repository, in a two-dimensional east-west cross section of Yucca Mountain are presented.

### Session VII

1) "Application of Kalman Filter for Analysis of Contaminant Transport in Ground Water Originating from Point Sources", by B.K. Panigrahi, and J.C. Hwang.

The identification of locations and strengths of pollution sources is performed with the help of a sequential stochastic model. This effort incorporates the measurement and modeling errors associated with any site modeling study. Results from a series of preliminary numerical experiments with a single point source and a constant injection rate are presented.

### Poster Session

1) "Evaluation of Uncertainty Associated with Contaminant Migration in Ground Water - A Technically Feasible Approach", by W.L. Wingle, and E.P. Poeter.

Complex probabilistic, yet user friendly software utilizing all available site data (soft and hard data) is developed to make a conjunctive interpretation of data describing the subsurface. Indicator and Bayesian approaches are used to characterize the data uncertainty, and conditional stochastic indicator simulations are conducted to represent the range of subsurface realizations based on the available data.

## IMPRESSIONS/CONCLUSIONS:

The current trend in state-of-the-art ground water, flow and transport, modeling is stochastic simulation. This may be conducted with the help of various approaches such as Kriging, Co-kriging, Indicator Kriging, Particle Methods, Probabilistic Methods, Monte Carlo (repeated) Realizations, Fractal Heterogeneity, Conditional Simulation, Adaptive Grids, etc. It will be to the CNWRA's benefit to get involved in as many of the above research areas as possible. Another important issue that this conference touched upon is Model Standardization and Quality Assurance. At least two states have already established verification criteria that the numerical models must abide by. It is very likely that more states will soon follow. IGWMC and the ASTM Task Force on Ground Water Models are actively working on developing and/or judging such regulatory criteria. It is, in my opinion, imperative for CNWRA to participate in such efforts from their inception.

**RECOMMENDATIONS:**

The author has requested all pertinent information from IGWMC and ASTM. Upon receipt of this material CNWRA staff should get involved with these model standardization and quality assurance efforts.

**SIGNATURES:**

| | |
|---|---|
| Amvrossios C. Bagtzoglou | 2/28/92<br>2-28-1992 |
| Research Engineer | |

**CONCURRENCE SIGNATURES AND DATE:**

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| Budhi Sagar | 3/2/92<br>3-2-1992 |
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## ATTACHMENTS

## ABSTRACT

A Performance Comparison of Different Analytical and Numerical Saturated Zone Contaminant Transport Models



Forest Arnold, Roy F. Weston, Inc., 215 Union Boulevard, Suite 600, Lakewood, CO 80228


A common objective in saturated zone contaminant transport modeling is estimating the concentration reaching a distant receptor such as a well field or surface water body. Often this receptor is a considerable distance beyond the area of a site investigation so that limited calibration data is available for contaminant transport modeling. There are a variety of numerical and analytical methods available to depict contaminant transport in porous media.

Different models include variables in the governing equations to represent dispersion, chemical decay, retardation and biodegradation. These governing equations are simplifications of the numerous interactions which occur at the micro-scale (< 10 cm) in natural porous media. Different results would be expected depending upon the presence or absence of certain factors in the governing equations and by their mathematical formulation. In order to assess these differences, a site in Minnesota was modeled using twelve commonly used numerical and analytical techniques.

Predicted groundwater contamination at a distant receptor point 4,000 feet from a constant source was found to vary over two orders of magnitude from 0.1% to 15% of the initial concentration. Although this type of test is not a true benchmark or field validation test and might be subject to some user bias, there is a wide range in performance of these models. This performance difference suggests that practitioners might want to use multiple methods in representing a given site under a situation of limited calibration data, in order to bracket the predictive variability inherent in the models.

## INTRODUCTION

A common objective in saturated zone contaminant transport modeling is estimating the concentration reaching a distant receptor such as a well field or surface water body. Often this receptor is a considerable distance from the area of detailed site investigations so that limited data is available for model calibration. This occurs frequently in wellhead protection, risk assessment and in Superfund site investigations (Javendel, 1984).

Often a simple model is used and a conservative estimate is made for the effects of dispersion, retardation and biological and chemical decay. This approach deliberately ignores these effects so receptor concentrations will be overestimated. If the simulated concentration reaching the receptor is low, then the perceived risk is low and no additional effort is expended to refine or calibrate the model.

There are many analytical and numerical modeling techniques available to assess contaminant transport problems. Different models include variables in the governing equations to account for advective movement, as well as for factors such as dispersion which alter contaminant movement patterns, or for factors such as retardation, chemical decay and biodegradation which decrease the amount of a contaminant which will move with ground water flow over time and distance. The equations representing these factors are physical and mathematical simplifications of the numerous phenomena which occur at the micro-scale ( < 10 cm) in natural porous media (Ruben, 1983).

In order to assess some of these performance differences a site in Minnesota was modelled using equivalent input data in 12 commonly used numerical and analytical models. This exercise makes it possible to assess the variability in performance of the different models.

## METHODS

Identical values of hydraulic conductivity, gradient and dispersion and decay were used in each code. The compounds of concern were Benzene, Toluene and Xylene (BTX) compounds from a gasoline pipeline leak. A low value of retardation was applied to all models which included retardation parameters. The decay values used were kept quite low, so that the results were comparable between model.s

As a further aid in comparing the different model outputs, the initial concentrations were set at 100%. This allows the results to be compared in terms of the percent of the initial concentration that reached the receptor point.

All of the models considered, except SLAEM (Strack, 1989) consider dispersion in the governing equation. The SLAEM model and AST123D combine chemical decay and biodegradation under a single decay term. Similarly, the Rapid Assessment Nomograph considers a decay term which covers both chemical decay or biodegradation. Bioplume II

(Bedient, et al, 1989) is the only model that directly estimates biodegradation based upon dissolved oxygen levels. Retardation is considered in most of the models except HPS (Galya, 1987), Hydropal Slug source (Watershed Research, Inc., 1988), and Random Walk (Watershed Research, Inc., 1988). The BTX compounds are preferable for this type of comparison because they have low retardation properties. Based upon field studies in Minnesota, they are subject to some biological decay so that a realistic estimate at the receptor point should include a conservative level of decay (Pfannkuch, 1984).

Not all of the numerical models or analytical models consider all of the large scale factors known to effect contaminant transport. Only Bioplume II, AT 123D, New MOC, Conmig, and the Rapid Assessment nomograph cover all of the relevant parameters. If there are geologic inhomogeneities present, AT123D and the nomographs cannot represent these. Only MOC, Bioplume II and SLAEM can represent geologic inhomogeneities in solving the flow and contaminant transport equations.

Of the codes used in this exercise, only MOC, Bioplume II and SLAEM are immune to numerical dispersion. All others might introduce some numerical dispersion errors which could be significant at a distance of 4,000 feet and 10 years travel time. These effects might vary with site conditions, time step, grid size and parameter choices.

## HYDROGEOLOGIC SETTING

The site modeled was the Superfund portion of the Koch Refinery Site near Rosemount, Minnesota in Dakota County. A short term pipeline spill has introduced gasoline into the unsaturated zone where it has reached the water table. There is a monitoring well network in place as part of Superfund cleanup activities. Ground water flow is northeastward where it discharges to the Mississippi River about 4,000 feet from the site. BTX compounds have been detected in the monitoring wells.

The unconfined upper aquifer at the site is comprised of glacial outwash from 60 to 330 feet thick around the refinery and approximately 160 feet thick in the modeled spill area. The outwash area consists of unconsolidated sand and gravel. This material was deposited by meltwater from the Superior Lobe of the St. Croix phase of the Wisconsinian period of glaciation. It is underlain by older till layers deposited during earlier phases of glaciation. The ground water velocity in the upper aquifer is estimated to be 400 ft/yr based upon slug tests and pump tests that were completed during site investigations.

## RESULTS

Table 1 presents a summary of the factors considered by the numerical and analytical models used, typical modeling time, and the predictions. In comparing the predictive results

**Table 1**
**A Comparison of Model Variables and Predictions**

| Model Name | Variables Included: Dis-persion | Retard-ation | Chemical Decay | Biodegra-dation | Time to Run | Results % of initial conc. |
|---|---|---|---|---|---|---|
| <u>NUMERICAL MODELS</u> | | | | | | |
| AT123D (Yeh, 1981) | x | x | x | x | hrs-day | 0.1 |
| Bioplume II (Bedient, 1989) | x | x | x | x | days-wk | 4 |
| Conmig (Walton, 1989) | x | x | x | x | 1-2 hrs | 5 |
| Hydropal Slug (Watershed, 1988) | x | | | | 1-2 hrs | 6 |
| MOC (Old) (Konikow, 1978) | x | x | | | days-wk | 15 |
| MOC (New) (Konikow, 1978) | x | x | x | x | days-wk | 4 |
| Random Walk (Watershed, 1988) | x | | | | hrs | 13 |
| SLAEM (Strack, 1989) | | x | x | x | days | 3 |
| <u>ANALYTICAL MODELS</u> | | | | | | |
| CDT Nomograph (Dragun, 1989) | x | x | | | 1-2 hrs | 6 |
| HPS (Galya, 1987) | x | | x | | hrs-day | 5 |
| Rapid Assessment Nomograph (Guswa, 1987) | x | x | x | x | 2-4 hrs | 15 |
| Wilson-Miller Nomograph (Kent, 1982) | x | x | x | | 1-2 hrs | 8 |

of the different models, the same values were used for dispersion, retardation and decay, but not all models consider all factors.

The values predicted for percent of initial concentration remaining range over two orders of magnitude, from 15% of Old MOC which does not consider chemical or biological decay (Konikow and Bredehoeft, 1978) and the Rapid Assessment Nomograph (Guswa, 1986) to 0.1% for AT123D (Yeh, 1981). The analytical methods predicted values in the middle of the range from 5% to 15% of the initial concentration remaining. There appears to be a larger range of predicted concentrations when comparing the numerical models than the analytical models (0.1% to 15% vs. 5% to 15%). Not surprisingly, the predictions are lower in the models that consider more factors.

Since the retardation factors for BTX compounds are low and would only vary over a narrow range, it appears that the results are the most sensitive to the decay term (either chemical or biological). It is interesting that the results from the Random Walk code are comparable to many of the other models although it does not consider retardation and decay. In this case, 7 of the 12 results would be above the applicable regulation for the river.

The results of the models which consider more factors appear to be lower. Yet it is common practice to avoid more complex models if there is limited data. This approach, which is viewed as more conservative, may give higher results. The impact of using a simpler model might be less realistic predictions which could have regulatory consequences.

In this exercise, the time required to use a different model varied from 1 to 2 hours for the CDT nomograph to days to weeks for a MOC run. Typical modeling time would include development of site input data, gridding and model runs required to reach a satisfactory solution. Table 1 indicates that there are relatively short time requirements for running analytical models. It is possible to run 2 nomographs, the Slug Source Package and the Random Walk package in Hydropal in a day. AT123D and SLAEM are easy to use and can be run in a few days. Although this might seem repetitive initially, the range of results and the importance of the decay terms could be assessed relatively quickly in some detail before embarking on the more lengthy and arduous process of running a complex numerical model like Bioplume II.

## DISCUSSION

This exercise demonstrates that the choice of model adds another source of variability in predicting contaminant transport. The decision to do additional modeling in order to consider parameter sensitivity and model introduced variation is often difficult due to time and resource constraints. The analytical models and more user friendly numerical models would be the quickest way to bracket the effects of model induced variability.

Any steps that can help the modeler assess, refine and improve the conceptual model of the site in order select a model with the appropriate variables is important. Without model variability bracketing, calibration and sensitivity analysis for a single model might be inadequate for a distant receptor analysis due to limited geological information and calibration points (which is usually the case in remediation and non research situations).

In an advection dominated system such as is found at this site, a hyperbolic representation like the particle tracking methods used in Random Walk and MOC may give different results than parabolic representations in finite difference/finite element methods (National Academy of Sciences, 1990).

It should be recognized, that this is not a true benchmark and field validation test (Hern and Melancon, 1986) and may be subject to some user bias due to limited site data. Even with more calibration data it is possible to reach nonunique solutions with different modelers using the same data set (Freyburg, 1988). A post audit over time will indicate differences between modeled results and actual field performance (Konikow, 1986).

There is considerable research being conducted in parameter optimization methods and improving our understanding of micro scale transport phenomenon. Unfortunately, for the practitioner there is often too little data available to use parameter optimization methods effectively and no way to quantify complex micro scale models for necessary modeling variables (e.g. retardation parameter). True benchmark studies and field validation tests are expensive and time consuming and might not be available for all of the models available, and that are being developed.

This performance comparison reflects the type of results that would be found for a simple site with relatively rapid ground water velocity. It may not be representative of other types of situations, such as different aquifer parameters, well field interactions, geologic inhomogeneities, surface water body interactions, shorter or longer distances, and for different time periods.

## SUMMARY

Using the same input data for a single site, the results from 8 numerical models and 4 analytical models are compared. The predicted concentrations at a distant receptor point ranged from over two orders of magnitude from 0.1% to 15% of the initial concentration depending upon the model chosen.

Most modelers deal with transport models with parameter related and mathematically introduced variability problems with limited time and money constraints. Using multiple models and sensitivity analysis to bracket the reasonable results for a particular site is adding additional time demands to already limited resources.

The philosophy of using multiple models and bracketing runs counter to the way that most modelers are trained. Unfortunately, single model results contain more uncertainty which is counterproductive to formulating workable policy decisions. As this exercise demonstrated, the choice of which model to use resulted in an almost even (7 of 12) chance in opposite policy decisions.

The consequences of this model induced uncertainty were not significant in this case due to the considerable dilution potential of the Mississippi River. In other situations however, there might have been public health, environmental, or financial consequences.

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