Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

ACTS
A multi-media contaminant transport modelling platform

M.M. Aral,[1] M.L. Maslia,[2] J. Guan,[1]

[1]*Multimedia Environmental Simulations Laboratory (MESL), School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, Georgia, USA.*
[2]*Division of Health Assessment and Consultation, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, Georgia, USA.*

Abstract

In an attempt to determine if there are links between environmental pollution and increased risk to human health, the Agency for Toxic Substances and Disease Registry (ATSDR) conducts health assessments, health consultations, exposure investigations, and health studies. Quantifying the fate and transport of pollutants and the uncertainty associated with the analysis is a key step in these studies. To assist engineers and health scientists in conducting such analyses, ATSDR and the Multimedia Environmental Simulation Laboratory (MESL) program at Georgia Tech have developed software to assist with environmental multi-media fate and transport computations in a user-friendly environment. This software is identified as the "**A**nalytical **C**ontaminant **T**ransport analysis **S**ystem" (**ACTS**). In this paper, we describe general features of this software and the models contained therein. Further demonstration of the capabilities and use of ACTS software in site-specific cases can be found in other publications of the authors as referenced in this paper.

1 Background

The occurrence, presence, and persistence of contaminants in air, soil, surface water, and groundwater has resulted in public awareness of environmental

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

health issues and this has lead to public concern about the potential for increased risks to human health. The difficulty in assessing human exposure to contaminated environmental media is compounded by several factors including: lack of measured exposure data, uncertainty about the start of contamination, spread and movement of a contaminant plume, and the lack of "off-the-shelf" tools or procedures that may involve multidisciplinary approaches needed to identify the link between multi-pathway environmental analysis and increased health risks in humans.

The Agency for Toxic Substances and Disease Registry (ATSDR), a Public Health Service agency of the United States Department of Health and Human Services, is mandated by the U.S. Congress to evaluate the public health threat of hazardous waste sites using environmental characterization data, community health concerns, and health outcome data [1]. In a comprehensive health assessment study, the linking of site specific environmental characterization databases with population exposure may often times become a difficult task. To assist with comprehending the link between environmental contamination and the potential for increased health risk, ATSDR is conducting research on exposure-dose reconstruction [2]. One of the objectives of this research program is to address the concept of total exposure characterization using novel approaches, and, in the process, develop simulation tools that can quickly provide reliable information needed for the completion of health assessment studies. In this paper we describe the **A**nalytical **C**ontaminant **T**ransport analysis **S**ystem (**ACTS**) software, which is a collection of analytical models developed to evaluate migration and fate of contaminants in air, soil, surface water, and groundwater environments within a user-friendly computational platform [5]. The use of the software in site specific applications is beyond the scope of this paper. These applications can be found in the following studies [3, 4, 5, 9].

2 Exposure assessment approach

Evaluation of dynamic and complex environmental systems can be accomplished through physical, conceptual, or mathematical models. However, mathematical modeling provides the only practical first step for considering the transport and fate of mixed chemical compounds through environmental media. The methodology being used by MESL in ATSDR's research on exposure-dose reconstruction is described by Aral et al. [3] and incorporates spatial kinetic principles and simulation tools through a database management system. The proposed system, is user friendly, supports the evaluation of critical aspects of exposure assessment analysis, and is intended to be modular in the sense that users will be able to include selected aspects of the analysis based on the importance of a particular environmental process. Thus, the analytical system is flexible and adaptable to varying environmental, geochemical, and chemical processes. The evaluation and management system being developed (Figure 1), consists of four primary modules: (1) database development module; (2) analytical, numerical, and

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

statistical analysis module (spatial and compartmental simulation methods); (3) coupling of multimedia simulation methods though a geographic information system; and (4) interpretation and presentation tools module. The methodology used allows for a unified yet flexible approach to total exposure characterization.

Within the pathways analysis module shown in Figure 1, Maslia et al. [9] describe a paradigm for determining human exposure to hazardous substances as consisting of four activities: (1) contaminant source identification, (2) site characterization and digital databases that include environmental and demographic information, (3) multimedia pathway transport of contaminants, and (4) routes of human exposure. It is activity number (3), exposure pathway transport of contaminants that is addressed by the ACTS system software, and this is the focus area of this paper.

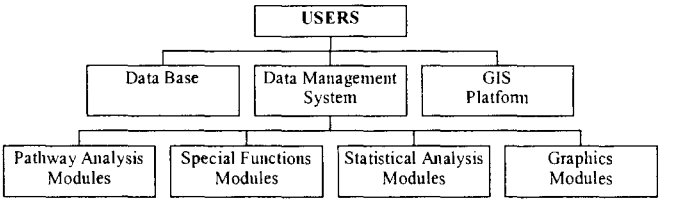

Figure 1. Proposed Exposure Assessment Management System

3 Analytical contaminant transport analysis system (ACTS)

The ACTS software has been developed to provide professionals in the fields of hydrogeology, environmental engineering, and environmental health with compact analytical tools to evaluate the migration and fate of contaminants in multimedia environments, air, soil, surface water, and groundwater (Figure 2). ACTS version 4.5 has been released publicly [5], although work continues on updating and enhancing the software. The fate and transport models included in the software are dynamic models that can be used to assess steady-state and time-dependent contaminant concentrations introduced to soil layers or contaminants released to air or water.

During the development of the ACTS software, emphasis was been placed on the creation of a unified, user-friendly, WINDOWS(TM) based software framework, with the capability to perform uncertainty analysis.

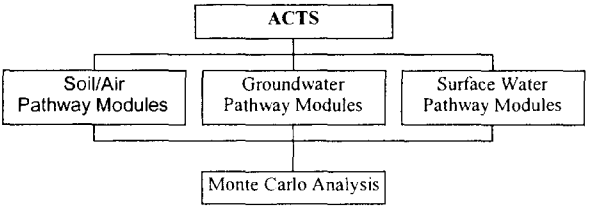

Figure 2. General outline of the ACTS software platform

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

Major functions currently performed by the ACTS software include:

i. Use of WINDOWS(TM) based application environment.
ii. WINDOWS(TM) based data entry in all applications.
iii. Capability to read input data files from earlier runs and spreadsheets.
iv. Use of WINDOWS(TM) based utility programs such as NOTEPAD.EXE or WRITE.EXE or any other compatible program to view, edit or print data bases.
v. Allocation of default values to some input parameters/variables through Chemical database input file.
vi. Capability to edit Chemical database to develop customized databases.
vii. Capability to view the results in customized graphics forms.
viii. Depending on user-selected options:
    - Simulation of emission rates from the source.
    - Simulation of contaminant dispersion in the air pathway.
    - Simulation of one-dimensional unsaturated zone transport.
    - Simulation of one-, two- and three-dimensional saturated zone transport with constant and variable dispersivity models.
    - Simulation of in-stream or estuary concentrations due to contaminant loading using several surface water mixing models.
ix. Uncertainty analysis in input parameters for all pathways.
x. Generation of random distributions for Monte Carlo simulations.
xi. Performance of statistical analyses of Monte Carlo simulation results.
xii. Graphical presentation of Mote Carlo simulation results.

Using the capabilities of ACTS software, publication-ready results can be developed using the presentation utilities included within ACTS. For each pathway, the ACTS software package comes with sample problems that provide input values and simulation results so that users of ACTS can identify and become familiar with data input and output operations. We briefly discuss below the analytical models contained in ACTS software. Owing to brevity, detailed mathematical descriptions of these models will not be presented here, but can be found in the ACTS User's Manual [5]. The ACTS User's Manual also includes an extensive list of references indicating the sources of the models used in the ACTS software. These also will be omitted in this paper due to limitations of space.

3.1 Soil/air pathway module

The soil/air pathway module consists of a chemical database, an emissions module, and an air dispersion module. The chemical database contains physical properties for selected chemicals. These chemical properties can be modified utilizing the chemical database "Edit" commands.

The emissions module contains four models that can be used to calculate emission rates from land-based (soil) contamination sources. These models can simulate a single chemical or multiple chemicals selected from the ACTS chemical database. The four emission models included in the ACTS are: (1)

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

Farmer's model for estimating emissions from a constant contaminant source buried below the soil surface [5]; (2) Thibodeaux-Hwang model for estimating time-varying emissions of volatile chemicals buried below the soil surface [5, 13]; (3) Cowherd particulate emissions model for estimating emission rates of respirable soil particles [5, 12]; and (4) Jury unsaturated zone model for estimating chemical flux volatilizing from soil and the time-dependent concentration profile within the unsaturated zone [7].

The air dispersion module provides access to two atmospheric dispersion models. The Box model is based on simplified mass balance equations and can be used to estimate concentrations near an emission source with the assumption that steady-state contaminant emissions from the source uniformly mix with a fixed volume of air inside the "box". The Gaussian dispersion models used in ACTS incorporate both steady-state and unsteady state models with the assumption that the distribution of chemicals within the contaminant plume is Gaussian in the vertical and crosswind directions. The models used in this module of ACTS generally follow the analysis discussed in the work of Turner [11]. Figures 3 and 4 show the models included in Air Pathway.

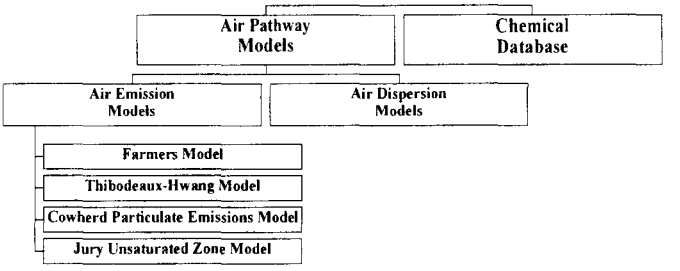

Figure 3. ACTS air emission models.

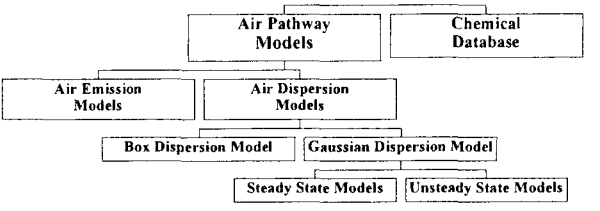

Figure 4. ACTS air dispersion models

3.2 Groundwater pathway module

ACTS groundwater module provides one, two, and three-dimensional analytical solutions, which can be used to simulate transport of dissolved phase contaminants through saturated porous media. In the unsaturated zone, the transport of contaminants is treated as a one-dimensional problem. In

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

developing the groundwater pathway module, the reports, technical papers and books by numerous authors were utilized [5].

For modeling fate and transport in the saturated zone, the ACTS software provides two options: (1) models with constant dispersion coefficients, and (2) models with variable (time-dependent) dispersion coefficients. For constant dispersion coefficients, ACTS contains analytical solutions for models simulating one-, two-, and three-dimensional flow for a variety of source types and boundary conditions. A feature that is built into ACTS is the ability to analyze contaminant source conditions that change over time. This is accomplished using the method of superposition.

The ability to simulate fate and transport with time-dependent dispersion coefficients (simulating spatial variability of dispersion coefficient) makes the ACTS software unique among environmental multimedia modeling software. In this module, ACTS provides general analytical solution for the two-dimensional solute transport equation with variable dispersion coefficients for an infinite aquifer domain. Specific solutions are presented for two contaminant source classifications (point and line sources), three types of contaminant source releases (instantaneous, continuous, or with a user specified initial distribution), and four dispersion coefficient functions (constant, linear, asymptotic, and exponential) as described in Aral [5]. The options that are available in this module are shown in Figures 5, 6 and 7.

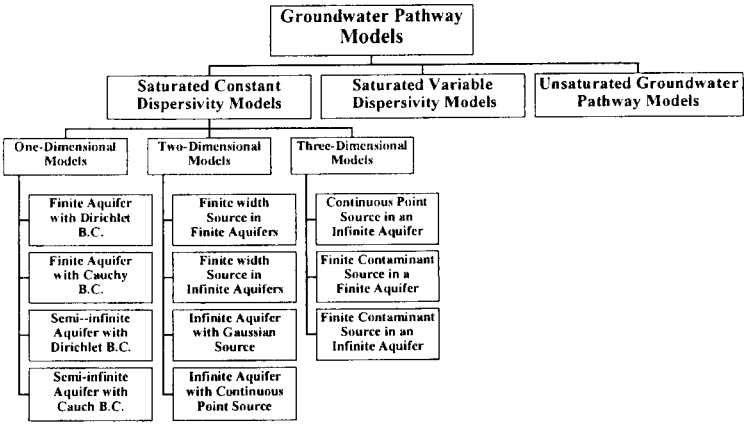

Figure 5. ACTS saturated constant dispersivity models.

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

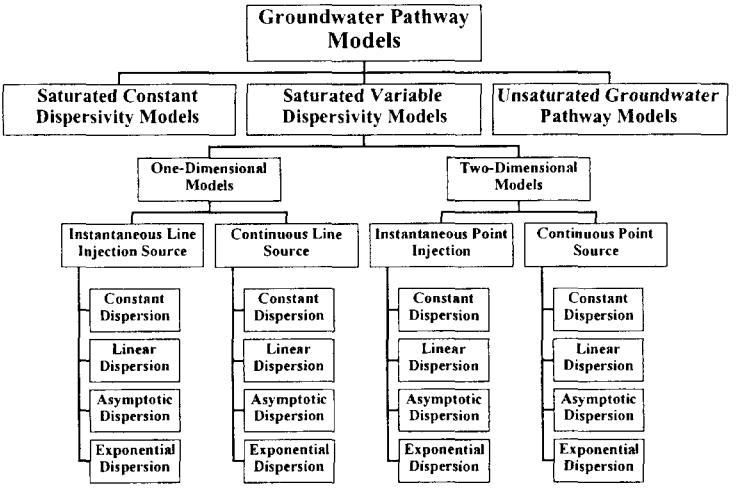

Figure 6. ACTS saturated constant variable dispersivity models

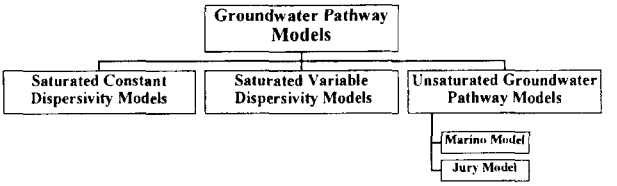

Figure 7. ACTS unsaturated constant dispersivity models

3.3 Surface water pathway module

The surface water pathway module of the ACTS software consists of several analytical models that can be used to simulate the fate and transport of contaminants within a surface water body and the deposition on the shoreline and river sediments from both routine and accidental releases of liquid effluents. A wide variety of mathematical models exit in the literature for evaluating hydrologic transport of contaminants within a surface water body, and these models may range from simple algebraic models to sophisticated multidimensional models requiring numerical solutions. For the ACTS platform, however, the emphasis has been placed on simple analytical models to maintain the "user-friendly" framework of the software. In preparing the surface water pathway module for ACTS, reports and technical papers by numerous authors were utilized extensively [5].

The models implemented in the ACTS software for the surface water pathway are grouped into three main categories. These categories are the near-field mixing, far-field mixing, and sediment transport models. Included in each of these groups are several subcategories of models, that reflect various surface water discharge conditions and surface water body

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

environments. The near-field mixing module includes: (1) the surface point discharge model, (2) the submerged point discharge model, and (3) the submerged multiport diffusers model. The far-field mixing module includes analytical solutions for four water bodies: (1) rivers with transverse mixing or longitudinal advection and dispersion, (2) estuaries, (3) small lakes and reservoirs, and (4) oceans and great lakes. The sediment module includes solutions for three types of water bodies: (1) rivers (Fletcher-Dotson model or Onishi mixing-tank model), (2) estuaries, and (3) lakes. The options that are available in this module are shown in Figures 8, 9 and 10.

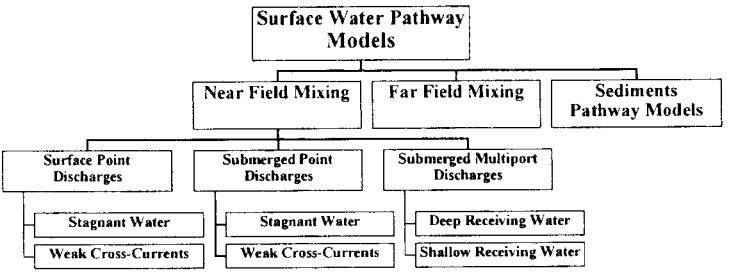

Figure 8. ACTS near field mixing models

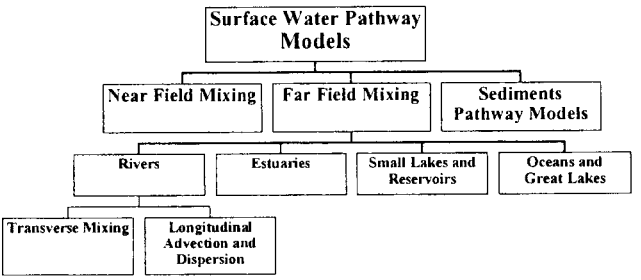

Figure 9. ACTS far field mixing models

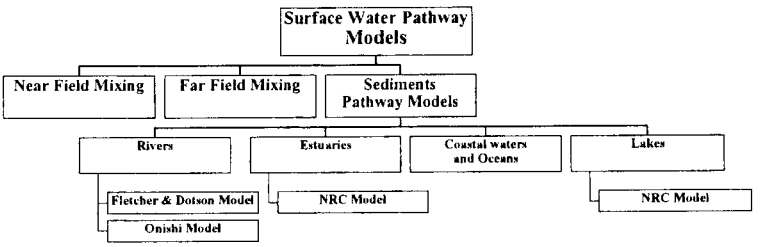

Figure 10. ACTS sediment pathway models

Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

3.4 Monte Carlo simulation module

To analyze cases involving uncertainty in input parameters, the Monte Carlo method is dynamically linked with all pathway models included in the ACTS software (Figure 2). In the Monte Carlo analysis mode, all or a selected subset of input parameters of a particular model may be characterized in terms of six statistical distributions provided in the ACTS software. Thus, a unique feature and advantage of the ACTS software is the ability to conduct uncertainty analysis using Monte Carlo simulation techniques without having to export input parameters and rely on external or third-party software to conduct the uncertainty analysis.

4 Conclusions

In a risk evaluation process, one must link contaminant levels originating from numerous contaminant sources, multimedia fate and transport processes, human or ecological exposure to these contaminants and toxicological impact of these contaminants in a comprehensive sequence of studies. In the spectrum of events that are considered in this process, numerous numerical and/or analytical models are often used. These tools should also include capability for uncertainty analysis. In this presentation an overview of the modeling tools developed and used in MESL and ATSDR are discussed. A brief demonstration of the features and use of the software tool is also included in the conference presentation.

Acknowledgments

The development of the software described in this paper was supported by Cooperative Agreement award number U50/ATU499828-06 by the Agency for Toxic Substances and Disease Registry (ATSDR). The authors would like to express their appreciation to Dr. Henry Falk, Assistant Administrator, ATSDR, for his continued support of the project.

References

[1] Agency for Toxic Substances and Disease Registry (ATSDR). Public Health Assessment Guidance Manual. Lewis Publishers, Chelsea, Michigan, 1992.

[2] Agency for Toxic Substances and Disease Registry (ATSDR). Exposure-dose reconstruction program: overview of strategy, March 1993. Agency for Toxic Substances and Disease Registry, Atlanta, 1993.

[3] Aral, MM, Maslia, ML, Williams, RC, and Abraham, JE (1995). ATSDR's exposure-dose reconstruction program: case studies in public health analysis of exposure to environmental contamination.

Abstracts and Papers, 1995 Pacific Rim Conference on Occupational and Environmental Health, Sydney, Australia, October 4-6,1995.

[4] Aral, MM., and Liao, B. Analytical solutions for two-dimensional transport equation with time-dependent dispersion coefficients. Multimedia Environmental Simulations Laboratory Report MESL-01-96, School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, 1996.

[5] Aral, MM. Analytical contaminant transport analysis system (ACTS). Multimedia Environmental Simulations Laboratory Report MESL-02-98,School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, 1998.

[6] Aral, MM. and Maslia, ML. Multi-Pathway Environmental Exposure Assessment Using "ACTS and "SAINTS" Software. Multimedia Environmental Simulations Laboratory Report MESL-05-98, School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, 1998

[7] Jury, WA, Russo, D, Streile, G, and El Abd, H. Evaluation of volatilization by organic chemicals residing below the soil surface. *Water Resources Research*, 26(1), pp.13-20, 1990.

[8] Marino, MA, Distribution of contaminants in porous media flow. *WaterResources Research*, 10(5), pp. 1013-1018, 1974.

[9] Maslia, ML, Aral, MM, and Radtke, TM, Conducting exposure assessment of populations by integrating environmental transport models, demographic analysis, and geographic information systems. Proceedings, Assessing and Managing Health Risks from Drinking Water Contamination: Approaches and Applications, Rome, Italy, September 13-17, 1994, International Association of Hydrological Sciences Publication No. 233, 221-233, 1995.

[11] Turner, DB. Workbook of atmospheric dispersion estimates: an introduction to dispersion modeling. CRC Press, Boca Raton, Florida, 1994.

[12] U.S. Environmental Protection Agency (USEPA). Rapid assessment of exposure to particulate emissions from surface contaminated sites. Office Washington, DC, 1985.

[13] U.S. Environmental Protection Agency (USEPA). Superfund exposure assessment manual. Office of Remedial Response, EPA Report EPA/540/1-88/001, Washington, DC, 1988.