United States
Environmental Protection
Agency

Environmental Research
Laboratory
Athens GA 30613

Research and Development

EPA-600/S3-84-052 May 1984

EPA

Project Summary

Air Land Water Analysis System (ALWAS): A Multi-Media Model for Toxic Substances

W.A. Tucker, A.Q. Eschenroeder, and G.C. Magill

The Air Land Water Analysis System (ALWAS) is a multi-media environmental model for describing the atmospheric dispersion of toxicants, the surface runoff of deposited toxicants, and the subsequent fate of these materials in surface water bodies. ALWAS depicts the spatial and temporal distribution of contaminant concentrations in a watershed and the air above it. Linked in ALWAS are three submodels that provide for independent and partially coupled usage modes — Dispersion and Deposition of Toxics (DiDOT); a modification, called NPSDEP, of the Nonpoint Source Model; and Exposure Analysis Modeling System (EXAMS).

DiDOT quantifies both wet and dry deposition rates over hourly, daily, and longer averaging periods. NPSDEP describes surface runoff of contaminants and EXAMS simulates their fate in surface waters.

DiDOT, which was developed in the study, is based on a Gaussian plume approach modified to account for deposition. Its meteorological and emission input requirements are similar to those of standard, short-term air quality assessment models. Input parameters include settling velocity, dry deposition velocity, and precipitation scavenging ratio. Guidance for estimating these parameters is provided.

ALWAS is appropriate for evaluating multi-media water quality problems of watersheds as large as 10^4 km^2. The full range of ALWAS capabilities may be exercised for hydrophobic organic chemicals of relatively low vapor pressure. By careful selection and linkage of the submodels, ALWAS may be applied to investigate the environmental behavior of a broad range of toxicants including highly soluble or volatile organics and heavy metals.

The full report incorporates detailed software documentation and a user's manual. The sensitivity of model results to uncertainties in key input parameters is investigated for a hypothetical simulation of benzo(*a*)-pyrene behavior in a small urban watershed.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Most recent progress in environmental modeling has involved a single medium (i.e., air quality, surface water quality, groundwater quality, or biological systems). Many pollutants, however, are released to more than one medium and are subject to intermedia transfer. Significant effects may occur in more than one medium or may be most important in a medium other than the one into which a pollutant is released. These multi-media environmental problems are receiving increasing attention as more of them are recognized (e.g., acid rain, volatilization and ground-water recharge from hazardous waste lagoons, and pesticide losses by volatilization). Multi-media environmental models for assessing such problems have not been available.

This project was intended to partially fill the gap by developing a model to describe the effect of atmospheric emissions, nonpoint source runoff, and point discharges of toxic pollutants on surface water quality. The Air Land Water Analysis System (ALWAS), one of the first models of its type, has not been calibrated or verified for any field situation, although its individual single-media model components have been used frequently on a stand-alone basis. For these reasons, ALWAS is considered a "first generation" multi-media model with room for improvement and extension.

The work included a review and evaluation of existing air quality models to identify any that would be suitable for linking with the Nonpoint Source Model (NPS) and the Exposure Assessment Modeling System (EXAMS). A suitable air model would describe both wet and dry deposition processes for toxic pollutants and would be applicable at a river basin scale (length scales of up to 100 km) over short-time frames in order to interface with NPS.

The review of available air models revealed that no accessible and documented models that fit these criteria were available. Most air quality models do not account for deposition processes adequately. Some that do treat deposition are specifically designed for the acid rain problem and are neither pertinent to toxic pollutants nor to the river basin spatial scale. Models designed to simulate acid rain must follow pollutants up to 1000 km. Consequently, they use multiple-station weather data to define plume trajectories. A local weather station is likely to represent adequately the winds and mixing conditions within a river basin unless the terrain is mountainous. The average separation distance of National Weather Service Stations is greater than the model application scale so model domain will rarely include more than one surface weather station.

From this review, it was apparent that an air quality model had to be developed specifically to link with NPS and EXAMS. The result was the Dispersion and Deposition of Toxics model (DiDOT). The review also showed that minor modifications of NPS and EXAMS were required in order to facilitate their linkage into ALWAS. The NPS modification is called NPSDEP.

ALWAS can simulate the effects on surface water quality of multi-media toxicant releases to the environment. It is most suitable for persistent organic chemicals that tend to adsorb to particulate matter, but ALWAS, or various combinations of its submodels, may also provide valuable multimedia information for metals and more soluble organics, given care in its application.

A technical discussion of the assumptions and rationale for the software development is provided. A User's Guide for ALWAS is presented that emphasizes portions of the software developed specifically for ALWAS. The User's Guide incorporates methods for estimating some of the critical ALWAS input parameters such as the deposition velocity, settling velocity, scavenging ratio, and air degradation half-life (assuming quasi-first order reactions).

The purpose of ALWAS is to assist in the assessment of water quality problems associated with toxic chemicals released to the atmosphere. The combined effect on surface water quality of toxic releases to several media — including air, nonpoint source runoff, direct discharge, and ground water — may also be evaluated. Analysis of ground-water impacts is limited because the user must know the rate and quality of ground-water recharge to the surface water body. The model will be particularly useful in determining the most effective strategies for controlling water quality effects of toxic chemicals regardless of the ultimate source and in evaluating the potential impacts of new chemicals entering commerce.

The basic flow of the model is from air to land surface to surface water body, with the direct transfer from air to surface water body also accounted for. Atmospheric point sources (smokestacks) and area sources (arising from vehicle use, residential heating, etc.) can be simulated. Wet deposition, caused by the scavenging of airborne contaminants by precipitation, is simulated as is dry deposition resulting from such processes as gravitational settling, impaction, or dissolution of gases. Gaseous and particulate contaminants are treated uniformly by the model. This treatment is consistent with recent findings that many toxic organic contaminants that exist as gases at atmospheric pressure and temperature nonetheless will behave as particulates with respect to deposition processes, since the fraction of the airborne mass that is adsorbed to ambient aerosols is primarily responsible for atmospheric deposition. Distinction between contaminants that are primarily particulate, as opposed to those that exist primarily as a vapor, is specified through the gravitational settling velocity, which would be zero for vapors. The dry deposition velocity and the scavenging ratio apply both to vapors and particles.

The model is applicable at a wide range of spatial scales from a calibrated NPS watershed (limited to about 5 km^2) to a major river basin covering 10^4 km^2. Scaling up to 10^4 km^2 presents technical problems in both the atmospheric dispersion model (DiDOT) and NPS. DiDOTs applicability to large spatial scales is limited because one of its assumptions is questionable at downwind distances approaching 100 km. The assumption is that the wind is uniform, allowing for no meandering within the application area. Even under ideal terrain and meteorological conditions, the assumption of uniform winds may only be valid within about 20 km of the measurement point. If the application area consists of mountainous terrain or a river valley, the scale over which the uniform wind assumption applies may be reduced even further. The alternatives to the uniform wind assumption — multiple station wind data or solution of the Navier-Stokes equations — are impractical, however. Both approaches significantly increase computing expenses and would require additional field data not generally available.

ALWAS is a time-dependent model whose fundamental time step is one hour. DiDOT and NPSDEP respond at that time scale whereas EXAMS interfaces with those two models after temporal averaging over a user-determined number of days. The time dependence of DiDOT is different mathematically from that exhibited by NPSDEP and EXAMS. DiDOT uses a standard air dispersion approach that assumes that steady state conditions exist for each hourly time step. This is possible because the atmosphere responds quickly and the contaminants are resident in the air domain for a short period of time. The approximation is inaccurate under low wind speeds of variable direction and at very large distances from the source. The approximation is accurate only if pollutants are emitted to the model's air domain and transported through it within the hour and do not return because of a reversal in wind direction.

On the other hand, both NPSDEP and EXAMS solve differential equations that follow the contaminant through the domain from time step to time step such that current conditions depend on the past history of loading, transport, and transformation. NPSDEP follows a daily time step on days without rain and an hourly time step on rainy days. EXAMS response times are expected to vary widely, depending primarily on the size and flushing time, and the user may specify an appropriate averaging time at integral multiples of one day for loading provided by DiDOT and NPSDEP. The appropriate averaging time would be less than or approximately equal to the contaminant half-life in the aquatic ecosystem as determined by an independent run of the steady state version of EXAMS.

ALWAS is principally designed for organic pollutants that tend to adsorb to particulate matter and are relatively persistent on the land surface. ALWAS, or specific combinations of its component sub-models, may be used to assess multi-media effects of a broader class of pollutants, however, including heavy metals or relatively hydrophilic organics. NPS runoff and subsurface water quality algorithms do not simulate soluble constituents. Both DiDOT and EXAMS, however, account for both soluble and adsorbed contaminants so that these two submodels can be used to determine the effects of direct deposition of hydrophilic organics in water bodies. This feature is especially useful for a lake whose surface occupies a large fraction of its watershed — Lake Superior, for example.

EXAMS is not presently designed to simulate the chemistry of metals in aquatic ecosystems. Air dispersion and deposition of metals, however, is expected to be faithfully simulated by DiDOT, and NPSDEP is suitable for describing land surface processes for relatively insoluble metals. Thus, DiDOT and NPSDEP could be used to study metals loadings to surface water bodies (from air deposition and runoff) and the relative contribution of various source types to the overall loading, but ALWAS could not be used to describe the resulting surface water quality effects.

Other limitations of ALWAS are principally related to the memory and operating system limitations of the PDP 11/70 computer system for which the model has been designed and the costs associated with handling the intermediate outputs of DiDOT that must be transferred to NPSDEP and EXAMS. These affect the spatial resolution of deposition rates and area source emissions and the total number of point sources that may be simulated. These limitations may be overcome very simply within the inherent structure of the model by increasing the capacity of various storage arrays if the model were to be implemented on a larger computer or one with virtual addressing capability. The cost of storing and handling the larger arrays, however, may limit such a scale-up for many applications. The resolution limitations of the software, as it currently exists, may not be a serious drawback for analysis of many deposition-related water quality problems.

An inherent limitation of ALWAS is its inability to appropriately account for volatilization of pollutants from the land or water back to the air. Although EXAMS quantifies the rate of volatilization from the water surface, this contaminant is not fed back to DiDOT as a pollutant air emission; it simply disappears from the model. On the other hand, NPSDEP does not account for volatilization of pollutants from the land surface. The reasons for not accounting for volatilization are several-fold, but principally relate to the technical problems of incorporating feedback into an already complex software structure, particularly in light of the fact that this is a "first-generation" multi-media model. The first-order effect on water quality of deposition of airborne contaminants was of primary interest in this development effort, rather than the second-order effect of volatilization followed by partial redeposition. The limitations suggest that the model be used principally for chemicals having relatively low vapor pressures, although we have not identified a precise range of vapor pressures over which the model is appropriate.

ALWAS may be used to study the environmental impacts of aerial pesticide applications so long as the drift losses, droplet size, effective height of release, and area of application are known. Given this information, ALWAS can be used to evaluate human exposure by inhalation, deposition of pesticide on non-target areas, and the combined impacts from drift and deposition. Use for pesticide evaluation may encounter some problems, however. First, DiDOT describes phenomena having characteristic length scales of 10^3 to 10^5 meters ($1\text{-}10^4 km^2$). On the other hand, pesticide applications may only extend over 10^2 - 10^3 meters (0.01 - 1 km^2). DiDOT cannot resolve the actual resultant spatial variability in pesticide concentrations. ALWAS may be used to simulate intermittent sources; however, the procedure would be cumbersome if many intermittent sources were included. This factor, coupled with the mismatch of length scales, suggests a reasonable approach to simulating the effects of pesticide application in a large river basin. Individual pesticide spraying events would not be simulated; rather, large portions of the basin would be assumed to be treated on specific days. The model would not resolve fine spatial variations.

Other, perhaps more serious, drawbacks to the use of ALWAS for pesticides are inherent in NPS, which does not account for volatilization and does not simulate the subsurface movement of soluble contaminants.

Methods are available for estimating drift losses, droplet size, and effective height of release for pesticidal input to ALWAS. Several investigators have performed field studies and developed empirical models for estimating the parameters of droplet release, and these may be useful for guidance in developing ALWAS input parameters for application to pesticide spray drift and deposition.

ALWAS has been applied in a hypothetical simulation of benzo(*a*)pyrene behavior in a small urban watershed.

Features

DiDOT

DiDOT can handle two contaminants in a single run. To interface with NPSDEP, one of these contaminants must be total suspended particulates and the other one may be any toxic pollutant, either vapor or particulate. Under the recommended mode of operation, the model simulates the behavior of the total airborne contaminant, which may be partially vapor and partially adsorbed to ambient aerosol. DiDOT does not explicitly account for the particle size distribution of particulate contaminant, so the deposition parameters should represent the mass weighted average of the distribution of the parameters. Methods for estimating these parameters are based on the mass median diameter of the particulate contaminant.

DiDOT's use of meteorological and source characteristics data is consistent with standard procedures used in most EPA-supported air quality models. This feature is intended to make the model easy to use for those familiar with standard air modeling procedures. DiDOT is also consistent with standard air modeling procedures in its use of Gaussian dispersion algorithms, plume rise formulas, ASME dispersion parameters, and stability classes based on wind speed and solar radiation. Its method for accounting for limited mixing under an inversion lid is also consistent with standard approaches.

DiDOT diverges from standard air quality models in its deposition algorithms. The dispersion algorithms used in DiDOT represent a synthesis and application of current research and mathematical analysis of the deposition process. To describe the dry deposition process from point sources, DiDOT applies a rigorous analytical solution that accounts for both gravitational settling and surface depletion.

The surface depletion model correctly accounts for the fact that pollutants are deposited on the ground, thus reducing ground-level concentrations relative to the values that would be observed if deposition were not occurring, leading to a vertical gradient of concentration at the surface. The source depletion model, on the other hand, preserves the Gaussian shape for the vertical concentration profile. It accounts for upwind deposition by adjusting the source emission rate, i.e., subtracting the surface integral of the upwind deposition flux from the emission rate. This approximation adjusts the source strength artifically by adjusting the volume of material in the plume in proportion to the concentration, rather than a surface depletion model in which deposition occurs at the ground. The assumptions of no deposition or source depletion result in overestimation of ground level concentrations. For the source depletion model, this leads to an over-estimate of the deposition rate as well.

Wet deposition processes are simulated via a scavenging ratio approach. The basic assumption is that the rainfall concentration is proportional to the ground level air concentration. Theoretically, several precipitation scavenging processes should not follow this pattern. These include "in-cloud" scavenging or rainout and the irreversible scavenging of an elevated plume. Nonetheless, for many contaminants under diverse meteorological conditions, the assumption proves relatively accurate. The scavenging ratio for toxic organic pollutants can be estimated to within an order of magnitude. During rainfall, DiDOT does not account for upwind wet deposition in determining the ground level air concentration.

Although DiDOT is primarily designed to simulate dispersion from continuous sources, it can be adapted to simulation of an intermittent source such as a chemical spill, or a pesticide application. This is accomplished by performing multiple runs with a selected subset of meteorological data.

NPSDEP

NPSDEP is the result of relatively minor modifications to NPS. NPS is a continuous simulation model that represents the generation of nonpoint source pollutants from the land surface. The model simulates surface and subsurface hydrologic processes, snow accumulation and melt, sediment generation, pollutant deposition, and pollutant transport for any specified period of meteorological data.

NPS inputs include parameters that allow the user to adjust the model to a specific watershed. Most of these parameters are specified by physical (observable) characteristics of the watershed; however, several of the parameters cannot be determined from observations, and the model must be calibrated before application to any watershed.

NPS permits simultaneous simulation of five user-specified contaminants. These contaminants are assumed to migrate with sediment entrained in surface runoff. Consequently, subsurface water is assumed to be clean. This constraint limits the validity of the model to pollutants that are strongly associated with sediments including hydrophobic organics and heavy metals. The contaminants are assumed to be conservative on the land surface, which implies that the model is most useful for non-volatile, persistent pollutants. For volatile, degradable contaminants, NPS loadings outputs may be useful as an upper bound.

NPS allows monthly variations in land cover, pollutant deposition (accumulation) and pollutant removal (e.g., by street cleaning).

The only significant modifications to NPS that are incorporated in NPSDEP relate to the deposition processes simulated by DiDOT. Where NPS allowed monthly variations in deposition rates, NPSDEP accepts daily variations. NPS permitted land-use-dependent ratios between contaminant and sediment (potency factors) that were assumed to be the same for eroded sediment and deposited sediment, but NPSDEP allows two separate potency factors per land use — one for eroded sediment from the land surface and one for the deposited sediment from DiDOT. Monthly variations in the potency factors are permitted. Thus, NPSDEP can simulate the combined impacts of deposited contaminant and some independent source of nonpoint pollution.

EXAMS

EXAMS describes the transport and chemical transformation of organic chemicals in surface water bodies. It is a multiple compartment model in which the cells are linked by advection and turbulent exchange. Cells may contain mostly water (littoral, epilimnion, hypolimnion, etc.) or mostly sediment (benthic), with different input requirements. Each cell consists of water, sediment, and biomass in variable proportions.

Chemical processes are simulated on the basis of either equilibrium partitioning or first-order kinetic processes. Equilibrium partitioning among a (5 x 3) matrix of possible forms is established for up to five ionic forms (valences of −2, −1, neutral, +1, +2) and between dissolved, sediment adsorbed, and biosorbed phases. Processes simulated by first-order kinetics include hydrolysis, oxidation, volatilization, microbial transformation, and photolysis.

The dynamic version of EXAMS used by ALWAS determines the dynamic response to time-varying loading rates.

Inputs

ALWAS requires six basic categories of inputs — meteorological data, pollutant source data, pollutant fate properties, calibration data for NPSDEP, characteristics of the physical environment (primarily for NPSDEP and EXAMS), and interfacing data.

Meteorological Data

Each sub-model of ALWAS requires different kinds of meteorological data. Both DiDOT and NPSDEP require hourly meteorological data in formats compatible with standard reporting formats of the National Weather Service.

Pollutant Source Data

DiDOT and EXAMS require data characterizing sources of the pollutant to the environment. DiDOT treats three kinds of pollutant sources: point sources, traditional area sources, and distant city-sized area sources. Traditional area sources represent air emissions from transportation, small institutional and commercial sources, residential heating or solvent use, land use activities — in short, all small sources that are too numerous or otherwise inconvenient to inventory individually. Distant cities are treated by a virtual point source approach. The data required to characterize sources in DiDOT are typical of those required by other air quality models, and are available in standard state-maintained emissions inventories.

Pollutant Fate Properties

Chemical specific inputs are required primarily by DiDOT and EXAMS. DiDOT uses the settling velocity, deposition velocity, scavenging ratio, and atmospheric degradation half-life. These, in turn, may be estimated using procedures presented in the report and knowledge of particle size, Henry's law constant, vapor pressure, and molecular weight, or other fundamental properties. EXAMS requires similar inputs, solubility in water, octanol/water partition coefficient, rates of hydrolysis, photolysis, and oxidation.

Calibration Data for NPSDEP

NPSDEP requires calibration data — time series of water flow and quality at the discharge point of an upland watershed. The availability of such data is critical to the site-specific application of ALWAS but may not be needed for application to generic, "typical" environments.

Characteristics of the Physical Environment

NPSDEP requires as input various physical features of the watershed — area, length of overland flow path, slopes, elevation, land use characteristics, portions of watershed that are pervious and impervious, soil characteristics, etc.

EXAMS relies extensively on a user-specified description of the water body, since it does not solve equations that describe its hydraulics. If multiple cells are specified, the user must quantify the advective and turbulent exchanges between cells. This demands an in-depth knowledge of flow patterns in the water body, which may be achieved via field studies and/or independent numerical modeling using models that solve the equations of motion. In lieu of such information, the user may rely on the descriptions of typical aquatic ecosystems contained as a default input data file within the EXAMS data base.

Interfacing Data

The geometrical relationships between the DiDOT receptor locations (points at which deposition rates are calculated), NPSDEP catchments, and EXAMS cells are within this category. Each of the models has a unique way of describing specific locations within its domain, and these are interrelated in a straightforward fashion.

As should be clear from the foregoing discussion, the data requirements are extensive, leading to significant costs in data gathering, formatting, and handling prior to full implementation of ALWAS. Most of these inputs, however, are routinely available from environmental data banks, including those maintained by EPA, the National Climatic Center, and the U.S. Geological Survey.

Outputs

The fundamental ALWAS outputs are the surface water quality outputs presented by EXAMS. These include the total contaminant concentrations, as a function of time, in each EXAMS cell, and the partitioning of that total contaminant among various ionic, dissolved, sediment adsorbed, and biosorbed forms. DiDOT also presents summary air quality outputs including long-term average concentrations over the watershed and the extreme hourly and daily average concentrations. NPSDEP provides flow, sediment transport, and toxicant loading outputs at monthly and annual intervals, as well as short term output for major storms.

William A. Tucker, Alan Q. Eschenroeder, and Gary C. Magil are with Arthur D. Little, Inc., Cambridge, MA 02140.

Kenneth F. Hedden *is the EPA Project Officer (see below).*

The complete report, entitled "Air Land Water Analysis System (ALWAS): A Multi-Media Model for Toxic Substances," (Order No. PB 84-171 743; Cost: $34.00, subject to change) will be available only from:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at:

Environmental Research Laboratory
U.S. Environmental Protection Agency
Athens, GA 30613

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

BULK RATE

Official Business
Penalty for Private Use $300

PS 0000329
U S ENVIR PROTECTION AGENCY
REGION 5 LIBRARY
230 S DEARBORN STREET
CHICAGO IL 60604

☆ U.S. GOVERNMENT PRINTING OFFICE: 1984-759-102/964