ALASKA DEPARTMENT OF ENVIRONMENTAL CONSERVATION
Division of Spill Prevention and Response
Contaminated Sites Program

Fate and Transport Modeling Guidance

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TABLE OF CONTENTS

1.0 Introduction

Fate and transport models have become an integral tool for contaminated site investigations and the selection of remedial techniques nationwide. Under the site cleanup rules (18 AAC 75.325-390), a responsible party may propose an alternative cleanup level for the migration to groundwater pathway using site-specific data and a fate and transport model (18 AAC 75.340(e)(2)). However, modeling for other pathways, such as contaminant migration to surface water, air pathway modeling, and other pathways and receptors is also accepted and in some cases may be required. The Alaska Department of Environmental Conservation's (ADEC) Contaminated Sites Program (CSP) uses contaminant fate and transport models to help determine site specific aquifer characteristics; as tools for predicting contaminant concentrations at exposure points; and to assist with the evaluation and selection of the most effective remedial alternative. CSP recognizes that the use of fate and transport models will continue to grow, and regulatory agencies will be relying on information obtained through modeling to assist with site management decisions. When adequately constructed, documented, and verified fate and transport models can provide an acceptable line of evidence supporting risk management decisions.

Fate and transport modeling is most appropriately used in conjunction with other lines of evidence. CSP project managers want to ensure that modeling results are protective of human health and the environment. The effective use of predictive fate and transport models as management decision tools requires the establishment of their functionality, performance characteristics, and applicability to the site being considered. Generally, models transform empirical values of input parameters into predictions of chemical concentrations in media which can then be utilized to estimate risk.

Note: Fate and transport model input parameters are just as important as the mathematical components of the model and therefore results critically depend on model inputs.

The purpose of this guidance is to provide general guidelines and criteria for the selection and application of fate and transport models, and to promote the appropriate use of models. This guidance is not a substitute for professional judgment that must be applied in the selection and application of modeling. This guidance considers any predictive tool that attempts to describe either the past or future fate and transport of contaminants to be either qualitative or quantitative, analytical or numerical. The guidance outlines the criteria for selecting a model, and the elements to evaluate and document to ensure model calculations are appropriate for their intended use.

2.0 Selecting a Modeling Program in the Public Domain

The department limits modeling programs to those which are in the public domain for the following reasons:

1. Proprietary modeling programs typically require purchase by CSP which adds to the overall cost of the project. These costs must in turn be recovered by the responsible party.
2. Contaminated site project files, including results of modeling and the tools used, are considered public information and must be available to the public for review.
3. As a government regulatory department, not a research organization, CSP lacks the necessary staff resources to evaluate computer models that are not in the public domain. Review of mathematical computations and computer source code is time intensive, requires specific staff

expertise; therefore review of unpublished private domain modeling programs for individual sites cannot be feasibly accomplished by CSP staff.

For the purposes of this guidance, "public domain modeling programs" are defined as readily available, without access fees, widely distributed, and generally accepted models. The majority of the public domain models have received extensive peer-review, and case histories describing their limitations and drawbacks have been published in the scientific literature. Many of the public domain modeling programs were developed by government agencies, such as the U.S. Environmental Protection Agency (USEPA), U.S. Geological Survey (USGS), and U.S. Department of Defense (DoD). When a public domain program has been modified it can no longer be considered a public domain program. A modified public domain model can still be proposed for use if it is peer reviewed, widely distributed, and generally accepted. Compared to public domain modeling programs, proprietary modeling programs, without proper review and general acceptance, provide a lower level of confidence in making site cleanup decisions.

Choosing the appropriate model requires site-specific evaluation that considers the heterogeneous nature of transporting media, contaminant types and mixtures, and the distribution of the contamination.

Although the department does not maintain a list of approved fate and transport models, many sources provide publicly available models, downloadable software and manuals. Some of these are listed below. Consultants are encouraged to work with the CSP project manager assigned to their specific site prior to proposing to use a model or submit modeled data.

The following websites offer public domain models:

U.S. Environmental Protection Agency Vapor Intrusion Screening Level (VISL) Calculator. https://www.epa.gov/vaporintrusion/vapor-intrusion-screening-levels-visls. The United States Environmental Protection Agency (USEPA) constructed this calculator to support vapor intrusion evaluation. The excel spreadsheet calculator lists volatiles chemicals, provides recommended screening-level concentrations for indoor air, soil gas, and groundwater, and allows calculation of site-specific screening levels based on user-defined target risk levels, and exposure scenarios.

Integrated Groundwater Modeling Center, Colorado School of Mines (IGWMC). http://igwmc.mines.edu/software/freeware_list.html The Integrated GroundWater Modeling Center (IGWMC) is an internationally oriented information, education, and research center for groundwater modeling. Provides downloads for free modeling software in the public domain.

U.S. Geological Survey. http://water.usgs.gov/software/ The software and related documentation on these web pages were developed by the U.S. Geological Survey (USGS) for use by the USGS in fulfilling its mission. The software can be used, copied, modified, and distributed without any fee or cost. Use of appropriate credit is requested. The software is provided as a minimum in source code form as used on USGS computers.

Center for Exposure Assessment Modeling (CEAM). https://www.epa.gov/exposure-assessment-models CEAM was established in 1987 to meet the scientific and technical exposure assessment needs of the United States Environmental Protection Agency (USEPA) as well as state environmental and resource management agencies. CEAM offers exposure assessment techniques for aquatic, terrestrial, and multimedia pathways for organic chemicals and metals.

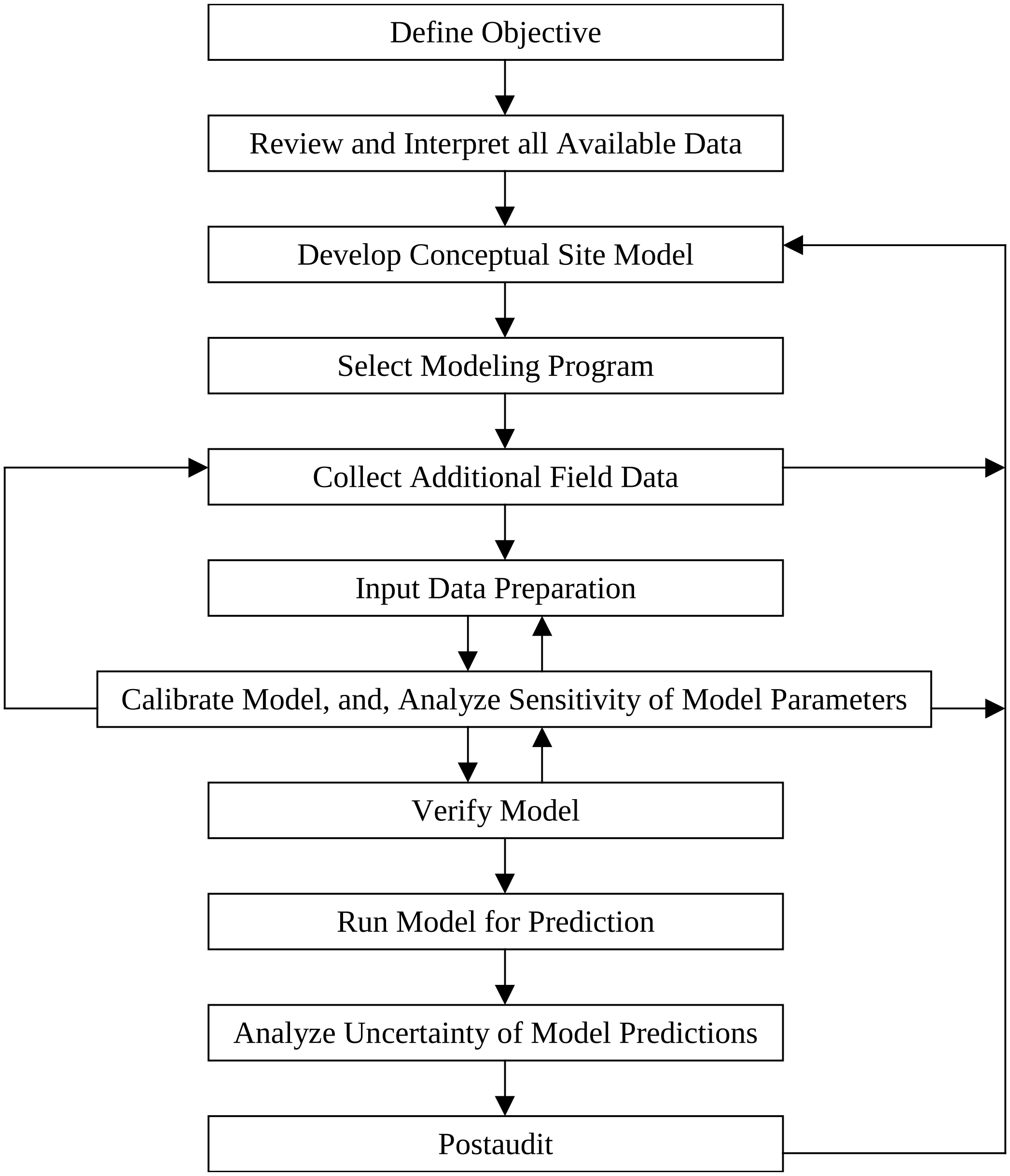
USEPA OnSite OnLine Tools for Site Assessment: https://www.epa.gov/land-research/models-tools-and-databases-land-and-waste-management-research Contains a suite of calculators for assessing subsurface contaminant transport.

Army Corps of Engineers. http://www.erdc.usace.army.mil/Media/Fact-Sheets/Fact-Sheet-Article-View/Article/476776/groundwater-modeling-system/ The Department of Defense, in partnership with the Department of Energy, the U.S. Environmental Protection Agency, the U.S. Nuclear Regulatory Commission and 20 academic partners, has developed the DoD Groundwater Modeling System. GMS provides an integrated and comprehensive computational environment for simulating subsurface flow, contaminant fate/transport, and design of remediation systems.

3.0 Modeling Work Plan

Figure 1 outlines the steps involved in contaminated sites model application. A thorough site characterization effort must precede any modeling at a contaminated site. If a responsible party will use modeling, a modeling work plan must be submitted to CSP for approval prior to use. The modeling work plan may be a subsection of a comprehensive work plan that describes all proposed work at a contaminated site. The proposed modeling work plan should include the components in the following subsections.

Figure 1 Steps in Contaminated Sites Model Application



3.1. Modeling goals

The goals and reasons for the modeling should be specific and measurable. For example, modeling might be conducted in order to predict benzene concentrations in groundwater at a certain distance from a source of specified concentration, or, the prediction of vapor concentrations arising from a well-defined source in an enclosed space of specific dimensions. Having a specific goal helps determine, at a later time, if the modeling exercise has achieved the goal.

3.2. Conceptual Site Model for Modeling

Based on available data, regional inferences, and professional judgment, a geologic and hydrogeologic conceptual site model should be prepared and included in the modeling work plan. Please see ADEC's Policy Guidance on Developing Conceptual Site Models, available at: http://dec.alaska.gov/spar/csp/guidance_forms/csguidance.htm. The conceptual site model should be graphical (maps, cross-sections, block diagrams) with associated descriptions. If the conceptual site model will be simulating ground water flow, it must indicate whether subsurface is a porous or a fractured medium. It should consider chemical and physical properties of the contaminants that may affect their movement. The conceptual site model must quantify the presence of permafrost and corresponding influence on fluid flow, if applicable. It must describe the temperature and pressure conditions of the transporting media.

For modeling of the vapor intrusion pathway, the conceptual site model should be developed by conducting thorough building surveys. The building surveys at a minimum should document building foundations, ventilation systems, preferential pathways, sensitive receptors, existence of background contaminant sources and building occupancy. Finally, the conceptual site model should also discuss data gaps, assumptions, and uncertainties and it should be continually refined as more data is obtained.

3.3. Technical Approach

Narrative should be included which describes technical considerations necessary to achieve the stated goal, such as, numerical or analytical, modeling dimensions (1-D, 2-D or 3-D), saturated or unsaturated flow, multiphase or single phase, reactive or non-reactive, dispersion, retardation, and/or degradation.

3.4. Computer Model

The work plan should identify the computer model selected. The capacities and limitations of the model should be discussed, including how specifically it applies to the site-specific conceptual site model. Site-specific input parameters are preferred. The work plan should reference the specific reports where the data has previously been presented in addition to presenting the site-specific data, sample numbers, dates collected, and specific sample locations. Non site-specific input parameters should have good justifications. The source of these parameters should be identified, for example, USEPA's Soil Screening Guidance (1996) documents, ADEC Contaminated Sites' *Guidance on Developing Cleanup Levels under Methods Two and Three* (2016) or scientific literature. The work plan should specify if input parameters have been assigned assumed values and justify the basis for the assumptions. The fate and transport parameters should be for the temperature and pressure conditions described in the conceptual site model versus standard temperature and pressure conditions. Submit computations to derive the parameter values at site-specific temperature and pressure conditions from the standard temperature and pressure conditions. Boundary and initial conditions should be described.

3.5. Sensitivity analysis

The use of extreme or non-representative assumptions or parameter values is a common weakness of mathematical models. Therefore, it is important to identify the critical parameters and conduct a sensitivity analysis for the most critical parameters. A sensitivity analysis is the process of varying inputs over a reasonable range (range of uncertainty in the value of the parameter) and observing the relative change in model response. The sensitivity of one parameter versus others is also evaluated. The purpose of the sensitivity analysis is to demonstrate the sensitivity of the simulations by varying input values. Sensitivity analyses are also beneficial in determining the direction of future data collection activities. Data for which a model is relatively sensitive would require future characterization, as opposed to data for which the model is relatively insensitive, which would not require further field characterization (Ohio EPA, 2007). See also Anderson and Woessner (1992), Zheng and Bennett (1995), and ASTM D5611-94 (2016).

When the input parameters vary widely and the model is designed to ultimately predict a contaminant concentration, an upper or lower 95 percentile confidence limit of the average should be used on the conservative side dependent on the influence of the predictive contaminant concentration for an exposure assessment. If the range of parameter values is known with confidence, then parameters should be chosen to represent the bounding case of maximum risk to human health and the environment (i.e. worst case scenario).

3.6. Model calibration

The work plan should include a plan to calibrate the model to reproduce appropriate field-measured parameters. The field-measured parameters will be different for different models and for different transporting media. Calibration establishes that the model can reproduce field conditions. Models have no predictive value if they cannot reproduce observed concentrations.

Calibration consists of changing values of input parameters in an attempt to match field conditions within acceptable criteria. Calibration requires that field conditions be properly characterized. Lack of proper characterization may result in a calibration to a set of conditions that do not represent actual field conditions.

Since some inputs are highly variable and the data is limited, these values are typically adjusted and extrapolated through an iterative process until an acceptable "match" is made. As calibration proceeds, data gaps often become evident. The modeler may have to redefine the conceptual site model and collect more data. When the best calibrated match is achieved, a final input data set should be established and demonstrated to be reasonable and realistic. The degree of accuracy and how precise the match should be is governed by the defined purpose of the modeling. Each modeler and reviewer will need to use professional judgment in evaluating the results. There are no universally accepted "goodness-of-fit" criteria that apply in all cases. However, it is important that the modeler make every attempt to minimize the difference between model-simulated and field conditions. Additional information for calibrating a ground water model can be found in ASTM D5981-96 (2008; Ohio EPA, 2007).

Documenting the degree of model calibration is important since it helps demonstrate how well the model estimates reality. Documentation can be in two forms: qualitative and quantitative. Qualitative is the simpler of the two, and involves using words, maps, tables and graphs to demonstrate that the model-derived predictions are consistent with the behavior that is expected based on field data. Quantitative analysis involves a statistical comparison of modeled results to values measured in the field. Many model post-processors include statistical packages that can provide an efficient tool for quantifying a model's degree of accuracy (Ohio EPA, 2007).

For initial assessments, it is possible to obtain useful results from models that are not calibrated. Potential applications include screening and guiding data collection activities. Risk calculations should not be made from uncalibrated model results unless a sensitivity analysis was conducted and critical input values represent worse case scenarios (Ohio EPA, 2007).

3.7. Model verification

Plan to reproduce a second set of field data using the set of calibrated parameter values and stresses. Because of uncertainties in the calibration, parameter values of a calibrated model may not represent the contaminated site conditions. If the parameter values established during calibration are changed during verification, the model should be calibrated again with the changed parameter values. By reproducing a second set of field data, model verification establishes greater confidence in the model. With only one set of field data, it may not be possible to verify a model. A second set of field data collection is often possible at sites with multiple observation wells. CSP may accept a calibrated but unverified model for predictions as long as careful sensitivity analysis of both the calibrated and the predictive models are performed and evaluated.

3.8. Uncertainty analysis

Describe the uncertainty associated with the modeling of a given problem. The uncertainty in modeling exists because uncertainties in transport mechanism, sink/source within the transporting media, temporal and spatial variation of model parameters, initial and boundary conditions, and, matrix heterogeneity.

3.9. Prediction

Upon completing calibration, sensitivity analysis, and field-verification, the model can be used to predict future scenarios.

The predictive simulations should be viewed as estimates and not as a certainty. There is always some uncertainty in predictive models. The simulations are based on the conceptual site model, the input parameters, and the model algorithms. The model's limitations and assumptions, as well as the differences between field conditions and the conceptual site model will result in errors in simulations. In an attempt to minimize these errors, models are calibrated by adjusting inputs until the model closely reproduces field conditions within some acceptable criteria. However, the time period over which a model is calibrated is typically small compared to the length of time used for predictive simulations. Relatively small errors observed during the time period over the model calibration or history matching may be greatly magnified during predictive simulations because of the larger time period typically used in predictive simulations.

The growth in errors resulting from projecting model simulation into the future may need to be evaluated by monitoring field conditions over the time period of the simulation or until appropriate cleanup criteria have been achieved.

Predictive simulations are often conservative. That is, given the uncertainty in model input parameters and the corresponding uncertainty, model input values are selected that result in a "worst-case" simulation. Site-specific data may be used to support a more reasonable worst-case scenario. Or stated another way, site-specific data should be collected to limit the range of uncertainty in predictive models. If long-term action is necessary, it may be necessary to refine and update the model as additional data are collected and future stresses are observed (see Post Audit

Section) (Ohio EPA, 2007).

3.10. Post-audit of the modeling

Plan to conduct post-audit several years after the modeling study is completed. Collect new field data to determine whether the prediction was correct. Analyze what went wrong with modeling and means to improve it. If site remediation work reduces risks posed by the contaminated site to acceptable levels, and, monitoring proves that the risks are acceptable, a post-audit may not be necessary.

A sufficiently calibrated and field-validated model uses historical data to predict the future; however, it is difficult to predict the magnitude, location, and duration of future stresses. As a result, performance monitoring (validation) of predictive simulations often show the flow system did not behave as predicted. Post-audits utilize the additional field data collected after the model study is completed to evaluate the accuracy of the prediction. The new data should be used to recalibrate the model to update and improve the simulation. These periodic updates allow appropriate "corrective actions" to be made (e.g., modifications to an extraction well system). Anderson and Woessner (1992) and Konikow (1986) provided discussions on post-audit methods that can be utilized to re-calibrate a model. Many investigators have suggested not extending transient predictive simulations for more than twice the number of years for which there is transient calibration and verification data (Ohio EPA, 2007).

4.0 Modeling Report

A final modeling report should describe model predictions, technical analysis, input parameters, results of parameter sensitivity and model uncertainty analysis. Critical input and output files should be in the report's appendix, also in portable computer disks. The report should have sufficient information for an independent reviewer to duplicate model runs.

5.0 Model Review

CSP may hire a term contractor to review the modeling work plan and modeling results. In accordance with state law, all expenses incurred for project oversight, including review of fate and transport models, must be reimbursed by the responsible party. If the modeling program is not available within CSP, the consultant must provide a copy to the department, complying with any copyright laws. Model acceptance may require contaminant levels monitoring, and, institutional controls.

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