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Democratized Environmental Modeling: A New Paradigm

By Jeffrey T. Rominger, Ph.D. and John M. Kondziolka, M.S., E.I.T.

Increased access and ease of use have made modeling a staple in environmental projects of all kinds.

It is tempting to take modeling results at face value – to simply trust that the models encountered in environmental work, powered by complicated software and rendered with enhanced graphics, must be right.

Models have become omnipresent in environmental work. The National Research Council broadly defines an environmental model as "a simplification of reality that is constructed to gain insights into select attributes of a particular physical, biological, economic, or social system" (NRC, 2007). In other words, a model is a tool used to help answer a question about the environment. These models can address groundwater, surface water, air, and receptor exposure, among other topics. Today, models are commonly relied upon by both sophisticated as well as novice users in almost every aspect of environmental work, including site investigation, remedial design, cost allocation, and exposure and risk assessment, to the point that the use of environmental models has now been "democratized." However, the widespread use of models and the increasing reliance on complicated, parameter-driven models does not necessarily mean that these models are inherently trustworthy or that the answers

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I N S I D E

Letter from the Editors

May 2020

Dear Colleague,

In this issue of *Trends*, we explore the topic of environmental modeling.

Our first article discusses the widespread use and increasing reliance on modeling in a broad range of scientific scenarios, including limitations and drawbacks to consider. The second article provides several examples of novel but scientifically defensible environmental model applications that demonstrate the versatility and evolving capabilities of environmental modeling. The third article introduces the concept of the living site model, how it can be applied, and its advantages.

Gradient contributors to this *Trends* issue include Drs. Jeffrey T. Rominger and Amy Dale; John Kondziolka, M.S.; Matthew Mayo, M.S., GISP, CPG, P.G.; and Shuo Zhao, M.S. Contributing author Dr. Kelly G. Pennell of the University of Kentucky wrote the guest editorial on vapor intrusion modeling.

We would also like to acknowledge the contributions of Bruce Jones, who has been the long-time graphic designer for our Trends newsletter. After working on over 75 issues, he retired this winter. Thank you, Bruce!

We hope this issue of *Trends* illuminates the myriad applications of environmental modeling and best practices for their use.

Yours truly,

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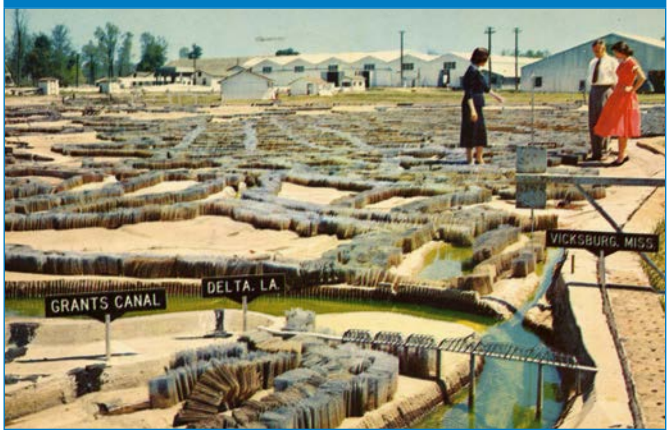
they provide to environmental questions are getting more "right." In fact, it is essential for modelers and non-modelers alike to understand the limitations of models and to be able to critique potentially unreliable model results.

THE MISSISSIPPI RIVER BASIN MODEL WATERWAYS EXPERIMENT STATION



Source: *Atlas Obscura*. Old Postcard of Site. Miss Preservation (Public Domain).

Several factors have contributed to the increased use and availability of environmental models, perhaps none more so than access to computing power. Whereas in the 1970s computers were scarce resources owned by large institutions, today laptop computers owned by individuals are capable of running many environmental models. Not only are computers cheaper and easier than ever to run, there is now widespread computer literacy among scientists as well as laypeople, making models more accessible than ever. And, as computing costs have come down, computational implementations of models are now cheaper, more versatile, and easier to implement than many laboratory experiments or physical models, making computer-based modeling the default tool for many applications.

The current paradigm of widely accessible computer-based models was not always the case. Following flooding in the Mississippi River Basin in the early 20th century, the U.S. Army Corps of Engineers developed a large-scale physical model of the Lower Mississippi Basin to model the impacts of dams and control structures on flooding and other hydrologic events (see figure). The model was enormous, covering nearly 200 acres, took decades to construct, was expensive to maintain and run, and was exclusive – very few had access to it. In many senses, this modeling approach was the antithesis of the democratized models that are widely available to users today. This Mississippi River physical model was abandoned in the 1970s (Cheramie, 2011) in favor of computer-based models of the river that were the forerunners of models in use, and widely available, today.

Whether computer-based or not, a commonality among environmental models is that they require judicious selection of the input parameters that affect model behavior and results. For example, in groundwater modeling, key parameters may include how strongly a chemical binds to soil particles. In air dispersion modeling, we need to know how strong the turbulent fluctuations are in air currents that cause mixing of chemical plumes. In the case of flooding in the Mississippi River Basin Model, key parameters include the amount of flow in the hundreds of small tributaries to the Mississippi as well as the channel "roughness" values, which determine how quickly water can move downstream. Lack of knowledge of key parameters can severely impair the reliability of the model results, though uncertainty in key parameters may not be immediately apparent to consumers of model results.

For this reason, there is a truism in environmental modeling that the results of a model are only as reliable as the quality of the input parameters and assumptions that are used to initialize, bound, and parameterize the model. Put more plainly, "Garbage in yields garbage out." It is tempting to take modeling results at face value – to simply trust that the models encountered in environmental work, powered by complicated software and rendered with enhanced graphics, must be right. This presumption is enabled by accessible user interfaces that may embed algorithms and key parameters in hidden lines of code, making them less apparent and less easily scrutinized. However, an environmental model is not just a software interface and a set of results. The model is every input, every algorithm, and every assumption used to initialize and run the scenario. Both modelers and non-modelers who rely on the model results must be familiar with, at minimum, the rationale for the model input and algorithm selection, the assumptions on which the model relies, and how to correctly interpret the model results.

In closing, modelers and non-modelers should ask the following types of questions in order to assess the reliability of a model and its results (see also U.S. EPA, 2009):

- Has the model been appropriately calibrated and validated, and has it undergone sensitivity testing?
- Do reliable data support the input values?
- Are the assumptions supporting the model appropriate?
- Which physical processes are not modeled, and can these be reasonably neglected?
- Is the model's level of complexity proportional to its intended objectives?

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The Right Tools for the Job: Versatility in Environmental Modeling

By Amy L. Dale, Ph.D and Matthew Mayo, M.S., GISP, CPG, P.G.

The continuous growth of new applications for modeling in environmental projects inspires creativity but requires discretion on the part of the scientists responsible.

Virtually any process can be described mathematically, and the potential applications of mathematical models to evaluations of chemical releases are seemingly endless. The closely related fields of chemical exposure modeling and contaminant fate and transport modeling as we know them today have undergone significant improvements and expansions over time, with thousands of researchers across numerous fields discovering new techniques each day and publishing an ever-evolving set of software tools applicable to an ever-widening set of issues. Regulators have long since recognized the value and validity of mathematical models in the assessment of chemical risks, and today models of all kinds are widely accepted as a core component of scientific analyses.

One of the major responsibilities of a mathematical modeler is knowing which tools are available and which is right for the job.

One of the major responsibilities of a mathematical modeler is knowing which tools are available and which is right for the job. Moreover, solving complex problems often requires linking several models together or applying an established model in a novel way. In this article, we highlight some innovative but scientifically acceptable uses of environmental models that demonstrate the versatility and wide applicability of environmental modeling.

Ignition Risks from Chemical Leaks: The dispersion of a gaseous leak will vary depending upon the characteristics of the gas and the space where the leak occurs – namely, gas density and viscosity, the dimensions of the space, the presence of obstructions, the strength and direction of air flow, *etc.* Computational fluid dynamics (CFD) models, which describe fluid flows at a higher resolution and with greater complexity than many other classes of environmental models, can account for each of these characteristics in detail and can be used to inform the likelihood that a particular release scenario will reach concentrations that could pose a hazard. Physical experiments, such as releasing a volume of the chemical into a constructed space and measuring the resulting concentrations, may be used to validate the CFD model. For example, CFD modeling can be used to assess the risk of an ignition occurring if a flammable chemical leaks from an indoor piece of equipment. An example of the output from this type of CFD model is shown below (see figure).

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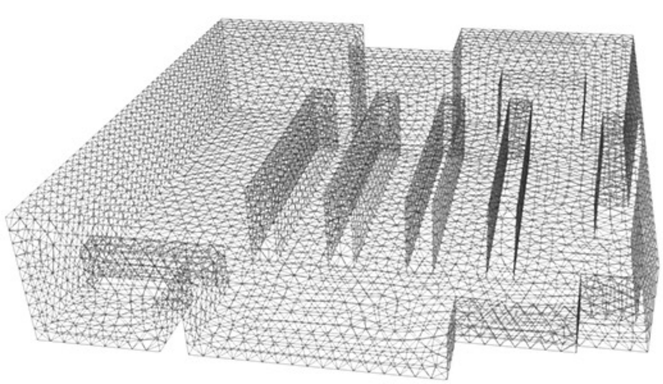
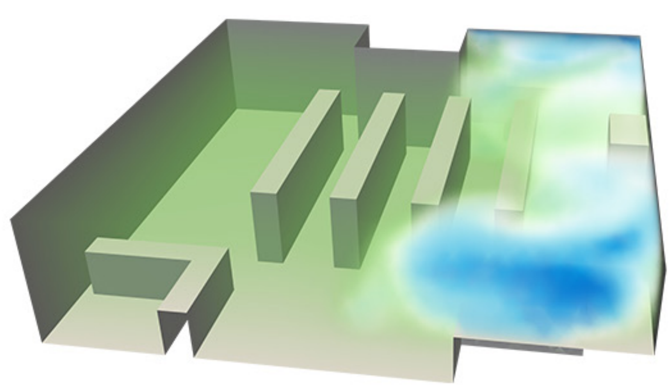
Computational Fluid Dynamics (CFD) Modeling of a Gaseous Leak



Spatial Discretization of Indoor Space



Projected Concentrations of Leaked Gas

The Right Tools for the Job: Versatility in Environmental Modeling

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Chemical Leaching through Liner Systems: Landfills, coal ash surface impoundments, and other water and waste control structures are often lined with engineered materials and/or hard-packed natural soils in order to reduce the rate at which chemicals leach from the structure and potentially cause adverse impacts to groundwater. Several analytical models and software packages are available for the evaluation of contaminant transport through liner systems (Rowe, 2012; U.S. EPA, 1997). One valuable application of these models is the analysis of new or alternative liner technologies and comparison of their performance to well-established technologies. Such models can, for example, help electric utilities make cost-benefit determinations for coal ash storage and disposal techniques.

Land Cover Classification Models: The potential for human exposure to chemicals in soil varies with land cover (Dixon *et al.*, 2006; Hilts, 1996). Land cover classification models provide information critical to establishing exposure scenarios and assessing variability in exposure potential over space and time. For large, mixed-use neighborhoods, for example, land cover classification models can be used to accurately and efficiently determine how ground cover and potential chemical exposures vary between properties and over time. Alternatively, land cover classification models can be used to quantify the extent of impervious surface areas, a controlling factor in stormwater runoff from sites.

In addition to the examples above, sophisticated models have been developed to assess the subsurface migration of groundwater plumes, mass loading of chemicals to waterways resulting from soil erosion and stormwater runoff, long-range atmospheric transport of industrial air emissions, the potential exposure of sewer workers to sewer gas, intrusion of soil vapor into basements in residential neighborhoods, impacts of climate change on water quality in U.S. rivers, and much more. With each new challenge that modelers accept, we gain new scientific insights.

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What's New at Gradient

Awards and Announcements

Barbara D. Beck was re-appointed as Associate Editor to *Toxicology and Applied Pharmacology*.

Joel Cohen has been elected Vice President of the Northeast Regional Chapter of the Society of Toxicology.

Joel Cohen was selected as a Primary Voter in the Association for the Advancement for Medical Instrumentation (AAMI) biological evaluation (BE)-working group (WG) 11: Allowable limits for leachable substances.

Julie Goodman has been appointed to the Board of Directors of the Academy of Toxicological Sciences.

Tom Lewandowski has been appointed to U.S. EPA's human studies review board.

Publications

Goodman, J.E., R.L Prueitt, R.D. Harbison, G.T. Johnson. 2020. Systematically Evaluating and Integrating Evidence in National Ambient Air Quality Standards Reviews. *Glob. Epidemiol.* https://www.sciencedirect.com/science/article/pii/S2590113320300031.

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By The Way...

Systematic review of climate models developed since the 1960s shows scientists have been getting it (mostly) right from the beginning.

Source: https://climate.nasa.gov/news/2943/study-confirms-climate-models-are-getting-future-warming-projections-right/.

The Living Site Model

By John M. Kondziolka, M.S., E.I.T. and Shuo Zhao, M.S.

Updating models over time brings them "to life," allowing for adaptive, responsive results.

Models can be an effective way to quantitatively synthesize the information available for an environmental system (Anderson *et al.*, 2015). While model results are the focus of most modeling exercises, the data used to construct a model can be a valuable repository itself, holding information such as scientifically defensible parameter values and a catalog of receptor locations. As discussed herein, there are benefits to regularly updating and maintaining environmental models, a concept that has been called a "living" site model (*e.g.*, Kress *et al.*, 2017; Berg and Sudicky, 2019).

WebGIS has become an effective way to allow real-time field sample location adjustments to be immediately viewed by stakeholders…

A living site model is regularly updated (*e.g.*, on an annual basis, or using real-time inputs) to incorporate new information. There are several benefits to maintaining a living site model, including more rapid deployment of the model when a specific question needs to be answered, distribution of the effort required to update the model over a longer period of time, and the added functionality of using the model as an up-to-date information repository. Two types of living site models, the first describing regular update intervals and the second describing real-time updates, are discussed below.

Regular update intervals have been used at one northeastern U.S. site to create a multiyear living site model. The initial model answered specific questions regarding contaminant travel times from a source to an observed groundwater plume. Following a field data collection effort, the model was refined and recalibrated, and then a moratorium on major model updates was put in place for two years, during which the model was used to answer exploratory questions (*e.g.*, How long will it take for this emerging contaminant to reach a receptor?), as well as to quickly retrieve answers to data repository questions (*e.g.*, How much was this well pumping in 2005?). Desired updates for the model were recorded during the two-year timeframe and, at the end of year two, were implemented to produce a new model, which will similarly be regularly updated.

Real-time and remote data acquisition methods have also been used to create living environmental data analysis and visualization tools. A WebGIS (Internet-based Geographic Information System) interface is a powerful tool that supports real-time updates to environmental site models. The COVID-19 case tracking map from Johns Hopkins University (https://arcg.is/0fHmTX; Dong *et al.*, 2020) is a recent public example of a WebGIS interface. Adjustments can be made to maps in real-time, from the field, on an interface accessed from a mobile device. The interface also provides a rapid, user-friendly way to access complex site data, such as sample chemical concentrations, surface elevations, and construction histories. WebGIS has become an effective way to allow real-time field sample location adjustments to be immediately viewed by stakeholders for site remediation in sensitive urban areas. Having remote, live access to historical aerial photo and data overlays has also provided crucial support to investigators as they locate structures left in place after site demolition.

As demand for rapid responsiveness increases, we expect to see increasing numbers of living site models. Numerical groundwater models, traditionally limited to regular update intervals, are migrating online for real-time access (*e.g.*, see the U.S. Geological Survey GWWebFlow tool at https://webapps.usgs.gov/gwwebflow/). The next generation of these models will likely include automated data retrieval to update the models in real time as new field data are collected from groundwater monitoring networks.

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By The Way...

"All models are just models," Dr. Anthony S. Fauci, science adviser to the White House coronavirus task force, has said. "When you get new data, you change them."

Source: The New York Times: The Coronavirus in America: The Year Ahead.

Guest Editorial: Narrowing the Gap: Conceptualizing Complex Problems in the Development of Vapor Intrusion Models

By Kelly G. Pennell, Ph.D., P.E.

Vapor intrusion models that include alternative pathways help bridge the gap between conceptual and numerical models.

Environmental scientists use models to inform decision making, prioritize locations for site characterization, assist in data interpretation, predict fate and transport of contaminants, and evaluate risk, among other activities. There are two common types of environmental models: conceptual models and numerical models. Conceptual models use visual and narrative descriptions of critical processes, while numerical models use equations to describe governing processes within environmental systems. New and emerging knowledge can fill the gap between conceptual and numerical models.

With nearly one million miles of public sanitary sewer mains…alternative pathways bring considerable uncertainty to vapor intrusion site assessments.

Vapor intrusion, the transport of subsurface contaminant vapors into indoor spaces, provides an example of how conceptual and numerical models can grow closer together by incorporating new information. Regulatory agencies encourage vapor intrusion conceptual site models (CSMs) to be developed and redefined as part of site assessment activities. For many years, vapor entry from alternative pathways (*e.g.*, contaminant vapor entry into buildings directly from piping conduits) was omitted from both conceptual models and numerical models. In 2013, Pennell *et al.* published a field study that helped redefine the generic CSM for vapor intrusion to include alternative pathway vapor entry (*i.e.*, sewer gas entry *via* a faulty toilet seal into an indoor space at a vapor intrusion site).

With nearly one million miles of public sanitary sewer mains and half a million miles of private sanitary sewer laterals buried across the United States, alternative pathways bring considerable uncertainty to vapor intrusion site assessments. Near sites contaminated with hazardous wastes, pipe deterioration may allow migration of contaminants into sewers. Subsequently, these pipes can potentially transport chemicals into buildings. Roghani *et al.* (2018) report that vapor intrusion exposure risks can extend hundreds of feet away from the main groundwater plume due to alternative pathways.

Recently, Shirazi *et al.* (2020) developed an open-access numerical modeling approach to describe fluctuations in indoor air trichloroethylene (TCE) concentrations due to alternative pathways, as well as characteristics that influence building air exchange rates (AERs). Aboveground processes, such as weather conditions, building characteristics, and AERs, have long been included in generic vapor intrusion CSMs, even though few vapor intrusion numerical models are available to systematically evaluate processes that influence AERs. Shirazi *et al.* (2020) compared the modeled data with field measurements, including AERs and TCE indoor air concentrations, from a research site in Layton, Utah (*i.e.*, Sun Devil Manor) that has been studied for years as part of a U.S. Department of Defense study. The CSM for Sun Devil Manor had previously been redefined due to the discovery of an alternative pathway at the site.

Shirazi *et al.* (2020) suggested that indoor air volatile organic compound (VOC) concentrations at vapor intrusion sites with alternative pathways may have larger temporal fluctuations than sites without alternative pathways; however, variations in AERs may also contribute to temporal fluctuations in indoor air VOC concentrations (but over a smaller range). While no model will ever be completely accurate, models such as the one used by Shirazi *et al.* (2020) provide opportunities to narrow the gap between conceptual and numerical models.

Kelly G. Pennell, a Gill Associate Professor of Civil Engineering at the University of Kentucky, conducts research to improve the detection and mitigation of exposure risks associated with legacy and emerging pollutants.

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Guest Editorial: Narrowing the Gap: Conceptualizing Complex Problems in the Development of Vapor Intrusion Models

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