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DPRA™

600 S. Andreasen Dr.
Suite A
Escondido, CA 92029
Tel. 760.781.1586
Fax 760.781.1588

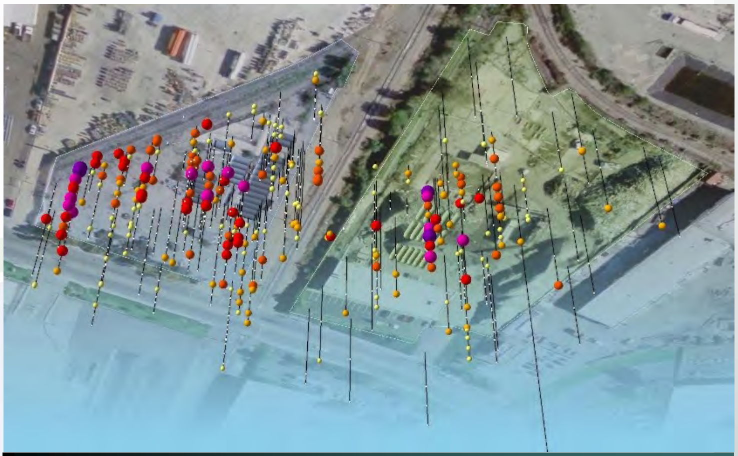
ZymaX FORENSICS

600 S. Andreasen Dr.
Suite B
Escondido, CA 92029
Tel. 760.781.1586
Fax 760.781.1588

www.DPRA.com

# Multiphase Modeling of Complex Field Sites

*By Ashok Katyal, Ph.D. and Robert Morrison, Ph.D.*



The critical input data needed for model development are either determined in the laboratories or estimated based on investigator's personal experience and literature values.

Hydrocarbons are organic compounds containing carbon and hydrogen. Carbon has interesting characteristics that allow it to develop strong bonds (single or multiple bonds) to itself and form long chain/rings and/or form bonds with many non-metals such as nitrogen, hydrogen, oxygen, chlorine, bromine, sulfur, and phosphorus. These characteristics determine properties such as solubility, volatility, adsorption, biodegradation/persistence, toxicity and how an organic compound behaves in the soil, atmosphere, surface and groundwater, and their impact on human and ecological health.

Several finite element and finite difference models have been developed (such as MOFAT, UTCHEM, NAPL, TOUGH2) to simulate fate and transport of organic species in soils, air, and water; continuity equations for water, oil and gas phases and the components' convection-dispersion equations are solved. The critical input data needed for model development are either determined in the laboratories or estimated based on investigator's personal experience and literature values, and later refined during the calibration; the initial parameters' values may be estimated as follows:

- Unsaturated zone flow characteristics (such as van Genuchten, or Brooks Corey parameters), porosity, variably saturated hydraulic conductivity function, and bulk density – soil samples are normally sent to qualified laboratories and parameters are estimated.
- Bulk fluid properties (specific gravity, inter-phase surface tensions, viscosity) – fluid samples are sent to qualified laboratories and parameters are estimated.
- Residual saturations (in the unsaturated and saturated zones) – soil samples are normally sent to qualified laboratories to estimate these parameters.
- Species' physicochemical properties (solubility, half life, distribution coefficient, dispersivity, diffusion, Henry coefficient, etc) are needed when fate and transport is simulated – most of such data are available in the current literature.

Multiphase modeling is highly complex (vis-à-vis groundwater) for several reasons such as:

- Initial conditions are difficult to define accurately – a snap shot measurements of the fluid levels (oil-water, and air-oil tables) is a quantitative indicator of the current free-phase oil volumes, and does not account for the NAPL (non-aqueous phase liquid) historically trapped in the saturated and unsaturated zones. These residual oil volumes (function of the historical fluid table fluctuations) can become free when fluid table fluctuations reverse and merge with the existing pool of free-phase hydrocarbon. An elaborate field sampling and/or numerical simulations are needed to estimate these volumes. Sometimes NAPL pools may not be connected (continuous) – if there are insufficient number of fluid level monitoring wells employed in the investigation, the NAPL volume will be overestimated. The likelihood of this happening increases when smaller product thicknesses are encountered.

*(Continued on page 2)*

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(Continued from page 1)

- Multiphase equations are highly nonlinear; the fluid phase conductivities (water, oil, and gas phases) are continuously changing and they are functions of the respective transient phase saturations (dependent on transient inter-phase capillary pressures, trapped oil saturations and the surface tensions). Porous media heterogeneities can significantly contribute to the solution instabilities and such behavior must be distinguished.
- Special calibration skills are needed to navigate through the parameters and identify those that are highly critical. It involves defining spatial distribution of hydraulic conductivity tensor and retention parameters, porosity, and residual saturations, fluid properties, and species physiochemical properties.
- Heterogeneities can have profound impact; clay lenses can significantly alter free NAPL flow, and NAPL can be trapped within these lenses and act as source of contamination for an extended period of time.
- Transient boundary conditions significantly add to the instabilities – fluid table fluctuations results in freeing and/or trapping of the hydrocarbon; it changes free-phase saturations and the effective free-phase permeability. Extraction wells produce significant fluid table fluctuations and can cause severe numerical difficulties – the computations will march forward with smaller time steps and need significant processor time.
- The complexity of simulations increases with the dimensionality of the problem. A three-dimensional multiphase formulation may not be practical for large scale problem due to unavailability of representative site-specific data, extraordinary high computational burden and cost of investigation.
- On large domains, a coarse mesh may cause unacceptable mass balance error, mesh aspect ratio in the lateral and vertical directions must be investigated – generally, mass balance error can be reduced by refining time step, and gradually ramping boundary and source/sink conditions.

One-dimensional models may suffice when flow is predominantly vertical and conservative estimates are sought. Two-dimensional vertical slice (x, z) or radial (r, z) multiphase models such as MOFAT (USEPA) are useful under most field conditions involving flow through the vadose zone and in the underlying aquifers. Vertically averaged models such as BIOSLURP are computationally highly efficient and can be used to investigate migration of LNAPL (light) and to oil, water, gas recovery systems – they are fairly stable under most field conditions and can be used to simulate large areas efficiently. A combination of one/two dimensional and vertically averaged models coupled in series can be used to simulate highly complex sites efficiently in cost-effective manner. Models are valuable tools and can be used to:

- Identify data gaps and help develop a cost-effective data collection strategy.
- Identify sensitive model parameters, and reduce uncertainty.
- Perform risk assessment – fate and transport investigations, and identify receptors that may be under potential risk.
- Assist in remedial design, and risk management.
- Assist in litigation support – identify sources of contamination and parties responsible for pollution, and estimate age of pollution (time of releases).

*For more information or to contact the authors, please email Paul Garcia at DPRA (Paul.Garcia@DPRA.com).*

**Dr. Ashok Katyal** has over 30 years experience providing consulting services in the environmental and water resources areas to several national and multinational companies, state, federal agencies, and law firms in USA. He has developed outstanding expertise in groundwater, surface water, and watershed areas. This was possible through extensive international experience (India 5 years, Kenya 6 years, Nigeria 1 year, in addition to 20 years in USA) working in the environmental, surface-groundwater interaction, irrigation and drainage systems, and watershed management areas. This diverse professional development enhanced during graduate work at Washington State University (USA) where his assistantship funding required developing, (1) 3D variably saturated subsurface flow and multi-component transport finite element model, and (2) the Furrow Irrigation Erosion Simulator (published by WSU as a special Research Bulletin, 1991). His Ph.D. dissertation, "Surface Irrigation Hydraulics as Influenced by Soil Texture and Plant Water Uptake", involved coupled solution of the overland continuity and momentum equations (surface flow, finite difference) and the variably saturated subsurface continuity equation (finite element). This tool was used to understand surface-subsurface water interaction, design irrigation systems, and for irrigation scheduling. Dr. Katyal is the author of MOFAT (USEPA), BIOSLURP, MOVER, MARS, BIOFT3D, SVE_3D, BIOSVE, SOILPARA, OILVOL, Metals_3D, and SAMAPS computer models.

**Dr. Robert Morrison** has a B.S. in Geology, a M.S. in Environmental Studies, a M.S. in Environmental Engineering, and a Ph.D. in Soil Physics from the University of Wisconsin at Madison. He has been working for over 35 years in the environmental field on issues related to soil and groundwater contamination. Dr. Morrison specializes in the forensic review and interpretation of scientific data for the purpose of identifying the source and age of a contaminant release and manages DPRA's environmental forensic practice group. Dr. Morrison is credited for coining the term "environmental forensics" and with Drs. Zhendi Wang (Environment Canada), Brian Murphy (Exponent), Paul Philp (University of Oklahoma), Cout Sandau (Trium, Inc.) and Steve Mudge (University of Wales) founded the International Network of Environmental Forensics (INEF) dedicated to this science, and authored the first textbooks on this subject.

Dr. Morrison has served on the editorial boards of *Ground Water*, *Groundwater Monitoring Review and Remediation* and was Editor in Chief of the *Journal of Environmental Forensics* for many years. He is the author of *Environmental Forensics: Principles and Applications* and *Environmental Forensics: A Glossary of Terms* published by CRC Press, Boca Raton, Florida and is co-author with Dr. Brian Murphy of *Introduction to Environmental Forensics* published by Academic Press, Oxford England. Dr. Morrison has worked as an expert witness and confidential consultant for the United States Department of Justice, the EPA and numerous law firms. Dr. Morrison has offered deposition and court testimony in over 50 cases. In his capacity as an expert witness and confidential consultant, Dr. Morrison has provided testimony in numerous cases, some with claims in the billions of dollars.

# Project Pitfalls (Part 2): Graphics

*By Justin R. Hone*

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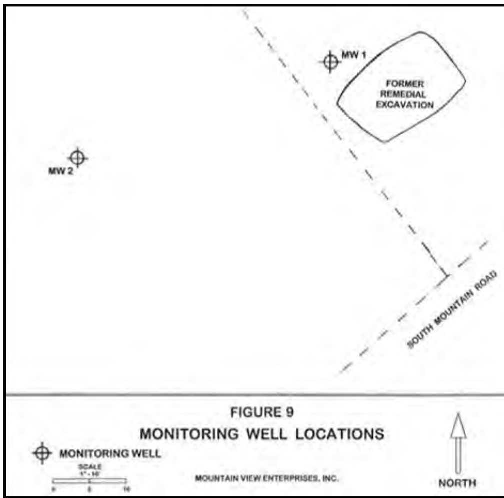
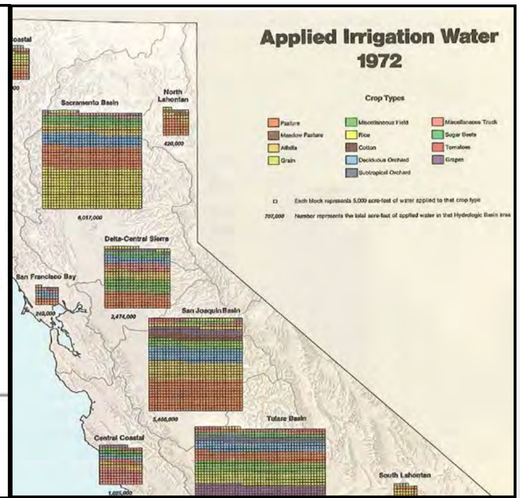
"A picture is worth a thousand words." So cliché, I know. Yet a bad picture is often worth that plus the cost of the court's ruling against your client. Effective graphics are essential at several steps in the litigation process. In our many years of supporting attorneys and experts, we've come across some interesting ways people chose to express their ideas, often at the over-simplified or over-complicated ends of the graphic spectrum. Shooting for and hitting the middle ground where comprehension and significance overlap can be quite challenging.




**Too simple.** *This is unprofessional. Can we take this seriously? This was the best they could do?*

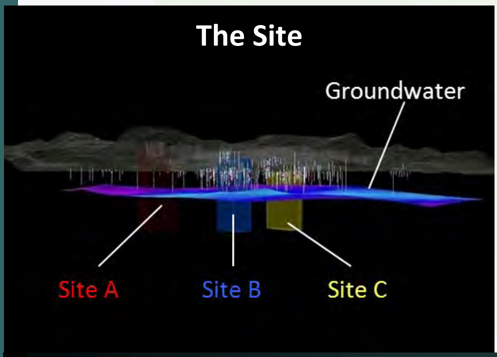


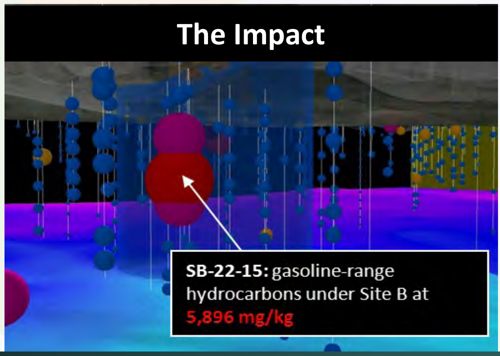

**Too complicated.** *I'm lost. Are they trying to confuse me? Where is this headed?*

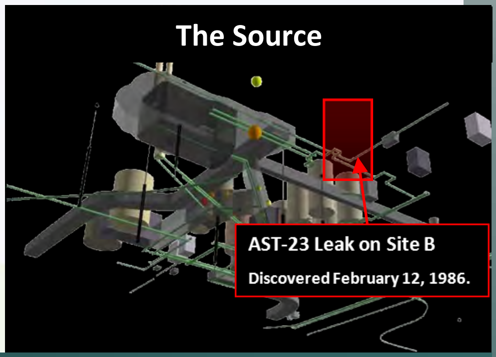
**Your expert in geochemistry probably wasn't the greatest art student.**
Experts know what they want to say, but they often lack the ability to present the information in a manner commensurate with their expertise. Often they go from one extreme of "pencil and sharpie" figures to the other, where excessive amounts of information are presented in a way that isn't immediately decipherable to the layperson (see examples above right). An effective exhibit should present data and opinions in a graphical, intuitive, and easy to understand manner. The collection of graphics below are one example where concepts are addressed individually as 'the site,' 'the impact' and 'the source.' This progression would likely be accompanied by a simplified graphic which compares source and impact spatially in either 2D or 3D, depending on the site parameters, the audience, and the intended message. In addition to visualizing the expert's opinion, we've found that our role often involves wrangling experts — keeping them in sync with the concepts that will convey properly and those that will need adjustment.

**In this economy?** Law firms and government agencies sometimes hire outside graphics companies to produce illustrations with varying degrees of success. While they are talented and creative individuals, they often don't work directly with the expert or understand his/her science. In our experience, they have no idea what the illustration is supposed to convey and simply provide a "polishing" service. Recently, DPRA worked on a case where a trial graphics company put a black border around our illustrations, added their company logo, and billed the firm thousands of dollars. Apart from the unnecessary expense, we've found that steering the expert toward meaningful graphics begins on day one, not the final days before trial or mediation when graphics companies are typically launched. The expert's written opinion is not sacrosanct if it doesn't tie in well with the visual evidence, but "graphics only" firms usually won't step on the expert's toes to make these adjustments.

*For more information, please email the author at [justin.hone@dpra.com](mailto:justin.hone@dpra.com).*




An example of a professional, easy-to-understand graphic tableau which presents the interlinked concepts of site location, environmental impact, and probable source. While it possible to show all three of these ideas in one panel, it is not recommended. The expert should also be familiarized with the progression of ideas so as to reflect the same in his or her written opinions and/or testimony.

**Justin R. Hone** is a licensed professional geologist in the State of California and a Senior Associate at DPRA, where he leads the environmental forensics litigation support practice. He holds a BS in Geophysics from the University of California at Riverside. Mr. Hone has acquired managerial, business development, and scientific experience in both public and private company atmospheres. He has authored several peer-reviewed publications pertaining to environmental forensics including the Environmental Forensics chapter of the United Nations' Encyclopedia of Life Support Sciences. Mr. Hone typically provides project management to clients in need of litigation and expert witness support services, GIS modeling, and trial graphics.

## INTRODUCING OUR EXPERTS...

**Dr. Yi Wang** is the Director of ZymaX Forensics' Isotope Laboratory. He has a B.S. in Environmental Science, an M.S. in Environmental Chemistry, and a Ph.D. in Environmental Geochemistry. He has worked for over 20 years in the environmental field on issues related to soil and water contamination. He developed Compound Specific Isotope Analysis techniques at Brown and Princeton University and applied isotope forensics in the environmental field. Dr. Wang is a specialist in the analysis of isotope ratios for carbon, chlorine, hydrogen, nitrogen, oxygen, and sulfur. He has published over 45 articles and books on soil and water contamination topics and shared this information via lectures throughout the world. Dr. Wang has served as an expert for the U.S. Environmental Protection Agency (EPA) and the State Coalition for Remediation of Drycleaners (SCRD) on chlorinated solvent cases where environmental forensics was used to allocate responsibility and optimize remediation strategy.

**Mr. Smith** brings over 28 years professional experience in project, program and line management, environmental forensics, and remediation of contingent environmental liabilities affecting industry. At DPRA, he leads the practice in hydrogeology and site remediation as it relates to work for attorneys and their corporate clients. Mr. Smith is well known for his pioneering breakthroughs in the remediation of chlorinated solvents from soils and groundwater and is recognized for having successfully completed possibly the nation's first dense non-aqueous phase liquid (DNAPL) cleanup in groundwater to regulatory limits in 1999. He is well published and a recognized lecturer at international technical forums. Most recently Mr. Smith has co-authored, Encyclopedic Dictionary of Hydrogeology by Academic Press, March, 2009, a chapter on thermal effects in "Electrochemical Remediation Technologies for Polluted Soils, Sediments and Groundwater" published by John Wiley & Sons and is a Patent holder since 1994 for a Ground Contamination Remediation Process U.S. Patent No. 5,279,740 which is also patented in Canada, Europe, Australia, and Taiwan. With this experience, Mr. Smith pioneered a program that was demonstrated to be highly effective in re-engineering soil and groundwater remediation systems that typically resulted in a 50% reduction in client reserves for contingent liability.

**Dr. Shan Tan Lu** is the Laboratory Manager of ZymaX Forensics Laboratories. He has over 20 years of experience in forensic and petroleum geochemistry and has managed the Forensic Geochemistry Laboratory for ZymaX Forensics for over 10 years. He has developed environmental forensic analytical methods to determine fuel types from product samples and has also provided expert consulting services for petroleum geochemistry. Dr. Lu has also authored over 20 environmental journal articles related to forensic and petroleum geochemistry and analysis.