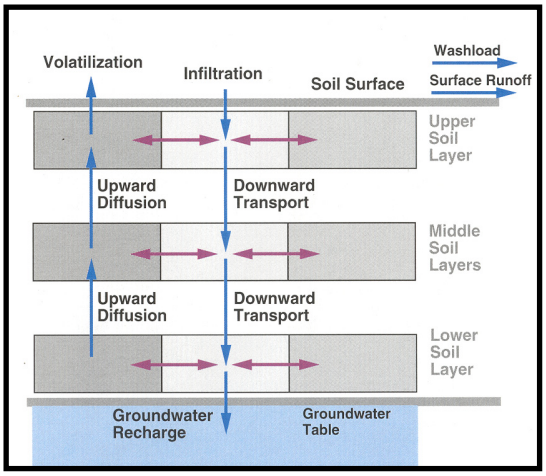
OAK RIDGE NATIONAL LABORATORY FACT SHEET
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Scientific Computing Within the ORNL Modeling & Simulation Group: Environmental Modeling

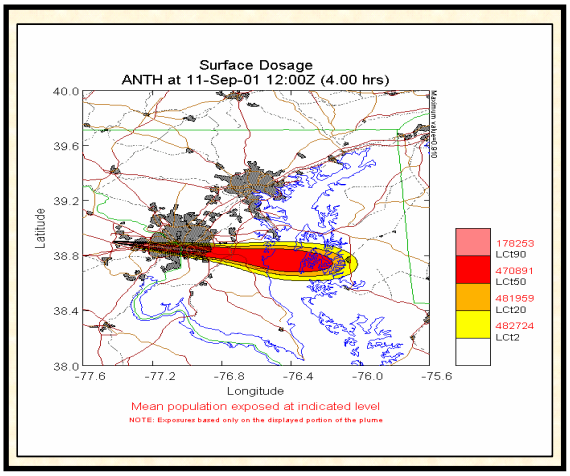
The ORNL Modeling and Simulation Group (MSG) develops sophisticated numerical solutions for a wide range of scientific, engineering, and operational applications. MSG's core competency is computational physics and engineering, and within this context we have extensive expertise modeling environmental systems. This problem solving scope includes the following.

- Contaminant transport as functions of *intramedia* mechanisms such as advection, diffusion, and transformation; and *intermedia* mechanisms such as deposition, evaporation, and adsorption.
- A broad range of radiological, biological, and chemical contaminants.
- Multiple media including air, water, sediment, man-made containment structures, compacted and fractured soils, as well as the human food chain.
- Multiple length scales including building interiors, industrial sites, regional rivers and estuaries, and complex mountain terrain.
- Deterministic, probabilistic, and optimal figures-of-merit using compartment-, Gaussian-, and physics-based solution techniques implemented with in-house and commercial software.
- An extremely broad set of applications including site-remediation studies of Gaseous Diffusion Plants (GDP's) for the Department of Energy (DOE); soil-sensitivity rankings for the Wisconsin Department of Natural Resources; radioactive nuclide dispersal within the Clinch River for DOE; characterization of catastrophic air-borne releases from nuclear, biological, and chemical sites for the Defense Threat Reduction Agency; as well as meteorological modeling support for the ORNL Emergency Response Meteorologist.

These applied scientific computing capabilities represent an extremely versatile environmental modeling resource for a broad range of R&D, industrial, homeland defense, and military applications. We welcome the opportunity to discuss your potential applications and ways MSG can contribute to a solution.

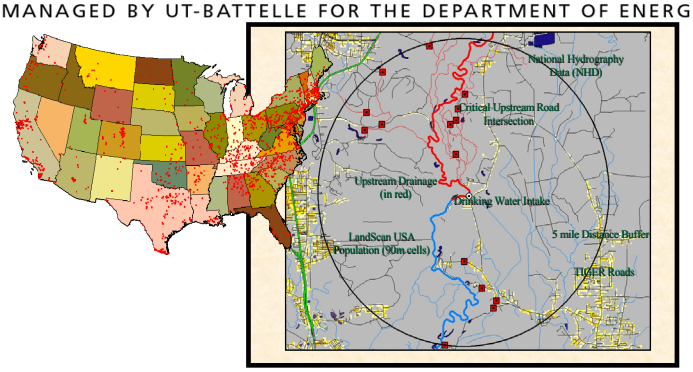


MSG acquired & extensively modified the SESOIL code then coupled SESOL with the PRISM probabilistic-driver code to study groundwater contamination at GDP's

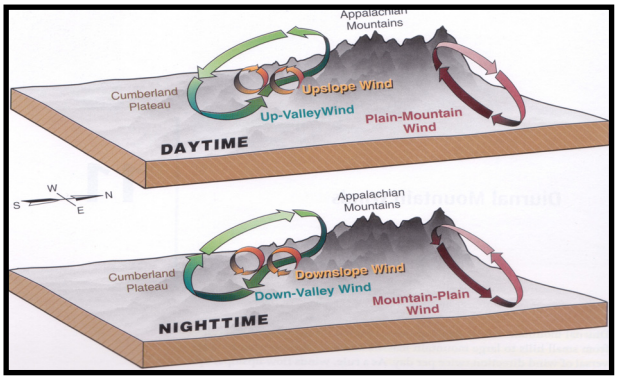


MSG co-developed the HPAC code to evaluate air-borne releases of nuclear, biological, & chemical agents. HPAC can also be coupled with GIS data bases to estimate at-risk populations

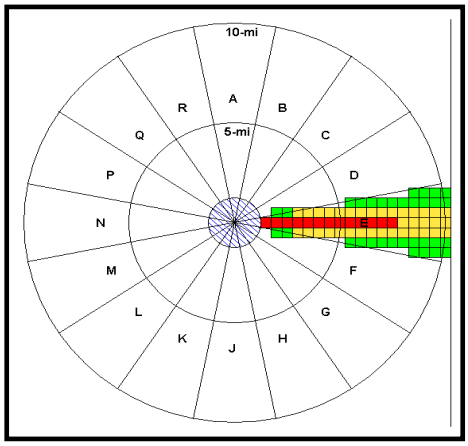
POC: David M. Hetrick
(865)576-7556/hetrickdm@ornl.gov
http://computing.ornl.gov/cse_home/cms/cmshome.shtml



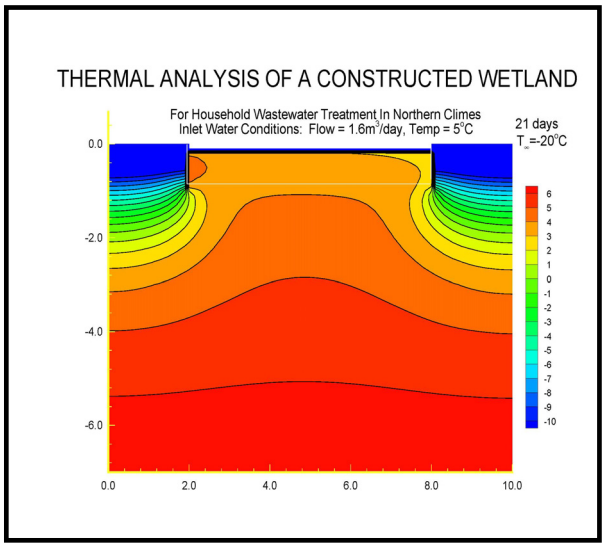
MSG developed the HYTRAS code to simulate waterborne fate & transport. HYTRAS can be coupled with GIS-derived infrastructure data to estimate, for example, drinking water contamination resulting from transport of NBC agents in water bodies & sediments



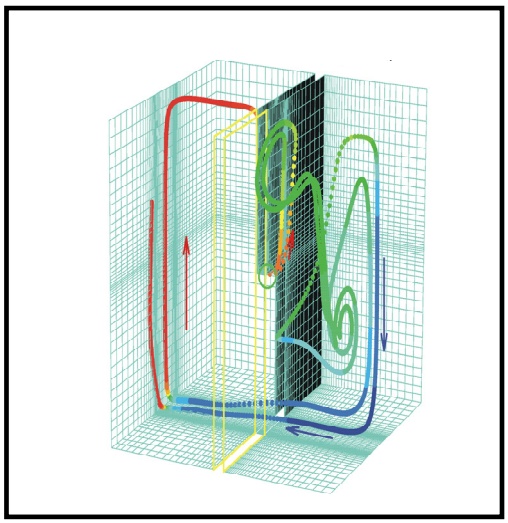
MSG models mountain meteorological processes within the Great Valley of Eastern Tennessee using the CAPARS software suite



MSG collaborated on development of the RASCAL code which will prepare human-dose projections resulting from radiological accidents



MSG utilized the in-house developed HEATING code to conduct a thermal analysis of a constructed wetland to quantify its hydraulic & pollutant-reduction performance under extreme wintertime conditions



MSG developed the PHI3D CFD code, in part, to study pollutant transport in confined spaces. This figure shows results from validation & verification effort for incompressible, laminar, buoyancy-driven flow between separate hot & cold rooms. Release point is bottom of door between the rooms, tracks are color-coded by temperature

POC: David M. Hetrick
(865)576-7556/hetrickdm@ornl.gov
http://computing.ornl.gov/cse_home/cms/cmshome.shtml