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TMVOC, A Numerical Simulator for Three-Phase Non-isothermal Flows of Multicomponent Hydrocarbon Mixtures in Variably Saturated Heterogeneous Media

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TMVOC is designed for studying subsurface contamination by volatile organic compounds (VOCs), such as hydrocarbon fuels and industrial solvents. It can model the one-, two-, or three-dimensional migration of non-aqueous phase liquids (NAPLs) through the unsaturated and saturated zones, the formation of an oil lens on the water table, the dissolution and subsequent transport of VOCs in groundwater, as well as the vaporization and migration of VOCs in the interstitial air of the unsaturated zone, and the reversible sorption of VOCs on the rock matrix of a porous medium. TMVOC accounts for differences in aqueous solubility and volatility of different VOCs that may be present in a NAPL. Thermal remediation treatments such as steam injection or electric resistance heating and associated phase change and flow effects can also be modeled. A simple half-life model for biodegradation is included as well.

In the TMVOC formulation, the flow system is assumed to be composed of water, non-condensable gases (NCGs), and volatile organic chemicals (VOCs). Mass transport occurs through multiphase advection and diffusion. There are no intrinsic limitations to the number of NCGs or VOCs. The necessary thermophysical and transport properties are computed by means of a very general thermodynamic formulation, which uses semi-empirical corresponding states methods. Any and all phase compositions in a gas-water-NAPL system are treated, including single, two-phase, and three-phase conditions (Fig. 1).

TMVOC is written in Fortran 77 and can be run on any platform for which a Fortran 77 compiler is available, including PCs. The code is implemented as a specialized module in the framework of the multi-purpose simulator TOUGH2, and retains the general process capabilities and user features of TOUGH2, including applicability to heterogeneous 3-D systems (Pruess, 2004). TMVOC is available for licensing from the Energy Science and Technology Software Center (ESTSC) of the U.S. Department of Energy (<http://www.osti.gov/estsc/>). Additional information is available on the TOUGH2 homepage, at <http://www-esd.lbl.gov/TOUGH2/>.

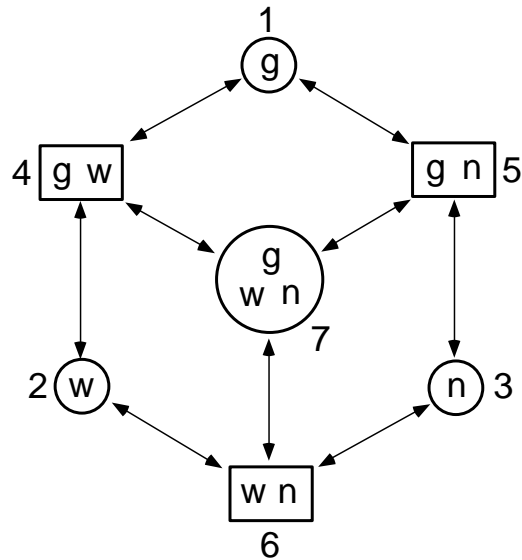


Figure 1. Phase compositions and phase changes considered by TMVOC. The phase designations are: g - gas, w - water (aqueous), n - NAPL.

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