How far will the LNAPL migrate? Tier 3

The Concawe Toolbox includes a new Tool developed by Andrew Kirkman based on LNAPL mass limitations included in the HSSM conceptual model integrated with LNAPL transmissivity relationships and LNAPL removal via Natural Source Zone Depletion (NSZD) using the Mahler et al. (2012) model. This Tier 3 section provides additional information about HSSM and UTCHEM, two tools that can be used to answer the question "How far will the LNAPL migrate?" The 2012 paper by Mahler et al. (2012) presents important findings on how NSZD limits LNAPL migration. Finally, an emerging LNAPL modeling method being developed by GSI's Dr. Sorab Panday is a promising new approach where LNAPL modeling can be performed using a commonly used groundwater model like MODFLOW.

Overview of HSSM

- "HSSM" is an acronym for Hydrocarbon Spill Screening Model.
- Uses analytical relationships to simulate LNAPL movement.
- Simulates vertical LNAPL flow through the unsaturated zone.
- Simulates formation and decay of an LNAPL lens at the water table.
- Assumes a circular lens that is not affected by a water table slope.
- Simulates dissolution of LNAPL constituents and dissolved plume migration.
- Older model that requires workarounds to run on 64-bit operating systems like Windows 10.
- NSZD cannot be simulated, so that LNAPL spreading predictions in HSSM will overestimate actual spreading.
- Can be downloaded here.

Overview of UTCHEM

- University of Texas chemical flood simulator developed for the oil industry.
- 3-D finite-difference numerical simulator for NAPL.
- Simulates multiphase, multicomponent, variable temperature systems and complex phase behavior.
- Accounts for chemical and physical transformations and heterogeneous porous media.
- Uses advanced concepts in high-order numerical accuracy and dispersion control and vector and parallel processing.
- Extremely powerful model but expensive and can be difficult to run.
- Due to its complexity, it is typically only used for more complicated LNAPL/environmental problems.
- Can be run either as a stand-alone program or accessed through GMS package (e.g., https://www.aquaveo.com/software/gms-groundwater-modeling-system-introduction)

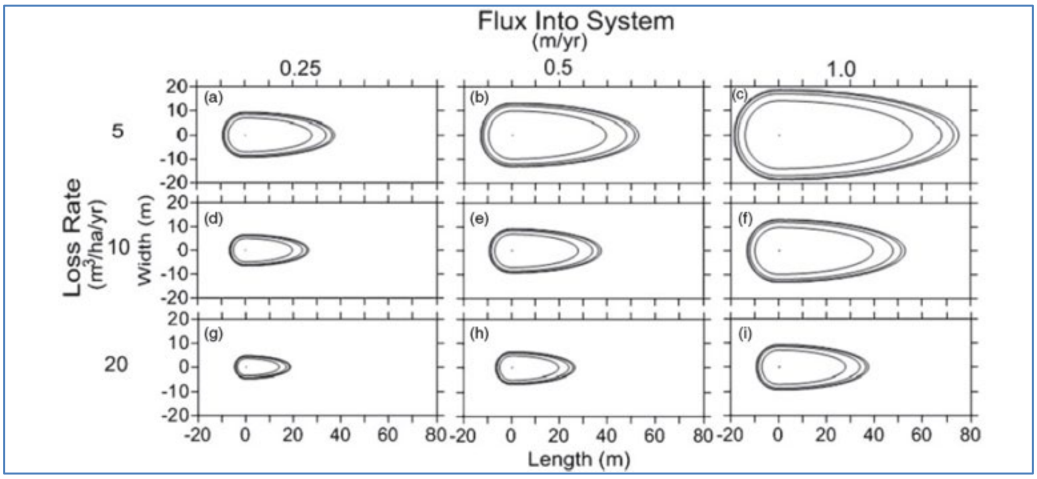
Video

A short video describing HSSM and UTCHEM can be viewed here.

Overview of Mahler et al. (2012) LNAPL Stability Paper

- "...natural losses of light nonaqueous phase liquids (LNAPLs) through dissolution and evaporation can control the overall extent of LNAPL bodies and LNAPL fluxes observed within LNAPL bodies."
- Uses proof-of-concept sand tank experiment where LNAPL is continually added but LNAPL body stabilizes due to losses via dissolution and evaporation.
- At actual LNAPL sites, LNAPL stability is rapidly achieved because of LNAPL losses via NSZD.

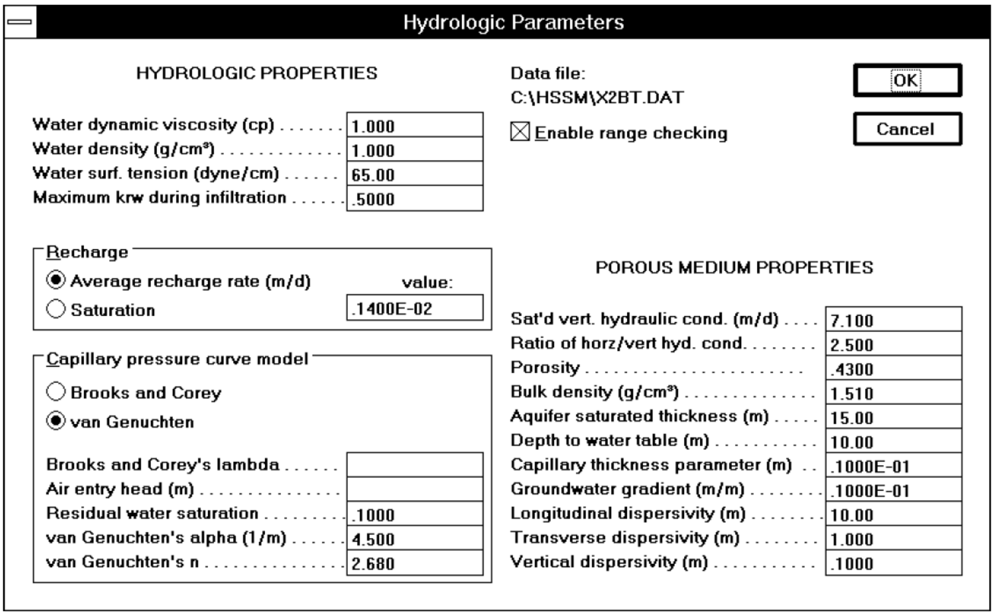
- Simple design charts are provided to show when LNAPL bodies will stabilize as a function of loading and NSZD rate, but these charts assume a constant LNAPL addition through time (a situation that is extremely infrequent at actual LNAPL sites).
- Key point: “...natural losses of LNAPL can play an important role in governing LNAPL fluxes within LNAPL bodies and the overall extent of LNAPL bodies.”
- The Concawe Toolbox Tier 2 model located under the question “How far will the LNAPL migrate?” developed by Andrew Kirkman uses key concepts from this paper to predict how far LNAPL can migrate.

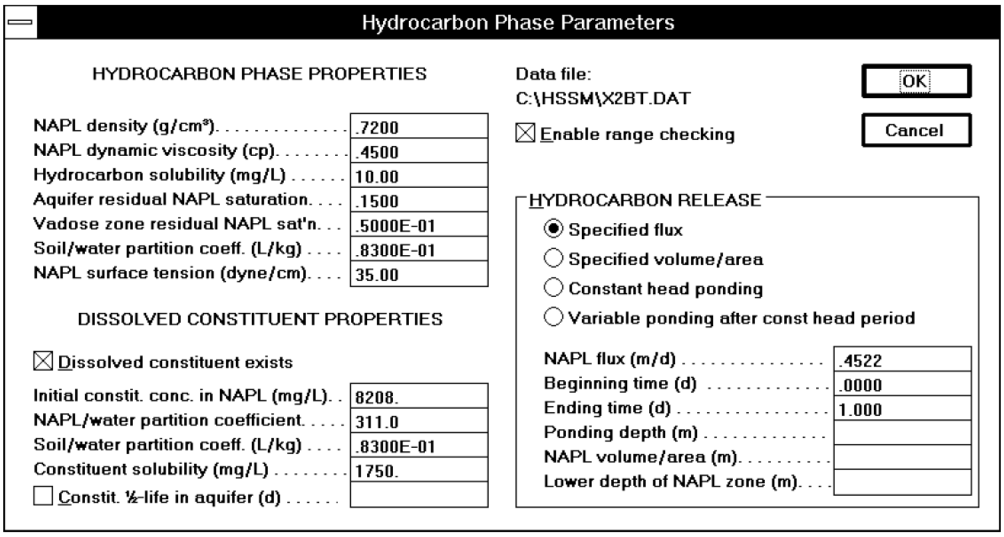


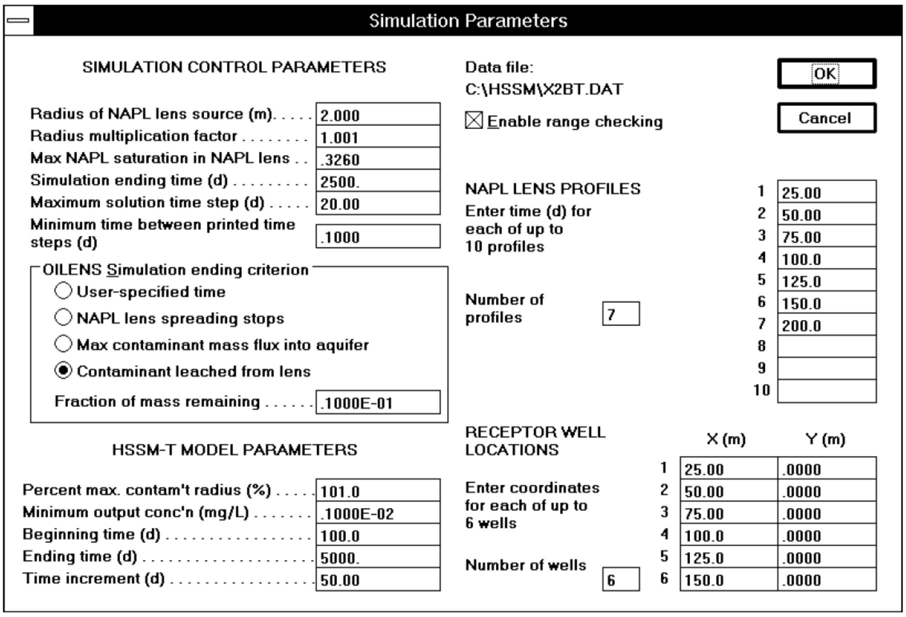
LNAPL body stabilization figure from Mahler et al. (2012). Each contour line is either 40 years (for panels a, b, c), 20 years (panels d, e, f), or 10 years (panels g, h, and i). (Reprinted with Permission)

Checklist of Input Data for HSSM

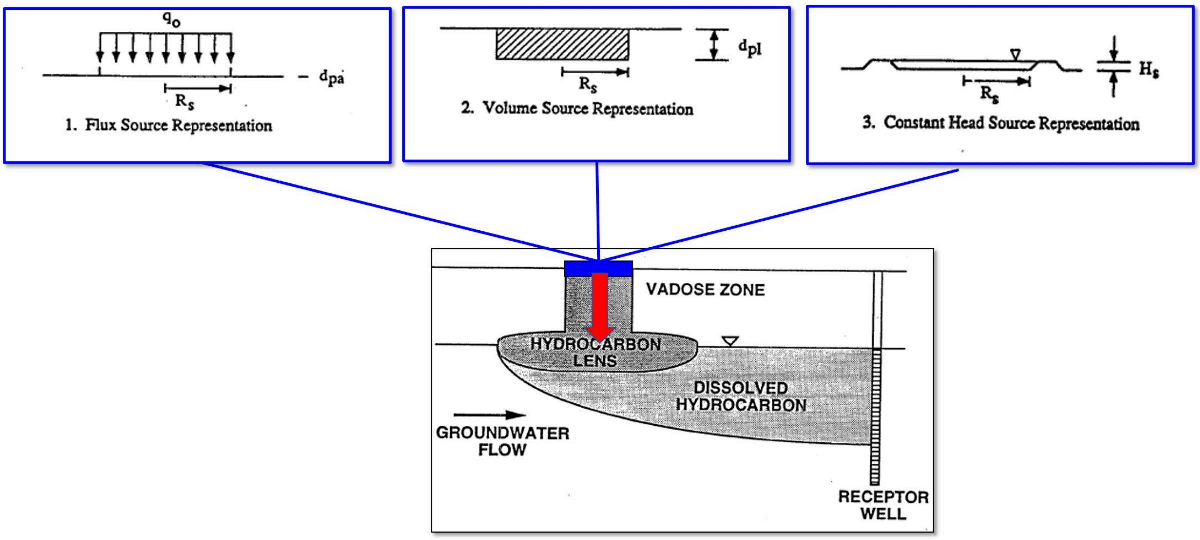
Appendix 3 of the HSSM User’s Guide (Weaver et al., 1994) lists key input data and provides support for parameter estimation. Key parameters with example values are reproduced below:







Users select one of three general release scenarios to the unsaturated zone and enter either an LNAPL flowrate over a certain time period, a volume of LNAPL released over a certain area, or a constant head of LNAPL in an impoundment.



General Flowchart for Running HSSM

Table 5 Outline of the HSSM-WIN Interface	
Interface Function	Section References
1. Installation of HSSM-WIN	4.2 and 4.3
2. Operation of the HSSM-WIN Interface, Summary of Interface Commands	4.4
3. Creation of Data Sets	4.5
4. Editing of Input Parameters	4.6.1 and 4.6.3 to 4.6.6
5. Running HSSM-KO and HSSM-T	4.5.3, 4.7
6. Graphing HSSM Results	4.5.4
7. Interpretation of HSSM Graphs	4.8
8. HSSM Output File Contents	6

Example Output from HSSM

Example output is shown below (Weaver et al., 1994).

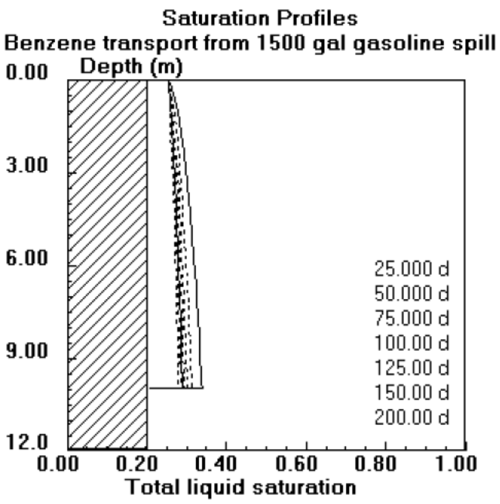


Figure 23 Typical saturation profiles

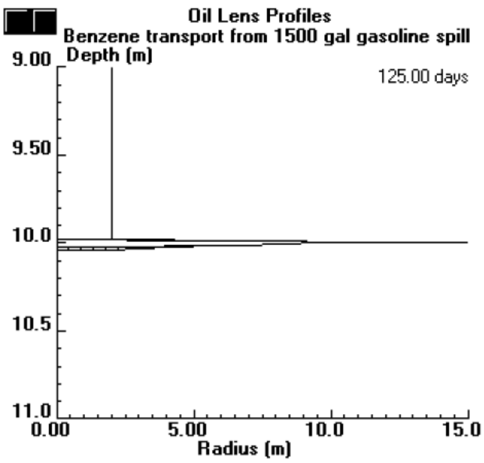


Figure 24 Typical NAPL lens profile

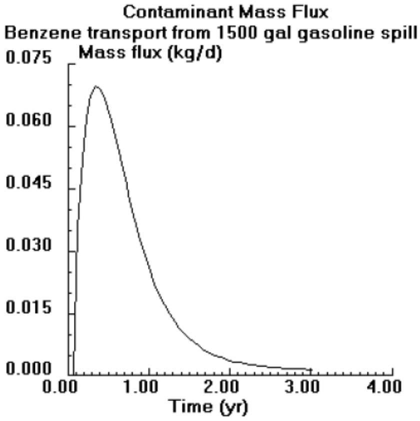


Figure 25 Typical contaminant mass flux history

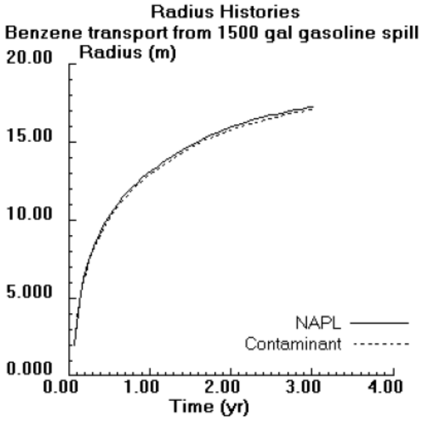


Figure 26 Typical NAPL lens radius history

UTCHEM Key Processes that Require Input Data

The UTCHEM Users Guide provides this list of processes. For each process there are required input data. The overall list of potential input data is determined by the nature of the UTCHEM simulation.

The major physical phenomena modeled in the simulator are:

- dispersion
- diffusion
- dilution effects
- adsorption for oil, surfactant and polymer
- interfacial tension
- relative permeability
- capillary pressure
- hysteresis in relative permeability and capillary pressure
- capillary trapping
- cation exchange
- phase density
- compositional phase viscosity
- phase behavior (pseudoquaternary)
- aqueous reactions
- partitioning of chemical species between oil and water
- dissolution/precipitation
- cation exchange reactions involving more than two cations
- in-situ generation of surfactant from acidic crude oil
- pH dependent surfactant adsorption
- organic biodegradation capability
- multiple organic species
- equilibrium and nonequilibrium organic dissolution in aqueous phase
- dual porosity option for simple phase tracer flow
- polymer properties: shear thinning viscosity, inaccessible pore volume, permeability reduction, adsorption
- gel properties: viscosity, permeability reduction, adsorption
- tracer properties: partitioning, adsorption, radioactive decay, reaction (ester hydrolization), dead-end pore (capacitance)
- temperature dependent properties: viscosity, tracer reaction, gel reactions, Surfactant phase behavior
- gas mobility reduction due to foam
- mixed-wet oil/water capillary pressure and relative permeability

Example UTCHEM Flowchart for a Surfactant Problem

An example problem in the GMS Tutorials Document (Aquaveo, 2021) outlines this process:

1. Contamination: Define media and contaminant properties, initial and boundary conditions, and release.
2. Dissolution: Equilibrium dissolution (only) from NAPL and conservative transport.
3. Pre-flush PITT: A partitioning interwell tracer test (PITT) to assess NAPL saturations is simulated.
4. Water Flush: A "pump and treat" simulation of 270 days of flushing using water. The results of this flush can be compared with the surfactant flush simulation.
5. Surfactant Flush: A SEAR simulation using a surfactant to enhance dissolution and recovery with a 60-day simulation time.
6. Post Flush: Simulation to determine recovery after the SEAR treatment is complete.

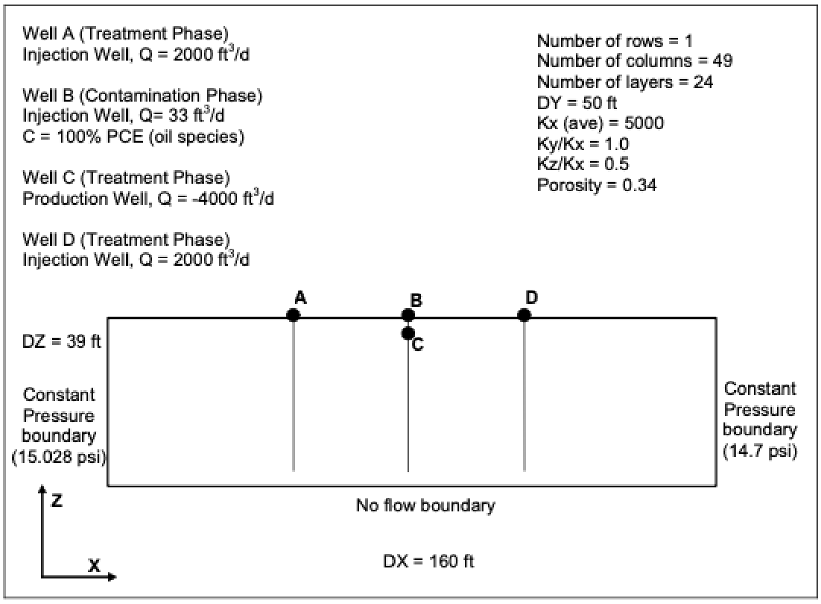


Figure 5-1 Sample Problem to be Solved with UTCHEM.

An Emerging LNAPL Model: The Panday LNAPL Simulator Based on MODFLOW

- Key Concept: Reduce governing multiphase flow equations using appropriate approximations to simplify and speed-up computations.
    - Solve only one (LNAPL phase) equation for evaluating LNAPL flow in the vadose zone and along the water table.
    - Assume air phase instantly equilibrates to movement of liquids.
        - Valid for unsaturated zone flow (this is not a petroleum reservoir).
        - Validated for flow of water in the vadose zone using Richards' Equation.
        - Eliminates air flow equation.
    - Assume water saturation is unchanged by neglecting water flow dynamics and water redistribution.
        - Appropriate at residual water saturations above capillary fringe.
        - Neglects depression of water table by pressure of overlying LNAPL so that lateral LNAPL spread will be larger than computed so impact is conservative.
        - Can bound impacts of LNAPL in capillary fringe and depression of water table.
        - Eliminates water flow equation.

    - Solve LNAPL flow equation only.
        - Simplify constitutive relationships such that air-filled pore space is the porosity available for LNAPL flow—reduces 3-phase relations to standard 2-phase air-LNAPL equations readily solved by available unsaturated zone flow codes.
- Why is it important and useful?
    - Can accommodate larger domain, finer grid, three-dimensional representation and structural complexity that may be difficult or impossible to represent and solve at a complex contaminated site with a multi-phase flow model.
    - Significantly alleviates computational burden.
        - Model runs quickly so that many alternative conceptualizations, parameter distributions, and ranges can be simulated to bracket likely behavior.
- Reduces parameterization burden (parameters are only needed for LNAPL phase).
    - Parameterization of unsaturated and saturated zones at a site is difficult.
    - Parameterization of multi-phase flow is difficult.
- **Key Point**: LNAPL migration can be performed with open source, public domain codes such as MODFLOW-USG or other unsaturated single phase flow codes.
- Current Status: A journal article is being prepared (Panday et al., in review) titled "*Simulation of LNAPL flow in the vadose zone using a single-phase flow equation".* The abstract is reproduced below.

  A simplified decoupled approach that considers flow only of the NAPL phase has been presented for simulating migration of LNAPL in the vadose zone and on the water table. The approach is applicable to several analyses of practical interest and can be readily adapted into existing vadose zone simulators by appropriate transformation of the constitutive relationships and parameters. Comparative examples demonstrate that results of LNAPL migration using the single-phase approach compare favorably to multiphase flow simulations in the vadose zone. The single-phase approach greatly reduces modeling effort and allows many more simulations to be performed within the same time period, than is possible with multiphase models. The main limitation of the single-phase approach is that it overestimates the spreading of LNAPL at the water table by about 10 to 20% in our comparative experiments for a flat water-table; these errors however reduce with increased water table gradients. The more rapid flow along the water table simulated by this approach as compared to the multiphase simulations is conservative for many examinations, however, this error is within the range of uncertainty in the impact of subsurface parameters such as intrinsic and relative permeability. If that is acceptable for an analysis, the single-phase approach presented here is a valid alternative for rapidly evaluating LNAPL migration in environmental settings.

References

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