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Atmospheric Dispersion Capability for T2VOC

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Author

Oldenburg, Curtis M.

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Curtis M. Oldenburg

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley CA 94720
USA

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Abstract

Atmospheric transport by variable-K theory dispersion has been added to T2VOC. The new code, T2VOCA, models flow and transport in the subsurface identically to T2VOC, but includes also the capability for modeling passive multicomponent variable-K theory dispersion in an atmospheric region assumed to be flat, horizontal, and with a logarithmic wind profile. The specification of the logarithmic wind profile in the T2VOC input file is automated through the use of a build code called ATMDISPV. The new capability is demonstrated on 2-D and 3-D example problems described in this report.

1. Introduction

An atmospheric transport capability has been added to T2VOC. The approach is applicable to the case of volatile organic compounds (VOCs) in the shallow subsurface that are transported by advection or diffusion across the ground surface and into moving air (i.e., wind) above the ground surface. Such transport is possible from contaminated sites and can be an effective process for removal of VOCs from soil. The approach is the same as developed by Oldenburg and Unger (2004) in earlier work for atmospheric dispersion of CO₂ that may potentially leak from geologic CO₂ storage sites. The new capability models all of the subsurface processes that T2VOC handles (see Falta et al., 1995; Pruess et al., 1999) and adds an atmospheric region with logarithmic velocity profile in which variable-K theory dispersion (Arya, 1999) is modeled. The actual changes to T2VOC to implement variable-K theory atmospheric dispersion are minor, but developing the initial logarithmic velocity profile corresponding to a given wind is tedious and requires the use of a build code to automate the task. In this brief report, we

describe the theory of variable-K dispersion, how to use the build code, and two examples to demonstrate the new capabilities.

2. Theory

In this section, we describe the theory and assumptions applicable to the transport of a dilute gas species, such as a VOC, evaporating from contaminated soil. If the VOC concentration in the gas phase is low enough (i.e., the gas is mostly air), the density and viscosity of the air-VOC mixture are not affected sufficiently by the VOC to alter the flow of the gas phase containing the VOC over the ground surface. In this case, the transport of the VOC is said to be passive because the VOC transport does not affect the flow field. Under the assumption of passive VOC transport, we discuss below the underpinnings of the use of an ambient wind profile and advection and dispersion in the lower layers of the atmosphere as developed in the atmospheric transport literature (e.g., Slade, 1968; Pasquill, 1974; Stull, 1988; Arya, 1999).

The mean turbulent transport of passive gas species in the atmospheric surface layer can be described by the advective-dispersive transport equation with variable eddy diffusivities (K_x , K_y , K_z) (Arya, 1999, p. 137). For the three-dimensional (x , y , z) transport of a component (such as a VOC) at concentration c , this equation is

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} - \frac{\partial}{\partial x} \left(K_x \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial y} \left(K_y \frac{\partial c}{\partial y} \right) - \frac{\partial}{\partial z} \left(K_z \frac{\partial c}{\partial z} \right) = 0 \quad (1)$$

For convenience in surface-layer transport modeling, the coordinate system can be arranged so that x is aligned in the downwind direction, making $v = w = 0$ where u is the ambient wind.

The ambient time-averaged wind profile near the ground surface has been shown theoretically to follow a logarithmic profile (e.g., Slade, 1968, p. 73). The logarithmic wind profile is valid over approximately the lower one-tenth of the atmospheric boundary layer, or approximately a few tens of meters above the ground surface. The logarithmic wind profile is given as:

$$u(z) = \frac{u_*}{k} \ln \left(\frac{z}{z_0} \right) \quad (2)$$

where $u(z)$ is the ambient wind velocity as a function of height, u_* is the friction velocity (a parameter that governs the shape of the wind profile near the ground surface for various surface types), k is von Karman's constant ($k = 0.4$), z is the elevation, and z_0 is a roughness height such that $u(z) = 0$ for $z \leq z_0$ and is also a function of various surface types (e.g., bare ground, grass, shrubs, etc.). The logarithmic wind profile is strictly applicable only to neutral stability conditions.

For the special case of constant eddy diffusivities and the assumption of a uniform wind velocity (u) with no shear (i.e., no velocity gradient), and assuming that advection dominates diffusion in the x -direction, solutions to Eq. 1 are given by the well-known Gaussian plume dispersion model, with constant eddy diffusivities D_{xx} , D_{yy} , and D_{zz} given by

$$D_{xx} = \frac{\sigma_x^2}{2t}, \quad D_{yy} = \frac{\sigma_y^2}{2t}, \quad D_{zz} = \frac{\sigma_z^2}{2t} \quad (3)$$

where σ_x , σ_y , σ_z are the standard deviations of concentration distributions at an observation or receptor point, and t is the travel time to the point (e.g., Arya, 1999, p. 132).

Although attractive because of its simplicity, the Gaussian plume model does not apply to situations with wind shear (i.e., a non-zero gradient of u with height) (Arya, 1999, p. 197-199), as appropriate for winds affecting VOCs evaporating from the ground surface. Instead, variable-K theory utilizing variable eddy diffusivities (K_x , K_y , K_z) is recommended for cases with wind shear and non-homogeneous turbulence such as will be found in the surface layer (Arya, 1999, p. 143). We have implemented variable-K theory and the assumption that K_z increases linearly with height as

$$K_z = k u_* z \quad (4)$$

(Arya, 1999, p. 143) into T2VOC. This model assumes neutral stability in the surface layer, and models the larger dispersion that occurs as the plume moves upward. There is no analogous formulation of K_y valid for short travel distances (< 10 km) in variable-K theory (Arya, 1999, p. 151). Nevertheless, the user can specify K_y formulations in the input file of T2VOCA as described below.

To summarize, we calculate eddy diffusivities from the variable-K diffusivity of Eq. 4 to produce an effective atmospheric dispersivity at every gridblock in the surface layer. Although it is normally negligible, the molecular diffusion coefficient is added to the eddy diffusivity with the largest term controlling the overall dispersion process. The single effective dispersivity is then used in the advective-dispersive transport equation for each chemical component to model surface-layer transport.

The assumptions that are made in this approach are as follows:

- 1) We assume the ground surface is flat (no topography) and horizontal.

- 2) We assume the dispersing component does not affect the flow field (wind) in the atmosphere, i.e., transport is passive. (Full density effects are considered in the subsurface.)
- 3) We currently use a logarithmic wind profile that assumes a stable atmosphere, and the wind velocity field is always horizontal and aligned with the x -axis.
- 4) In variable-K theory, there is no widely accepted formulation to use for lateral dispersion (K_y).
- 5) By using variable-K theory and logarithmic velocity profile, we assume implicitly that (1) the time scale is long enough that winds can be averaged, and (2) the length scale is relatively long. The relevant time scale can be considered to be from 1 month to several years, and length scale from 10 m to 1 km.

3. Implementation in T2VOC

The simulation of atmospheric advection and dispersion by the above methods requires the specification of a logarithmic wind profile within the TOUGH2 framework that will prevail throughout the simulation. This step involves generating a grid with sufficient layers (i.e., parallel to the ground surface) to discretize the wind profile to the desired accuracy. Next, a static gas-phase pressure profile in the z -direction is used along with a constant pressure difference between the upstream and downstream boundaries of the surface layer given by

$$\Delta P = P_2 - P_1, \quad P_1 > P_2 \quad (5)$$

where P_1 and P_2 are the upstream and downstream pressures, respectively, within a layer.

The phase velocity is computed using Darcy's equation

$$u = -\frac{k_D}{\phi \mu} \nabla(P - \rho g z) \quad (6)$$

where k_D is the intrinsic (Darcy) permeability, ϕ is the porosity, μ is the gas viscosity, ρ is the mass density of the gas phase, g is the gravitational acceleration and z is height. Setting the porosity of the surface-layer materials to unity, the velocity of the atmospheric air will be proportional to the permeability of the layer and pressure difference, ΔP , for horizontal layers. Given that ΔP is a constant for all layers, the individual permeability variations of the layers can be selected to produce a logarithmic wind profile. Note that the thickness of each layer must be constant to ensure a constant air velocity within the layer across the length of the domain. Note further that the permeability is a pseudo-permeability with no physical significance; its purpose is simply to create the desired velocity profile. Note also that the velocity in the surface layer must not be allowed to change significantly during the simulations because the dispersion process is assumed to be passive and the result of constant unidirectional wind. In essence, by this approach we have specified a velocity field for the surface layer that persists throughout the T2VOCA simulation. We have developed a build code (ATMDISPV) to automate the above steps for convenient initial condition development.

Numerical dispersion in the implicit and upstream-weighted TOUGH2 framework is on the order of one-half the grid spacing multiplied by the velocity. Because of the alignment of the grid with the unidirectional wind, numerical dispersion occurs only in

the flow direction (i.e., x -direction) in the surface layer. In the quasi-steady cases we are considering, advection dominates transport in the flow direction. In the vertical direction, the velocity is zero ($w = 0$), thus vertical eddy diffusion is untainted by numerical dispersion.

4. The Codes

Two codes are included in the package described here. These are (1) the modified T2VOC code called T2VOCA, and (2) the build code ATMDISPV used to generate T2VOCA input and related files.

4.1 T2VOCA

T2VOC has been modified to include atmospheric dispersion of all components under the assumption of variable-K theory. The new code is called T2VOCA where the A stands for atmosphere. Compilation of T2VOCA should be done as follows where it is assumed the T2 file is present in the same directory and the command is appropriate for the Portland Group Fortran77 compiler:

```
pgf77 -c -i8 -r8 t2cg22.f t2f.f t2voca.f meshm.f t2solv.f ma28.f
```

```
pgf77 -o xvoca t2cg22.o t2f.o t2voca.o meshm.o t2solv.o ma28.o
```

n.b.: Users should rename subroutines MULTI, RELP, and PCAP in t2f.f for compatibility with T2VOC and T2VOCA.

To execute xvoca, enter the command

```
xvoca <dispv.dat >out &
```

where dispv.dat is the T2VOCA input file and out is the T2VOCA output file. The T2VOCA input file is identical to the T2VOC input file described in Falta et al. (1995) and Pruess et al. (1999) except for the addition of a SELEC block with atmospheric dispersion parameters. The minor modifications for atmospheric dispersion are described below in the discussion of the dispv.dat file produced by the helper code ATMDISPV.

4.2 ATMDISPV

ATMDISPV is a build code that is used to establish gas- and hydro-static equilibrium conditions and a logarithmic velocity profile in the atmospheric region. ATMDISPV derives its name from “atmospheric dispersion for VOCs.” This build code reads from the control file atmdispv.dat and a file called vocinp.dat containing the CHEMP block to produce a T2VOCA input file called dispv.dat along with MESH and INCON files as per user specifications in atmdispv.dat. The dispv.dat file contains a SELEC block that specifies the needed parameters (location of source, a flag for setting K_y , and u^*) for computing atmospheric dispersion in T2VOCA. To compile ATMDISPV, use a Fortran77 compiler command such as the following (appropriate for PortlandGroup Fortran77):

```
pgf77 -o xatmdispv atmdispv.f
```

To execute ATMDISPV, simply enter the command

xatmdispv

The input variables and their definitions in the control file atmdispv.dat are presented in Table 1. As shown in Table 1, the input consists mostly of specifications that control MESH file generation, initial conditions, and ROCK properties. The ROCK properties and initial conditions for the fluids present (e.g., X_air50_water_init) are assigned to the subsurface part of the domain. The reference permeability applies to the atmosphere region. CHEMP data are read from vocinp.dat. The valley parameters allow users to define a valley within the domain, a capability that should only be invoked if users can verify that the present dispersion modeling assumptions are met. Examples of the atmdispv.dat control file are shown in Figures 1 and 2. The variables in Table 1 should become clearer upon study and execution of the example problems discussed in the next section.

The main purpose of the build code ATMDISPV is to automate the multiple preliminary steps normally associated with TOUGH2 simulations. This build code is especially useful for the tedious task of specifying the multiple layers in the atmosphere region that will control the logarithmic wind profile. The process of creating T2VOCA input files using the ATMDISPV build code consists of three steps that are controlled by the input values of the variables “model” and “INCON_MESH” in the control file atmdispv.dat.

Table 1. Variable Definitions for atmdispv.dat input file.

Variable	Definition
model	Controls stage of input file generation: = 0 gravity equilibrium = 1 steady-state flow = 2 final files with GENER blocks
INCON_MESH	Controls INCON and MESH file generation: = 0 no INCON or MESH file generation = 1 generate 1-D mesh = 2 generate full INCON from 1-D SAVE, and full MESH
nx_ups	Number of gridblocks in x-direction upstream of source.
nx_source	Number of source gridblocks in x-direction.
nx_dwns	Number of gridblocks in x-direction downstream of source.
ny_source	Number of source gridblocks in y-direction.
ny_dwns	Number of gridblocks in y-direction excluding source
nz_atm	Number of gridblocks in z-direction in atmosphere region.
nz_vad	Number of gridblocks in z-direction in vadose zone.
nz_sat	Number of gridblocks in z-direction in saturated zone.
ix_val_min	Starting x-direction gridblock for valley.
ix_val_max	Ending x-direction gridblock for valley.
iy_val_min	Starting y-direction gridblock for valley.
iy_val_max	Ending y-direction gridblock for valley.
iz_val_min	Starting z-direction gridblock for valley.
iz_val_max	Ending z-direction gridblock for valley.
width_source	Size of source in y-direction (m).
width_dwns	Width (y-direction) of system minus width of source (m).
height_atm	Height (z-direction) of atmosphere region (m).
height_vad	Height (z-direction) of vadose zone (m).
height_sat	Height (z-direction) of saturated zone (m).
length_ups	Length (x-direction) of system upstream of source (m).
length_dwns	Length (x-direction) of system downstream of source (m).
length_source	Length (x-direction) of source (m).
time_end	End time for simulation (see TOUGH2 User's Guide) (s).
dtime_start	Initial time-step (see TOUGH2 User's Guide) (s).
perm_x, y, z, pors	Permeability in x-, y-, and z-directions (m^2), porosity
irp, rp1, rp2, rp3, rp4, rp5	Relative perm. parameters (see TOUGH2 User's Guide).
icp, cp1, cp2, cp3, cp4, cp5	Capillary pressure params. (see TOUGH2 User's Guide).
nad, drok, cwet, spht	Rock properties (see TOUGH2 User's Guide).
com, expan, cdry, tortx	Rock properties (see TOUGH2 User's Guide).
gk, foc	Rock properties (see TOUGH2 User's Guide).
X_air50_water_init	Mass frac. air in water + 50 (see TOUGH2 User's Guide).
Xmol_voc_water_init	Mole fraction VOC in water.
Xmol_voc_gas_init	Mole fraction VOC in gas.
Sg_init_vad	Initial gas saturation in vadose zone

Table 1 (continued). Variable Definitions for atmdispv.dat input file.

Sw_init_vad	Initial water saturation in vadose zone.
Sw_init_sat	Initial water saturation in saturated zone.
T_ref	Temperature ($^{\circ}\text{C}$).
Pg_ref	Gas reference pressure in atmosphere region (Pa).
leak_VOC_rate	VOC leakage rate in source area (kg/yr/m^2).
rech_rate	Recharge rate or infiltration rate (m/yr).
v_star	Friction velocity (m/s).
von_karman	von Karman constant (set this to 0.4).
z_o	Roughness length (m).
K_ref	Reference permeability in atmosphere region (m^2).
xsource, ysource, zsource	Coordinates of center of source region (m, m, m).
dispflag	Flag for setting K_y . If dispflag = 0, $K_y = 0$, K_z is from variable-K theory. If dispflag = 1, $K_y = K_z$, K_z is from variable -K theory. If dispflag < 0, $K_y = K_z = -\text{dispflag}$.
dens_air	Density of air for calculating initial conditions (kg/m^3).
dens_water	Density of water for calculating initial conds. (kg/m^3).
visc_air	Viscosity of air for calculating properties of atmos. (Pa s).
grav	Acceleration of gravity (m/s^2).

Preliminaries

Users should create a directory referred to as the “run_” directory, and a subdirectory referred to as the “build_” directory. The T2VOCA simulations will be done in the run_ directory, and the construction of input files will be done in the build_ directory. Users should copy atmdispv.dat into the build_ directory. The source codes for T2VOCA and ATMDISPV can be compiled in any other directory (e.g., a higher-level “source_” directory) from which users will access the executables while in the build_ or run_directories.

Step One

In this step, a one-dimensional (1-D) column of gridblocks is generated that will be used to run a T2VOCA gravity-capillary equilibrium. The resulting one-dimensional steady-state equilibrium will then be automatically replicated to fill out a 2-D or 3-D region in the subsequent ATMDISPV run in Step Two. In the build_ directory, edit the atmdispv.dat file to have the desired specifications and set

model = 0

INCON_MESH = 1

Make sure there is a file called vocinp.dat that contains a CHEMP block is present in the build_ directory in order to specify and read VOC properties (see Pruess et al., 1999 for information about the CHEMP block). Run xatmdispv to produce MESH, INCON_grav, and dispv.dat files.

Copy the MESH, INCON_grav, and dispv.dat files to the run_ directory. Note the SELEC block in the dispv.dat file contains all of the parameters needed to specify atmospheric dispersion in T2VOCA. These are x , y , and z locations of the source, the variable that controls K_y (dispflag), and the friction velocity (v^*).

In the run_ directory, run xvoca using the MESH, INCON_grav, and dispv.dat files as MESH, INCON, and T2VOCA input file, respectively.

Copy the SAVE file back to the build_ directory for Step Two.

Step Two

This step reads from the SAVE file from Step One to create a full 2-D or 3-D simulation of gravity-capillary equilibrium with gas- and hydrostatic conditions. To accomplish Step Two, edit the atmdispv.dat file in the build_ directory to set

```
model = 1
```

```
INCON_MESH = 2
```

Run xatmdispv to produce MESH, INCON, and dispv.dat files.

Copy MESH, INCON, and dispv.dat files to the run_ directory.

Change to the run_ directory, and run xvoca using MESH, INCON, and dispv.dat files as MESH, INCON, and T2VOCA input file, respectively. This run should be quick because the initial condition is generated from replication of the 1-D column simulated in Step One.

Copy resulting SAVE file back to build_ directory for Step Three.

Step Three

This step computes the steady-state initial condition with logarithmic wind profile in the atmospheric region. In the build_ directory, edit the atmdispv.dat file to set

```
model = 1
```

```
INCON_MESH = 0
```

Run xatmdispv to produce MESH, INCON_steady, and dispv.dat files.

Copy MESH, INCON_steady, and dispv.dat files to the run_ directory.

In the run_ directory, run xvoca using the MESH, INCON_steady, and dispv.dat files as MESH, INCON, and T2VOCA input file, respectively.

The result should be a steady-state subsurface and atmosphere simulation with logarithmic wind profile in the atmospheric region. The SAVE file from this run can be edited to add in whatever subsurface VOC concentrations or NAPL saturations are desired as an initial condition, or GENER blocks can be added to specify VOC injection. The resulting SAVE file is the initial condition for the subsequent T2VOCA simulations of VOC transport in the subsurface and atmosphere regions.

5. Example Problems

5.1 Two-Dimensional Problem

This 2-D problem models a thin portion of saturated zone, a thick vadose zone, and an atmospheric region with average winds of 2 m/s at a height of 10 m. Non-aqueous phase liquid (NAPL) chlorobenzene (CB) is present in a part of the vadose zone and its evaporation and dissolution leads to a CB plume in the subsurface and atmospheric dispersion in the atmosphere region. The process of generating the input files and running this problem along with results are presented below.

Step One

Create a `run_` directory and a `build_` subdirectory. Copy the T2VOCA executable into the `run_` directory, and copy the ATMDISPV executable, the `atmdispv.dat` control file, and a file called `vocinp.dat` containing a CHEMP block appropriate for chlorobenzene (CB) into the `build_` directory. In the `build_` directory, edit the `atmdispv.dat` file so that it appears as in Figure 1 with `model = 0` and `INCON_MESH = 1`. Run `xatmdispv` to produce `MESH`, `INCON_grav`, and `dispv.dat` files. These files are the 1-D MESH file, a 2-D `INCON_grav` file, and T2VOCA input file (`dispv.dat`) for a gravity-capillary equilibrium run. (The `dispv.dat` file will obtain its CHEMP block from the `vocinp.dat` file present in the `build_` directory). Copy these files to the `run_` directory (rename `INCON_grav` to `INCON`), and run `xvoca` (`xvoca <dispv.dat >out &`). The result should be a rapid 1-D gravity-capillary steady-state. Copy the resulting `SAVE` file to the `build_` directory for Step Two.

```

0
1
5 5 20
1 0
20 8 2
31 31 51 51 31 31
1. 0.
10. 8.0 2.0
100. 400. 100.
3.156e11 0.1
1.0e-12 1.0e-12 1.0e-12 0.2
7 0.2 0.1 1.0 0.01 0.0
7 0.2 0.1 1.e-4 1.e10 1.0 0.0
2 2400.0 0.0 0.01
1.0e-10 0.0 0.0 1.0
0.0 0.0
50.00001 0.e-8 0.e-6
0.5 0.5 1.0 15.0 100.0e3
0.0 0.0
0.261 0.4 0.1 1.0e-2
100.0 .5 10.0 0.
1.16 1000.0 0.180318e-4 9.80665

! model =0 grav (writes INCON_grav), =1 steady (INCON_steady), =2 final (dispv.dat w/ GENER)
! INCON_MESH =0 no file generation, =1 generate 1d MESH, =2 generate full INCON from 1d SAVE
! nx_ups, nx_source, nx_dwns (x is flow direction)
! ny_source, ny_dwns (ny_dwns = ny - ny_source) (y is width direction)
! nz_atm, nz_vad, nz_sat (z is vertical direction)
! ix_val_min, ix_val_max, iy_val_min, iy_val_max, iz_val_min, iz_val_max (valley specs.)
! width_source, width_dwns (width_dwns = width - width_source) (y direction)
! height_atm, height_vad, height_sat (z direction)
! length_ups, length_dwns, length_source (x direction)
! time_end, dtime_start
! perm_x, perm_y, perm_z, pors
! irp, rp1, rp2, rp3, rp4, rp5
! icp, cp1, cp2, cp3, cp4, cp5
! nad, drok, cwet, spht
! com, expan, cdry, tortx
! gk, foc
! X_air50_water_init, Xmol_voc_water_init, Xmol_voc_gas_init
! Sg_init_vad, Sw_init_vad, Sw_init_sat, T_ref, Pg_ref
! leak_VOC_rate [kg/yr/m2] (4e6), rech_rate [m/yr]
! v_star, von karman, z_o, K_ref (permeability ref)
! xsource, ysource, zsource, dispflag
! dens_air, dens_water, visc_air, grav

```

Figure 1. File atmdispv.dat showing values for initial build of one-dimensional column of Step One.

Step Two

In the `build_` directory, edit the `atmdispv.dat` file by setting `model = 1` and `INCON_MESH = 2` so it looks like that in Figure 2. Run `xatmdispv` which will now read from the `SAVE` file containing the 1-D gravity-capillary equilibrium and replicate this throughout the full 2-D domain. This should produce `MESH`, `INCON`, and `dispv.dat` files. Copy these files to the `run_` directory and run `xvoca (xvoca <dispv.dat >out &)` to produce a 2-D gravity-capillary equilibrium and corresponding `SAVE` file. Copy the `SAVE` file back to the `build_` directory. This run should converge immediately because the 2-D steady state is simply a collection of 1-D columns at steady state. Therefore, the `xvoca` simulation part of Step Two can be omitted by copying the `INCON` file produced in Step One in the `build_` directory to `SAVE` and proceeding directly to Step Three. However, we include Step Two to emphasize the purpose of each step, namely, to produce a stable static equilibrium for the whole domain in anticipation of Step Three where we add in the wind.

```

1      ! model =0 grav (writes INCON_grav), =1 steady (INCON_steady), =2 final (dispv.dat w/ GENER)
2      ! INCON_MESH =0 no file generation, =1 generate 1d MESH, =2 generate full INCON from 1d SAVE
3      ! nx_ups, nx_dwns, nx_dwms (x is flow direction)
4      ! ny_source, ny_dwms (ny_dwms = ny - ny_source) (y is width direction)
5      ! nz_atm, nz_vad, nz_sat_ (z is vertical direction)
6      ! ix_val_min, ix_val_max, iy_val_min, iy_val_max, iz_val_min, iz_val_max (valley specs.)
7      ! width_source, width_dwms (width_dwms = width - width_source) (y direction)
8      ! height_atm, height_vad, height_sat (z direction)
9      ! length_ups, length_dwms, length_source (x direction)
10     ! time_end, dtme_start
11     ! perm_x, perm_y, perm_z, pors
12     ! irp, rp1, rp2, rp3, rp4, rp5
13     ! icp, cp1, cp2, cp3, cp4, cp5
14     ! nad, drok, cwet, spht
15     ! com, expan, cdry, tortx
16     ! gk, foc
17     ! X_air50 water init,Xmol_voc_water_init, Xmol_voc_gas_init
18     ! Sg_init_vad, Sw_init_vad, Sw_init_sat, T_ref, Pg_ref
19     ! leak_VOC_rate [kg/yr/m2] (4e6), rech_rate [m/yr]
20     ! v_star, von_karman, z_o, K_ref (permeability ref)
21     ! xsource, ysource, zsource, dispflag
22     ! dens air, dens water, visc air, grav

```

Figure 2. File *atmdispv.dat* showing input for build of steady-state 2-D hydro- and gas-static profile of Step Two.

Step Three

In the `build_` directory, edit the `atmdispv.dat` file by setting `model = 1` and `INCON_MESH = 0` so it looks like that in Figure 3. Run `xatmdispv` which will now read from the `SAVE` file containing the 2-D gravity-capillary equilibrium generated in Step Two and add in boundary pressures on the upstream and downstream sides of the atmospheric region to generate the wind across the system. The execution of `xatmdispv` should produce `MESH`, `INCON_steady`, and `dispv.dat` files. Copy these files to the `run_` directory (remember to copy `INCON_steady` to `INCON`). From the `run_` directory, run `xvoca` (`xvoca <dispv.dat >out &`) to produce a 2-D steady-state with wind in the atmospheric region and corresponding `SAVE` file.


```

1      ! model =0 grav (writes INCON_grav), =1 steady (INCON_steady), =2 final (dispv.dat w/ GENER)
0      ! INCON_MESH =0 no file generation, =1 generate 1d MESH, =2 generate full INCON from 1d SAVE
5 5 20      ! nx_ups, nx_source, nx_dwns (x is flow direction)
1 0      ! ny_source, ny_dwns (ny_dwns = ny - ny_source) (y is width direction)
20 8 2      ! nz_atm, nz_vad, nz_sat (z is vertical direction)
31 31 51 51 31 31      ! ix_val_min, ix_val_max, iy_val_min, iy_val_max, iz_val_min, iz_val_max (valley specs.)
1. 0.      ! width_source, width_dwns (width_dwns = width - width_source) (y direction)
10. 8.0 2.0      ! height_atm, height_vad, height_sat (z direction)
100. 400. 100.      ! length_ups, length_dwns, length_source (x direction)
3.156e11 0.1      ! time_end, dtime_start
1.0e-12 1.0e-12 1.0e-12 0.2      ! perm_x, perm_y, perm_z, pors
7 0.2 0.1 1.0 0.01 0.0      ! irp, rp1, rp2, rp3, rp4, rp5
7 0.2 0.1 1.e-4 1.e10 1.0 0.0      ! icp, cpl, cp2, cp3, cp4, cp5
2 2400.0 0.0 0.01      ! nad, drok, cwet, spht
1.0e-10 0.0 0.0 1.0      ! com, expan, cdry, tortx
0.0 0.0      ! gk, foc
50.00001 0.e-8 0.e-6      ! X_air50_water_init, Xmol_voc_water_init, Xmol_voc_gas_init
0.5 0.5 1.0 15.0 100.0e3      ! Sg_init_vad, Sw_init_vad, Sw_init_sat, T_ref, Pg_ref
0.0 0.0      ! leak_VOC_rate [kg/yr/m2] (4e6), rech_rate [m/yr]
0.261 0.4 0.1 1.0e-2      ! v_star, von karman, z_o, K_ref (permeability ref)
100.0 .5 10.0 0.      ! xsource, ysource, zsource, dispflag
1.16 1000.0 0.180318e-4 9.80665      ! dens_air, dens_water, visc_air, grav

```

Figure 3. File atmdispv3.dat showing input for build of steady-state wind profile of Step Three.

T2VOCA Simulation

The SAVE file produced can now be edited to specify VOC initial concentrations or saturations for a subsequent simulation of VOC flow and transport. We have done this by adding in non-zero NAPL saturation in the gridblocks located in the vadose zone below the region $100 \text{ m} < x < 200 \text{ m}$ and running out one year. Portions of the input and output files are shown in Figures 4 and 5, respectively. The grid and NAPL saturation after one year are shown in Figure 6, while the velocity field, water saturation, and CB mass fraction in the gas phase are shown in Figure 7. Note the low concentrations in the atmospheric region as wind strongly disperses and dilutes CB concentrations.

```

VOC dispersion model
ROCKS----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
atm 1      22.4000E+031.0000E+002.0007E-032.0007E-032.0007E-030.0000E+001.0000E-02
1.0000E-100.0000E+000.0000E+001.0000E+000.0000E+000.0000E+00
1      1.0000E-010.0000E+001.0000E+001.0000E-02
1      0.0000E+000.0000E+001.0000E+00
atm 2      22.4000E+031.0000E+004.3995E-034.3995E-034.3995E-030.0000E+001.0000E-02
1.0000E-100.0000E+000.0000E+001.0000E+000.0000E+000.0000E+00
1      1.0000E-010.0000E+001.0000E+001.0000E-02
1      0.0000E+000.0000E+001.0000E+00
atm 3      22.4000E+031.0000E+005.5149E-035.5149E-035.5149E-030.0000E+001.0000E-02
1.0000E-100.0000E+000.0000E+001.0000E+000.0000E+000.0000E+00
1      1.0000E-010.0000E+001.0000E+001.0000E-02
1      0.0000E+000.0000E+001.0000E+00
.
.
.
atm19      22.4000E+031.0000E+009.8851E-039.8851E-039.8851E-030.0000E+001.0000E-02
1.0000E-100.0000E+000.0000E+001.0000E+000.0000E+000.0000E+00
1      1.0000E-010.0000E+001.0000E+001.0000E-02
1      0.0000E+000.0000E+001.0000E+00
atm20      22.4000E+031.0000E+001.0000E-021.0000E-021.0000E-020.0000E+001.0000E-02
1.0000E-100.0000E+000.0000E+001.0000E+000.0000E+000.0000E+00
1      1.0000E-010.0000E+001.0000E+001.0000E-02
1      0.0000E+000.0000E+001.0000E+00
soil1      22.4000E+032.0000E-011.0000E-121.0000E-121.0000E-120.0000E+001.0000E-02
1.0000E-100.0000E+000.0000E+001.0000E+000.0000E+000.0000E+00
7      2.0000E-011.0000E-011.0000E+001.0000E-020.0000E+00
7      2.0000E-011.0000E-011.0000E-041.0000E+101.0000E+00

CHEMP----1----*---Chlorobenzene data----4----*----5----*----6----*----7----*----8
632.4      45.2      0.265      0.249      1.6
404.9      -7.587      2.26551      -4.09418      0.17038
112.559      -33.890      .5631      -4.522E-4      1.426E-7
1106.0      293.0      8.0E-6      283.15      1.00
-4.573      1.196E+3      1.37E-3      -1.378E-6      308.0
7.996E-5      0.      0.      0.
0.15      .0050      0.

PARAM----1----+---123456789012345678901234----+----5----+----6----+----7----+----8
8 2 99      9910000010002000040 03001 2.13e-05
0.0000E+003.1560E+071.0000E+01      dummy      9.8066E+003.0000E+00
1.0000e-4
1.000000E+05      0.000000E+00      0.000000E+00      1.500000E+01

TIMES----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
3 1
7.8894e+061.5779E+073.1560E+07

MULTI----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
3 3 3 6

SELEC----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
2

0.1000E+030.5000E+000.1000E+020.0000E+000.2610E+00

```

Figure 4. Portion of input file (dispv.dat) showing subset of layers generated for specifying logarithmic velocity profile.

^L
VOC dispersion model

THE TIME IS 0.36528E+03 DAYS

[illegible]

Figure 5. Portion of output file for T2VOCA run.

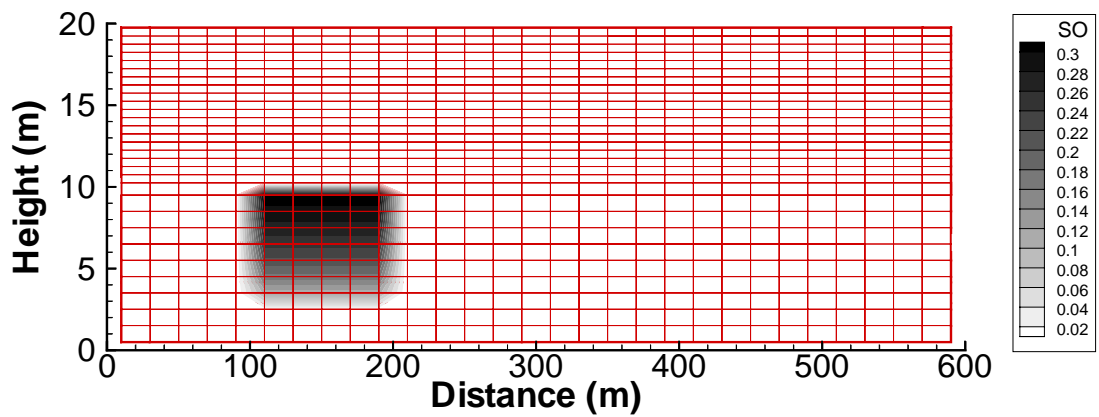


Figure 6. Grid and NAPL saturation after one year for 2-D example problem.

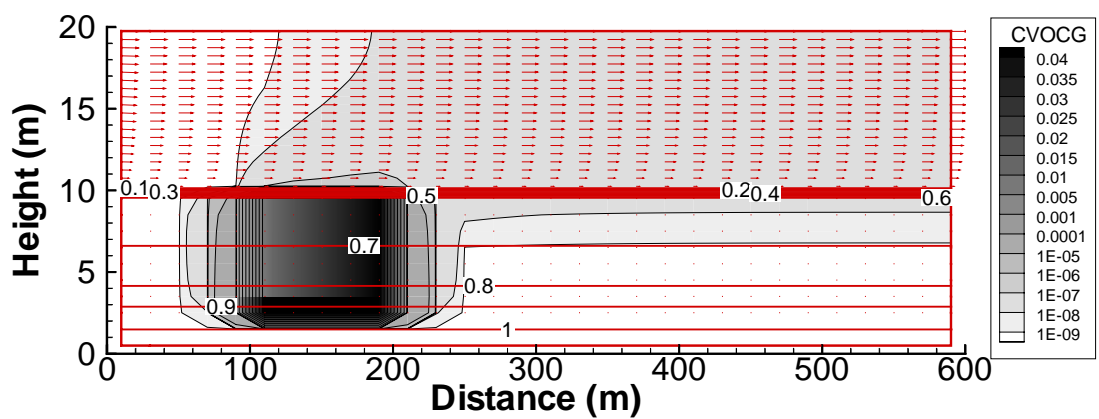


Figure 7. Results of water saturation and mass fraction VOC in the gas phase after one year.

5.2 Three-Dimensional Problem

A 3-D problem can be generated analogous to the 2-D case above. We based the 3-D system on the schematic specified by the sketch shown in Figure 8. Here is provided an abbreviated description of the process of developing a model grid and initial conditions for VOC transport for this problem. The atmdispv.dat control file for the 3-D case is shown in Figure 9 with model = 0 and INCON_MESH = 1 as appropriate for Step One. Note that the variable dispflag is set to 1, which makes $K_y = K_z$ where K_z is calculated from variable-K theory. Note that we honored the 500 m of distance downstream (x -direction) from the source but shortened the upstream distance to 100 m for a total x -length of 600 m. We used 10 gridblocks of 1 m height for the subsurface, and 20 gridblocks of 0.5 m height for the atmospheric region. We used uniform 50 m x 50 m (x - y) gridblocks in the x - and y -directions. The total number of gridblocks is 12 x 20 x 30 in the x -, y -, and z -directions. The grid is somewhat coarse for practical reasons; finer discretizations can be used depending on computer resources available.

Results are shown in Figure 10 for three planes with contours of mass fraction of CB in the gas phase and gas-phase velocity vectors after 1 year. As shown, the CB migrates downwards in the subsurface and disperses upwards and downwind above ground by variable-K theory dispersion. The CB concentrations in the atmosphere region are quite small due to dilution by the wind and dispersion.

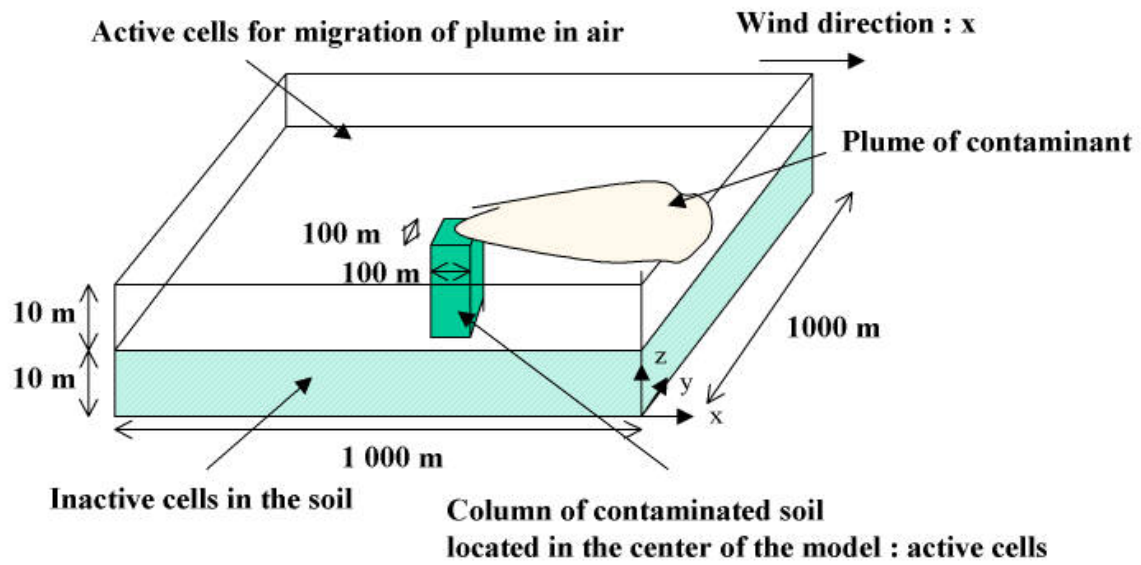


Figure 8. Schematic of 3-D problem domain specified by INERIS.

```

0
1
5 5 20
5 45
20 8 2
31 31 51 51 31 31
100. 900.
10. 8.0 2.0
100. 400. 100.
3.156e11 0.1
1.0e-12 1.0e-12 1.0e-12 0.2
7 0.2 0.1 1.0 0.01 0.0
7 0.2 0.1 1.e-4 1.e10 1.0 0.0
2 2400.0 0.0 0.01
1.0e-10 0.0 0.0 1.0
0.0 0.0
50.00001 0.e-8 0.e-6
0.5 0.5 1.0 15.0 100.0e3
0.0 0.0
0.261 0.4 0.1 1.0e-2
100.0 450.0 10.0 1.
1.16 1000.0 0.180318e-4 9.80665

! model =0 grav (writes INCON_grav), =1 steady (INCON_steady), =2 final (dispv.dat w/ GENER)
! INCON_MESH =0 no file generation, =1 generate 1d MESH, =2 generate full INCON from 1d SAVE
! nx_ups, nx_source, nx_dwns (x is flow direction)
! ny_source, ny_dwns (ny_dwns = ny - ny_source) (y is width direction)
! nz_atm, nz_vad, nz_sat (z is vertical direction)
! ix_val_min, ix_val_max, iy_val_min, iy_val_max, iz_val_min, iz_val_max (valley specs.)
! width_source, width_dwns (width_dwns = width - width_source) (y direction)
! height_atm, height_vad, height_sat (z direction)
! length_ups, length_dwns, length_source (x direction)
! time_end, dtm_start
! perm_x, perm_y, perm_z, pors
! irp, rp1, rp2, rp3, rp4, rp5
! icp, cp1, cp2, cp3, cp4, cp5
! nad, drok, cwet, spht
! com, expan, cdry, tortx
! gk, foc
! X_air50_water_init, Xmol_voc_water_init, Xmol_voc_gas_init
! Sg_init_vad, Sw_init_vad, Sw_init_sat, T_ref, Pg_ref
! leak_VOC_rate [kg/yr/m2] (4e6), rech_rate [m/yr]
! v_star, von_karman, z_o, K_ref (permeability ref)
! xsource, ysource, zsource, dispflag
! dens_air, dens_water, visc_air, grav

```

Figure 9. ATMDISPV control file atmdisv.dat for Step One.

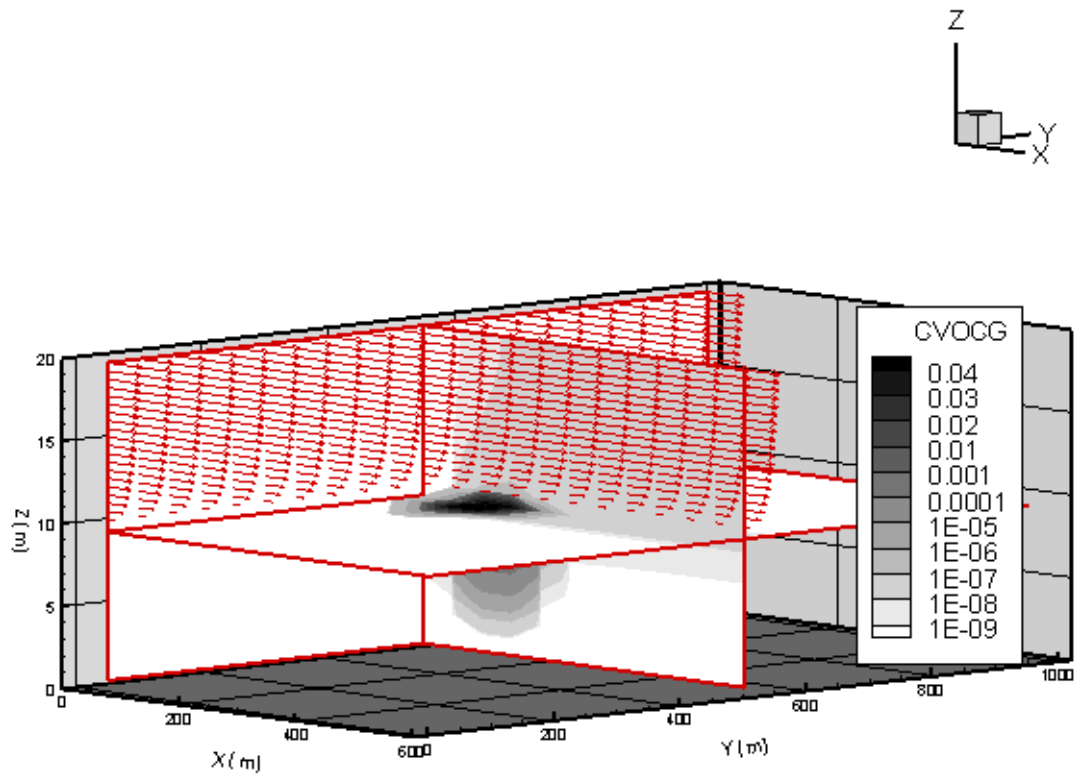


Figure 10. Results of 3-D coupled subsurface and atmospheric dispersion of CB from the shallow vadose zone after 1 year. Contours are mass fraction of CB in the gas phase. Vectors are gas-phase velocity (max. = 2 m/s).

6. Summary

T2VOCA and ATMDISPV provide atmospheric transport capability to T2VOC under specific assumptions relevant to variable-K theory. The use of the build code ATMDISPV for the problem specified involves three sequential steps which produce T2VOCA input, MESH, and INCON files with a steady logarithmic-profile wind in the atmosphere region. The SAVE file for this initial flow field can be modified or merged with other SAVE files to include non-zero VOC concentrations or NAPL saturations and then used as an INCON file for a T2VOCA simulation of coupled subsurface and atmospheric transport of VOC. Example problems demonstrate the mechanics of the approach and provide example simulation results.

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