TOUGH Short Course

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Berkeley, California

May 18-20, 2006

Multiphase-Multicomponent Flow with Volatile Organic Compounds (VOCs)

- T2VOC
- Phase Combinations
- Primary Variables and Variable Switching
- Secondary Parameters
- Input Format for Chemical Properties

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T2VOC

- T2VOC is a numerical simulator for modeling the transport of volatile organic chemical (VOC) contaminants in nonisothermal systems multiphase systems.
- Simulates processes such as
  - Migration of NAPLs in variably saturated media
  - Vacuum extraction of chemical vapors from the unsaturated zone
  - Air injection into the saturated zone for removal of volatile organics (air sparging)
  - Steam injection for removing NAPLs from contaminated soils…
- It is an extension of TOUGH2, also containing *t2voc.f*
- Reference: Falta, R.W., K. Pruess, S. Finsterle, and A. Battistelli (1995), *T2VOC User's Guide*, Report LBNL-36400, Lawrence Berkeley National Laboratory, Berkeley, Calif.

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Phase Combinations

- Large number of phase combinations possible in problems involving appearance or disappearance of phases.
- For a system in which three fluid phases can be present (w-aqueous, g-gas, n-NAPL) seven phase combinations are possible:

One-phase:	(1) w	(2) g	(3) n
Two-phase:	(4) w - g	(5) w - n	(6) g - n
Three-phase:	(7) w - g - n		

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Phase Combinations

- In T2VOC it is assumed that the aqueous phase never totally disappears (S_w stays larger than 10^{-4}).
- Number of possible phase combinations reduces to four:

One-phase:	(1) w	
Two-phase:	(2) w - g	(3) w - n
Three-phase:	(4) w - g - n	

- Initial conditions must include small amount of aqueous phase ($S_w > 10^{-4}$).

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Primary Variables

- T2VOC considers up to a four-component system
  - Water, air, VOC + heat
- Four primary variables needed to specify thermodynamic state (assuming local thermal/chemical phase equilibrium).
- The possible primary variables are:

Pressure,	P	
Temperature,	T	
Mass fraction of air in aq. phase,	X_{aw}	(X_w^a)
Mole fraction of VOC in gas phase,	$X_{mol,og}$	(X_g^c)
Mole fraction of VOC in aq. phase,	$X_{mol,ow}$	(X_w^c)
Gas phase saturation,	S_g	
Aqueous phase saturation,	S_w	

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Primary Variables

- The four primary variables (X1-X4) that are possible for the four phase combinations:

Phase(s)	X1	X2	X3	X4
w	P	X_{aw}+50	$X_{mol,ow}$	T
w - n	P	S_w	X_{aw}+50	T
w - g	P	S_w	$X_{mol,og}$	T
w - g - n	P	S_w	S_g+10	T

- Primary variables at grid block and time depend on phases.
- Number of unknowns can be reduced in some cases (more later).

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Phase Checking/Variable Switching

- Must be performed after each iteration for each grid block.
- After starting with aqueous conditions (1), appearance of NAPL causes phase transition to (2) in grid block.

	Phase(s)	X1	X2	X3	X4
(1)	w	P	X_{aw}+50	$X_{mol,ow}$	T
↓ (2)	w - n	P	S_w	X_{aw}+50	T
	w - g	P	S_w	$X_{mol,og}$	T
	w - g - n	P	S_w	S_g+10	T

- NAPL phase appears when $X_{mol,ow}$ exceeds solubility limit (at T).
- X2 becomes S_w (=1-10^{-6}) and X3 becomes X_{aw}+50.

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Phase Checking/Variable Switching

- Appearance of gas causes phase transition from (1) to (3).

	Phase(s)	X1	X2	X3	X4
(1)	w	P	X_{aw}+50	$X_{mol,ow}$	T
↓	w - n	P	S_w	X_{aw}+50	T
(3)	w - g	P	S_w	$X_{mol,og}$	T
	w - g - n	P	S_w	S_g+10	T

- If "bubble pressure" P_{bub} (= P_{VOC} + P_{vap} + P_{air}) is greater than total pressure P, then gas phase evolves and the variables are switched.
- X2 becomes S_w (=1-10^{-6}) and X3 becomes $X_{mol,og}$.

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Phase Checking/Variable Switching

- Check to see if third phase appears from two phases.

	Phase(s)	X1	X2	X3	X4
	w	P	X_{aw}+50	$X_{mol,ow}$	T
(2)	w - n	P	S_w	X_{aw}+50	T
(3)	w - g	P	S_w	$X_{mol,og}$	T
(4)	w - g - n	P	S_w	S_g+10	T

- From (2) to (4), gas phase evolves, and $S_g = 10^{-6}$.
- From (3) to (4), NAPL phase evolves, and S_g is reduced (multiplied by $1\text{-}10^{-6}$)
- Saturation of NAPL is $S_n = 1 - S_w - S_g$.

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Phase Checking/Variable Switching

- Phase saturations checked for phase disappearance.

	Phase(s)	X1	X2	X3	X4
	w	P	X_{aw}+50	$X_{mol,ow}$	T
(2)	w - n	P	S_w	X_{aw}+50	T
(3)	w - g	P	S_w	$X_{mol,og}$	T
(4)	w - g - n	P	S_w	S_g+10	T

- Transition from (4) to (2) if $S_g < 0$.
- Transition from (4) to (3) if $S_w + S_g > 1$ ($S_n < 0$).

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Secondary Variables

- Secondary parameters are functions of the primary variables.

Sections in T2VOC Manual	Parameter	Phase: gas	Phase: aqueous	Phase: NAPL
	Saturation	$S_g(S_w)$	S_w	$S_n(S_w, S_g)$
7.7 (p. 33)	Relative Permeability	$k_{rg}(S_g, S_w)$	$k_{rw}(S_w)$	$k_{rn}(S_g, S_w)$
7.1-7.4 (p. 24-28)	Viscosity	$\mu_g(P, \chi_g^c, T)$	$\mu_w(P, T)$	$\mu_n(P, T)$
	Density	$\rho_g(P, \chi_g^c, T)$	$\rho_w(P, T, \chi_g^c)$	$\rho_n(P, T)$
7.5 (p .29)	Specific Enthalpy	$h_g(P, \chi_g^c, T)$	$h_w(P, T)$	$h_n(P, T)$
7.7 (p. 33)	Capillary Pressure	---	$P_{cgw}(S_g, S_w)$	$P_{cgn}(S_g, S_w)$
7.6 (p. 31)	Water Mass Fraction	$X_g^w(P, \chi_g^c, T)$	$X_w^w(P, \chi_g^c, T)$	$X_n^w(P, \chi_g^c, T)$
	Air Mass Fraction	$X_g^a(P, \chi_g^c, T)$	$X_w^a(P, \chi_g^c, T)$	$X_n^a(P, \chi_g^c, T)$
	VOC Mass Fraction	$X_g^c(P, \chi_g^c, T)$	$X_w^c(P, \chi_g^c, T)$	$X_n^c(P, \chi_g^c, T)$
7.8 (p. 34)	Vapor Molecular Diffusivity	$D_g^w(P, \chi_g^c, T)$	---	---
	VOC Molecular Diffusivity	$D_g^c(P, \chi_g^c, T)$	---	---
	Tortuosity	$\tau_g(S_g, S_w)$	---	---
7.6 (p. 31)	VOC Henry's Constant	H_{gw}^c		
7.8 (p. 34)	Thermal Conductivity	$K(S_g, S_w, T)$		

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Input Format for Chemical Properties

- Chemical properties specified in block CHEMP (p. 41 of Manual)

T2VOC INPUT FORMATS

TITLE

ROCKS

MAT	NAD	DROK	POR	PER (1)	PER (2)	PER (3)	CWET	SPHT
COM		EXPAN	CDRY	TORTX	GK	FOC		
IRP		RP (1)	RP (2)	RP (3)	RP (4)	RP (5)	RP (6)	RP (7)
ICP		CP (1)	CP (2)	CP (3)	CP (4)	CP (5)	CP (6)	CP (7)

CHEMP

TCRIT	PCRIT	ZCRIT	OMEGA	DIPOLM
TBOIL	VPA	VPB	VPC	VPD
AMO	CPA	CPB	CPC	CPD
RHOREF	TDENRF	DIFV0	TDIFRF	TEXPO
VLOA	VLOB	VLOC	VLOD	VOLCRT
SOLA	SOLB	SOLC	SOLD	
OCK	FOX	ALAM		

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Input Format for Chemical Properties

- Data sets for common chemicals available in file *voc.dat*

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CHEMP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     11/94... VOC data sets prepared by George Moridis, LBL
CHEMP----1-Benzene-2----*----3----*----4----*----5----*----6----*----7----*----8
     562.2      48.2     0.271     0.212       0.0
     353.2  -6.98273   1.33213  -2.62863  -3.33399
    78.114-.3392E+020.4739E+00-.3017E-030.7130E-07
      885.    289.00 0.770E-05    273.10      1.52
0.4612E+010.1489E+03-.2544E-010.2222E-04     259.0
 0.411E-03 0.000E+00 0.000E+00 0.000E+00
 0.891E-01     0.001

CHEMP----1-Toluene-2----*----3----*----4----*----5----*----6----*----7----*----8
     591.8      41.0     0.263     0.263       0.4
     383.8  -7.28607   1.38091  -2.83433  -2.79168
    92.141-.2435E+020.5125E+00-.2765E-030.4911E-07
      867.    293.00 0.880E-05    303.10      1.41
-.5878E+010.1287E+040.4575E-02-.4499E-05     316.0
 0.101E-03 0.000E+00 0.000E+00 0.000E+00
 0.273E+00     0.001

CHEMP----1-Ethylbenzene-*----3----*----4----*----5----*----6----*----7----*----8
     617.2      36.0     0.262     0.302       0.4
     409.3  -7.48645   1.45488  -3.37538  -2.23048
   106.168-.4310E+020.7072E+00-.4811E-030.1301E-06
      867.    293.00 0.770E-05    298.10      1.79
-.6106E+010.1353E+040.5112E-02-.4552E-05     374.0
 0.258E-04 0.000E+00 0.000E+00 0.000E+00
 0.681E+00     0.001
…
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