TOUGH Short Course

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Radionuclide Transport for TOUGH2

- Description of EOS7R
- Physical Processes
- Primary Variables
- Input Formats

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EOS7R

- EOS7R is an equation of state module for simulation with:
  - Water, brine, air, 2 radionuclides, and heat
  - Radionuclides that decay and are water soluble and volatile
  - Adsorption onto solid grains
  - Molecular diffusion in aqueous and gas phases
- Assumptions
  - Radionuclides do not form non-aqueous phases
  - Salt precipitation does not occur
- Additional reference:
  - Oldenburg and Pruess, EOS7R: *Radionuclide Transport for TOUGH2*, Report LBL-34868, LBNL, Berkeley, Calif., Nov., 1995.
- Code executable created by compiling TOUGH2 with *EOS7R.f.* Additional instructions in *read.me* file.

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Radioactive Decay

- Exponential decay of mass (M) of radionuclide component (k)

$$\frac{dM^k}{dt} = -\lambda_k M^k$$
$$M^k = M_0^k \exp(-\lambda_k t)$$

- Half-life depends on decay constant λ_k

$$\frac{M^k_{t_{1/2}}}{M^k_{t_0}} = \exp(-\lambda_k t_{1/2}) = \frac{1}{2}$$
$$t_{1/2} = \frac{\ln 2}{\lambda_k}$$

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Sorption and Dissolution of Radionuclides

- Mass adsorbed onto solid grains by reversible instantaneous linear model

$$M^k = \phi \sum_\beta S_\beta \rho_\beta X^k_\beta + (1-\phi)\rho_R \rho_{aq} X^k_{aq} K_d$$

- Gas dissolution in the aqueous phase determined by Henry's law

$$P_k = K_h X^k_{aq} \quad \text{or} \quad X^k_{aq} = \left(K_h^{-1}\right) P_k$$

The amount of component k dissolved in aqueous phase is determined by the partial pressure and the "inverse of Henry's constant"

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Primary Variables

- EOS7R considers up to a five components plus heat
  - -Water, brine, parent radionuclide (Rn1), daughter radionuclide, air, and heat
- The possible primary variables are:

Pressure,	P
Mass fraction of brine,	X_b
Mass fraction of Rn1,	X_{Rn1}
Mass fraction of Rn2,	X_{Rn2}
Mass fraction of air,	X_{air}
Gas phase saturation,	S_g
Temperature,	T

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Primary Variables

- Two combinations of primary variables (X1-X6) are possible, depending on phase condition:

	X1	X2	X3	X4	X5	X6
1-phase (*aq.*)	P	X_b	X_{Rn1}	X_{Rn2}	X_{air}	T
2-phase (*aq.* + *gas*)	P	X_b	X_{Rn1}	X_{Rn2}	S_g+10	T

- When $P_{gas} > P_{aq}$, transition to 2-phase from 1-phase conditions
- When $S_g < 1$, transition to 1-phase from 2-phase conditions
- Number of unknowns can be reduced in MULTI block (see p.45, 162)
  - If gas is excluded, NK = 4 (NK = 5 otherwise)
  - If diffusion is ignored, NB = 6 (NB = 8 otherwise)

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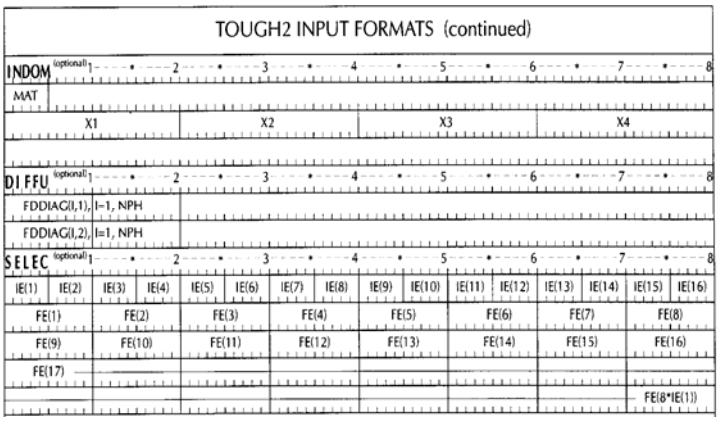
Input Format for EOS7R

- Properties related to diffusion, adsorption, radioactive decay and volatilization are specified in block `SELEC` (see p. 46 of Manual)

SELEC.1
SELEC.2
SELEC.3
SELEC.4
…



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