**Conceptual Model**

This model calculates the concentrations of LNAPL constituents downgradient of an LNAPL release over time.

A known volume of LNAPL is released to the subsurface. The LNAPL has several components whose volume fractions are known, and the density of the LNAPL is also known. The unidentified fraction of the LNAPL is a mixed petroleum product with unknown components, but with a known average molecular weight.

The LNAPL establishes a lens in the groundwater with a known width and average thickness. Groundwater flows through the LNAPL lens and dissolves the LNAPL constituents, reducing the remaining volume of LNAPL and changing its composition as the more soluble compounds dissolve out of the LNAPL. Equilibrium between the water and LNAPL within the lens is assumed, so that the concentration of constituents downgradient of the LNAPL are equal to the effective solubility of the LNAPL constituents. Effective solubility is the solubility of a pure phase component times its mole fraction in the LNAPL.

**Dimensions and units:**

T = time.

M = mass.

Mi = mass of constituent i.

MN = mass of LNAPL.

N = moles.

Ni = moles of constituent i.

NT = total moles of all constituents in LNAPL.

L = length

V = volume, or L3:

VN = volume of NAPL.

Vw = volume of water.

Vi = volume of constituent i.

Lw = liters of water.

**Input parameters:**

K = hydraulic conductivity (L/T).

i = hydraulic gradient (dimensionless).

w = width of LNAPL lens (L).

b = average thickness of LNAPL lens (L).

n = number of constituents in LNAPL.

ρN = density of LNAPL (MN/VN).

Δt = time step (T).

For each constituent i:

yi = volume fraction of constituent in LNAPL (Vi/VN)

ωi = molecular weight of constituent i (Mi/Ni.

Si = solubility of pure constituent i (Mi/Vw).

ρi = density of LNAPL constituent i (Mi/Vi).

**Variables:**

t = time (T);

Ci = water concentration of constituent i (Mi/Vw).

Ni = moles of constituent i (moli).

NT = total moles in LNAPL (molN).

xi = mole fraction of constituent i in LNAPL (moli/molN)

zi = mass fraction of constituent i in LNAPL (Mi/MN)

Sei = effective solubility of constituent i (Mi/Vw).

q = groundwater specific discharge (L/T).

**Superscripts and subscripts:**

i = constituent i;

k = time step k;

0 = initial value (time = 0);

**Program**

***Calculate specific discharge (groundwater flux) through the LNAPL area:***

1) 

***Calculate the volumetric flow rate of groundwater through the LNAPL:***

2) 

***Calculate the initial moles of LNAPL constituents and the total mols:***



For i = 1 to n

3) 

4) 

next i

***Calculate initial mole fractions and effective solubilities of each constituent:***

For i = 1 to n

5) 

6) 

next i

***Calculate initial mass fractions of each constituent:***

For i = 1 to n-1

7) 

next i

8) 

***Calculate density of other LNAPL components:***



For i = 1 to n-1

9) 

next i

10) 

***Main Loop: Calculate changes in composition of each constituent over time:***

For t = 0 to final time

*Write current water concentrations:*

For i = 1 to n

11) 

next i

*Calculate new moles of each LNAPL constituents, new mole fractions, and new effective solubilities:*

12) 

For i = 1 to n

13) 

14) 

next i

For i = 1 to n

15) 

16) 

next i

t = t + Δt

Loop

END