APPENDIX U

EXAMPLE CALCULATIONS

P = Partial Pressure (atm)

 $X = \text{Concentration of contaminant in groundwater} \left(\frac{mol}{L}\right)$ $K_H = \text{Henry's Law constant} = \frac{P}{X}$

The following example calculation converts the measured concentration of TCE in groundwater to the expected equilibrium concentration in soil gas using the Henry's Law constant for TCE:

$$K_H(TCE) = \left(11\frac{atm \cdot L}{mol}\right)$$

Molecular weight of TCE = 131.4 $\frac{g}{mol}$

Measured concentration of TCE in groundwater = $5.0 \frac{\mu g}{L}$

$$X_{TCE} = 5.0 \, \frac{\mu g}{L} \times \frac{1 \, g}{10^6 \, \mu g} \times \frac{1 \, mol}{131.4 \, g} = 3.8 \times 10^{-8} \frac{mol}{L}$$
$$P_{TCE} = 11 \frac{atm \cdot L}{mol} \times 3.8 \times 10^{-8} \frac{mol}{L} = 4.2 \times 10^{-7} atm$$
$$\frac{4.2 \times 10^{-7} atm}{1 \, atm} = 0.420 \, ppmv = 420 \, ppbv$$

The following example calculation converts the measured concentration of PCE in soil gas to the expected equilibrium concentration in groundwater using the Henry's Law constant for PCE:

 $K_H(PCE) = \left(18 \frac{atm \cdot L}{mol}\right)$

Molecular weight of PCE = 165.85 $\frac{g}{mol}$

Measured concentration of PCE in soil gas = 64 ppbv

$$64 \text{ ppbv} = 0.064 \text{ ppmv} = \frac{6.4 \times 10^{-8} atm}{1 atm}$$
$$X_{PCE} = 6.4 \times 10^{-8} atm \times \frac{1}{18 \frac{atm \cdot L}{mol}} = 3.6 \times 10^{-9} \frac{mol}{L}$$
$$3.6 \times 10^{-9} \frac{mol}{L} \times 165.85 \frac{g}{mol} \times 10^{6} \frac{\mu g}{g} = 0.59 \frac{\mu g}{L}$$