2. Gas solubility and water vapour source term $G_{sol,e,n}^P$

**Gas solubility**

In a two phase liquid/gas system, a part of the gas compound $n$ will be dissolved in the liquid phase and part will be in the gas phase. The equilibrium liquid phase concentration of the gas compound as a solute, $z_{eq,n}^L / z^L$, is related to the absolute partial pressure of the gas in the gas phase, $z_n^G p_a^G / z^G$ and the ambient temperature, where $z_n^G / z^G$ is the gas phase concentration and $p_a^G$ is the gas absolute pressure. The equilibrium concentration can be calculated using Henry’s Law,

$$z_{eq,n}^L / z^L = H_n^T z_n^G p_a^G / z^G$$

(3)

where $H_n^T$ is Henry’s coefficient for compound $n$ at temperature $T$. Values of $H_n^T$ for a range of compounds may be found in (Moody, Rodwell et al. 1992, Chapra 1997, Droste 1997, Sander 1999). (Sander 1999) also gives the following formula for the variation of Henry’s constant with temperature $T$ in Kelvin.

$$\frac{H_n^T}{H_n^0} = e^{-a_n \left( \frac{1}{T_0} - \frac{1}{T} \right)}$$

(4)

Effectively the solubility decreases exponentially with increasing temperature the decay rate being determined by values of $\alpha_H$.

In LDAT the changes in the liquid phase concentration are assumed to take place at a rate proportional to the difference between the actual concentration $z_n^L / z^L$ and $z_{eq,n}^L / z^L$.

$$\Delta \left( \frac{z_n}{z} \right) = -f_H \left( \frac{z_n}{z} - H_n^T z_n^G p_a^G / z^G \right) \Delta t$$

(5)

Where $f_H$ is the gas solubility mass transfer coefficient.

Thus with reference to equation (2)

$$G_{sol,e,n}^L = -f_H \left( \frac{z_n^L}{z^L} - H_n^T z_n^G p_a^G / z^G \right) z^L$$

And $G_{sol,e,n}^G = -G_{sol,e,n}^L \rho_{e,n}^L / \rho_{e,n}^G$

The values used for Henry’s coefficient in LDAT are given in Table 1. Note that an artificially high value is applied for Oxygen to facilitate the calculation of heat generation as the result of aerobic
degradation. This issue is discussed further in Section 4.

**Water vapour**

At any point in time the pore-space will contain water vapour as well as gas. In LDAT it is assumed that the water vapour pressure, $e_a$ kPa, is equal to the absolute partial pressure calculated as,

$$e_a = z_w^G p_a^G / z^G$$  \hspace{1cm} (6)

where $z_w^G / z^G$ is the water vapour gas phase concentration and $p_a^G$ is the absolute gas pressure.

If the temperature in the gas is $T$ °C there will be a vapour pressure related to $T$, $e_s(T)$, at which the volumetric water vapour concentration reaches the maximum value that the pore space can accommodate. $e_s(T)$ is known as the saturated water vapour pressure. In LDAT the change in $z_w^G / z^G$ over a time increment $\Delta t$ is assumed to be proportional to the difference between $e_s(T)$ and $e_a$, thus,

$$\Delta(z_w^G / z^G) = f_W \Delta t (e_s(T) - e_a)$$  \hspace{1cm} (7)

Where $f_W$ is a rate constant with units 1/kPa/day.

The function $e_s(T)$ (kPa) assumed for LDAT is that given by (Chapra 1997) quoting (Raudkivi 1979).

$$e_s(T) = 0.613 \exp \left( \frac{17.27 T}{237.3 + T} \right)$$  \hspace{1cm} (8)

Again with reference to equation (2)

$$G_{sol,e,n}^G = f_W (e_s(T) - e_a) z^G$$

And $G_{sol,e,n}^L = -G_{sol,e,n}^G \rho_{e,n}^G / \rho_{e,n}^L$