Reactive Tracer Equation

The concentration of a reactive tracer from a single channel, i, is

$$C_{r,i}(t) = f_i \, exp(-\lambda_i \, t) \frac{\rho_f \nu_i M_r}{Q} \frac{1}{2\sqrt{\pi \alpha_i \nu_i t}} exp\left[\frac{-(L_i - \nu_i t)^2}{4\alpha_i \nu_i t}\right] = \, exp(-\lambda_i \, t) \, C_{c,i} \tag{1}$$

(e.g., Carslaw and Jaeger, 1959, p. 50, Section 2.1, Case I; Toride et al., 1993) where M_r is the mass of reactive tracer and λ is the temperature-dependent first-order rate coefficient which, for constant reservoir temperature, is given by

$$\lambda = A \, exp\left(\frac{-E_a}{RT}\right) \tag{2}$$

where E_a is the activation energy, A is the pre-exponential factor, R is the gas constant T is the reservoir temperature (kelvin). Dividing Eq. (1) by the solution for concentration of a conservative tracer yields

$$\frac{C_{r,i}(t)/C_{c,i}(t)}{M_r/M_c} = C_{rel} = \exp(-\lambda t) \tag{3}$$

When the reservoir temperature varies between the tracer injection point and the fluid extraction well, the rate coefficient can be considered an effective value (λ_{eff}) which is dependent on the average (or effective) reservoir temperature and Eq. (2) is written as

$$\lambda_{eff} = A \, exp\left(\frac{-E_a}{RT_{eff}}\right) \tag{4}$$

or

$$\lambda_{eff} = A \int_0^1 exp\left(\frac{-E_a}{RT(x_r)}\right) dx_r = A \, exp\left(\frac{-E_a}{R\int_0^1 T(x_r) dx_r}\right) \tag{5}$$

and the effective temperature is

$$T_{eff} = \int_0^1 T(x_r) dx_r \tag{6}$$

where $x_r = x/L_i$ and L_i is the distance between the tracer injection point and fluid extraction well along channel i.

The choice of tracer depends on the sensitivity of change in tracer concentration to the change in the effective temperature, i.e., dC_{rel}/dT_{eff} (Plummer et al., 2012). This sensitivity is

$$\frac{dC_{rel}}{dT_{eff}} = \frac{A \, t \, E_a}{R \, T_{eff}^2} \, exp\left[-A \, t \, exp\left(\frac{-E_a}{R \, T_{eff}}\right) - \frac{E_a}{R \, T_{eff}}\right] \tag{7}$$

The concentration of a reactive tracer at the extraction well is

$$\frac{C_{r,i}(t)/C_{c,i}(t)}{M_r/M_c} = \sum_{1}^{nch} f_i exp\left(-A\ exp\left(\frac{-E_a}{RT_{eff,i}}\right)\ t\right) \tag{8}$$

where $T_{eff,i}$ is given by Eq. (6) and $T_i(x)$ is the temperature profile in channel i.