

# Units for LHHW Pre-Exponential Factor and Equilibrium Constant

The pre-exponential factor in the LHHW rate expression has very complex units which depend on the concentration basis selected, whether a reference temperature is specified, and the degree of concentration dependency of the driving force and adsorption terms. The concentration is converted to SI units before the rate is calculated. The pre-exponential factor has the units needed to make the

overall rate expression have SI rate units, that is,  $\frac{\text{kmol}}{\text{sec} \cdot \text{kg catalyst}}$  for the **Rate Basis** Cat (wt). When the **Rate Basis** is Reac (vol), the rate is instead in  $\frac{\text{kmol}}{\text{sec} \cdot \text{m}^3}$  units. In either case, the catalyst weight or reactor volume used is determined by the reactor where the reaction occurs.

The units for the pre-exponential factor can be written as

$$\text{units for } k = \frac{\left( \frac{\text{kmol}}{\text{sec} \cdot (\text{kg catalyst or m}^3)} \right)}{(\text{K or } ^\circ\text{R})^{TE} (\text{conc.})^{DFCE}}$$

where:

<i>TE</i>	=	Temperature exponent. If a reference temperature is specified, this is zero because the reference temperature cancels out the units of the temperature. If a reference temperature is <i>not</i> specified, this is <i>n</i> , the temperature exponent specified. The temperature unit can be Kelvin or Rankine based on the units specified for the reference temperature.
<i>conc.</i>	=	Units of concentration. This depends on the concentration basis selected. Molar concentration (kmol/m <sup>3</sup> ) Molality (mole/kg water) Mole fraction, mass fraction, or mole gamma (dimensionless) Partial pressure or fugacity (N/m <sup>2</sup> ) Mass concentration (kg/m <sup>3</sup> )
<i>DFCE</i>	=	Driving force concentration exponent. The sum of all the $\nu_i$ for all components in term 1 of the driving force expression. <b>Note:</b> When water is included in the reaction and molality basis is selected, mole fraction is used for water instead of molality, since the molality of water would just be a constant. As a result, exclude the exponent of water from the sum if basis is molality.

The equilibrium constants in the driving force and adsorption expressions may also have units. K1 in the driving force expression is always dimensionless, but K2 has units to make the second term of the driving force expression have the same units as the first; that is, it has concentration units from the above table to a power equal to the difference in the net concentration exponents of the two terms. In the adsorption expression, each equilibrium constant has concentration units inverse of the concentration it is multiplied by, so that each term is a dimensionless number.