Equation of State Reference / Documentation

[redacted] The main function of the EoS was to appropriately model the non-ideal behavior of CO_2 in the supercritical state. [redacted]

[redacted] This facilitated solubility calculations of CO_2 in aqueous solutions under non-ideal and non-isothermal conditions. The example Peng-Robinson formulation is as follows:

$$p = [RT/(V_m - b)] - [aA/(V_m^2 + 2bV_m - b^2)]$$

Where:
p - pressure (absolute)
V_m - molar volume (1 mole of gas or liquid)
R - ideal gas constant (8.3144621 J/(mol.K)
T - absolute temperature (K)
$A = [1 + k(1-T_r^{0.5})]^2$
$b = 0.07780RT_c/p_c$
$a = 0.45724\ R^2\ T_c^2/p_c$
and
T_c - critical temperature
p_c - critical pressure
$T_r = T/T_c$
$k = 0.37464 + 1.54226w - 0.26992w^2$, when $w > 0.49$