Contents

Pure Component Data Manager Help

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Introduction to PCDman

ChemSep is a software system for modeling distillation, absorption, and extraction operations. *ChemSep* was designed to be easy to use by students with no experience of engineering software, while having sufficient flexibility and power to appeal to expert users. In pursuit of these objectives *ChemSep*features a menu-driven, user-friendly interface. To facilitate the quick and easy simulation of chemical processes the program needs to have libraries of physical properties for most commonly used chemicals. There are libraries for pure compounds and databanks for pure compound data (PCD). ChemSep's default databank is called *chemsep1.pcd*. When an user wants to use a compound that isn't in this databank (s)he must be able to make a new library with the PCD information. The PCDman(ager) does just that.

Temperature Dependent Properties

Many properties can be estimated as simple functions of temperature. *ChemSep* includes many equations that can be used for this purpose/ Pure component temperature dependent physical properties from correlations published by the Design Institute for Physical Properties Research (DIPPR). However, any other quantity that depends on one dependent variable and up to five parameters may be calculated from the equations provided. The equations available in *ChemSep* are as hown in 1.

Table 1: Temperature correlations (t is temperature in Kelvin and $t_r = t/t_c$)

Key	equation
1	$y = a$
2	$y = a + bt$
3	$y = a + bt + ct^2$
4	$y = a + bt + ct^2 + dt^3$
5	$y = a + bt + ct^2 + dt^3 + et^4$
10	$\exp\left(a - \frac{b}{c+T}\right)$
11	$y = \exp a$
12	$y = \exp a + bt$
13	$y = \exp a + bt + ct^2$
14	$y = \exp a + bt + ct^2 + dt^3$
15	$y = \exp a + bt + ct^2 + dt^3 + et^4$
16	$y = a + \exp b/t + c + dt + et^2$
17	$y = a + \exp b + ct + dt^2 + et^3$
45	$y = at + bt^2/2 + ct^3/3 + dt^4/4 + et^5/5$
75	$y = b + 2ct + 3dt^2 + 4et^3$
100	same as 5
101	$y = \exp a + b/t + c\ln(t) + dt^e$
102	$y = at^b/(1 + c/t + d/t^2)$
103	$y = a + bexp(-c/t^d)$
104	$y = a + b/t + c/t^3 + d/t^8 + e/t^9$
105	$y = a/b^{1+(1-t/c)^d}$
106	$y = a(1 - t_r)^{[}b + c.t_r + d.t_r^2 + et_r^3]$
107	$y = a + b[(c/t)/sinh(c/t)]^2 + d[(e/t)/cosh(e/t)]^2$
114	$y = a^2(1 - t_r) + b - 2ac(1 - t_r) - ad(1 - t_r)^2 - c^2(1 - t_r)^3/3 - cd(1 - t_r)^4/2 - d^2(1 - t_r)^5/5$
115	$y = \exp a + b/t + c\ln t + dt^2 + e/t^2$
116	$y = a + b(1 - t_r)^{0.35} + c(1 - t_r)^{2/3} + d(1 - t_r) + e(1 - t_r)^{4/3}$
117	$y = at + b(c/t)/tanh(c/t) - d(e/t)/tanh(e/t)$
120	$y = a - b/(t + c)$
121	$y = a + b/t + c\ln t + dt^e$
122	$y = a + b/t + c\ln t + dt^2 + e/T^2$
207	same as 10
208	$y = 10^{a - \frac{b}{t+c}}$
209	$y = 10^{a(1/t - 1/b)}$
210	$y = 10^{a + b/t + ct + dt^2}$
211	$y = a\left[\frac{b-t}{b-c}\right]^d$

Technical Background

Process Modelling

More information

You can obtain updates to *ChemSep* Lite from our web site: www.chemsep.com. Read and/or download the latest technical reference material. ChemSep Case Stories are also available for download.