

# Contents

Introduction to PCDman . . . . .	3
Temperature Dependent Properties . . . . .	4
Technical Background . . . . .	6

# Pure Component Data Manager Help

**Harry A. Kooijman**

Amsterdam, The Netherlands

kooijman@chemsep.org

**Ross Taylor**

Clarkson University, Potsdam, New York

taylor@chemsep.org

Copyright © 2008 by H.A. Kooijman and R. Taylor. All rights reserved. This publication is public domain. No responsibility is assumed by the authors for any injury and/or damage to persons or property as a matter of products liability, negligence, or otherwise, or from any use or operation of any methods, products, instructions, information, or idea's contained in the material herein. The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in absence of specific statement, that such names are exempt from the relevant protective laws and regulation and therefore free for general use.

## 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 shown 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	$y = a + b \exp(-c/t^d)$
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](http://www.chemsep.com). Read and/or download the latest **technical reference material**. ChemSep **Case Stories** are also available for download.