A FAST INSIGHT INTO THE PRESSURE-DENSITY-TEMPERATURE RELATIONSHIP OF CELLULOSE

by

Ling LIN\textsuperscript{a*}, Ya LI\textsuperscript{b*}, Yongfang QIAN\textsuperscript{c}, and Yanping LIU\textsuperscript{d}

\textsuperscript{a}Ningbo Advanced Textile Technology and Fashion CAD Key Laboratory, Zhejiang Fashion Institute of Technology, Ningbo, China
\textsuperscript{b}National Engineering Laboratory for Modern Silk, College of Textile and Clothing Engineering, Soochow University, Suzhou, China
\textsuperscript{c}School of Textile and Material Engineering, Dalian Polytechnic University, Dalian, China
\textsuperscript{d}College of Ocean Science and Technology, Zhejiang Ocean University, Zhoushan, China

Original scientific paper
https://doi.org/10.2298/TSCI1804845L

An approximate pressure-density-temperature relationship of cellulose is derived by Taylor expansion technology with a knowing reference values for pressure, density, and temperature. The approximate formula can be used for fast prediction of relationship among pressure, density and temperature near its reference partner.

Key words: cellulose, pressure-volume-temperature relationship, polymers thermodynamics

Introduction

Cellulose has been widely used for mass-production of a wide variety of products, especially fabrics, paperboards and papers [1–4]. Pressure-volume-temperature or pressure-density-temperature relationship is used to control the thermophysical properties of cellulose. It is wellknown that temperature greatly affects both cellulose dyeing process and cellulose properties [5]. To have an optimal temperature for the dyeing process, we have to have a fast insight into the pressure-density-temperature relationship of cellulose, which is, however, of high non-linearity, and it is difficult to be used for practical applications.

In this paper we will give a simple explicit relationship among pressure, density, and temperature for easy applications.

Pressure-density-temperature relationship

The pressure-density-temperature relationship of cellulose can be expressed in the form [2]:

$$\rho = 1 - \exp \left(-P \frac{T}{T} - \frac{\rho^2}{T} \right)$$

(1)

This formulation is inexplicit, and it is difficult to have a fast insight into the relationship. We write eq. (1) the form:

* Corresponding author’s, e-mail: liyasuda@163.com
\[ F(P, \rho, T) = \ln(1 - \rho) + \frac{P}{T} + \frac{\rho^2}{T} = 0 \] (2)

In practical applications, we have reference values for pressure, density, and temperature. For example, when \( T = T_0 \), we have \( P = P_0 \), and \( \rho = \rho_0 \). Using Taylor series expansion [6], we have approximately the following linear pressure-density-temperature relationship:

\[ F(P, \rho, T) = \ln(1 - \rho_0) + \rho_0 + \frac{P_0}{T_0} + \frac{\rho_0^2}{T_0} + (P - P_0) \frac{\partial F}{\partial P}(P_0, \rho_0, T_0) + \]
\[ + (\rho - \rho_0) \frac{\partial F}{\partial \rho}(P_0, \rho_0, T_0) + (T - T_0) \frac{\partial F}{\partial T}(P_0, \rho_0, T_0) = 0 \] (3)

and the following non-linear pressure-density-temperature relationship:

\[ F(P, \rho, T) = \ln(1 - \rho_0) + \rho_0 + \frac{P_0}{T_0} + \frac{\rho_0^2}{T_0} + (P - P_0) \frac{\partial F}{\partial P}(P_0, \rho_0, T_0) + \]
\[ + (\rho - \rho_0) \frac{\partial F}{\partial \rho}(P_0, \rho_0, T_0) + (T - T_0) \frac{\partial F}{\partial T}(P_0, \rho_0, T_0) + \]
\[ + \frac{1}{2} (P - P_0)^2 \frac{\partial^2 F}{\partial P^2}(P_0, \rho_0, T_0) + \frac{1}{2} (\rho - \rho_0)^2 \frac{\partial^2 F}{\partial \rho^2}(P_0, \rho_0, T_0) + \]
\[ + \frac{1}{2} (T - T_0)^2 \frac{\partial^2 F}{\partial T^2}(P_0, \rho_0, T_0) + (P - P_0)(\rho - \rho_0) \frac{\partial^2 F}{\partial P \partial \rho}(P_0, \rho_0, T_0) + \]
\[ + (P - P_0)(T - T_0) \frac{\partial^2 F}{\partial P T}(P_0, \rho_0, T_0) + (\rho - \rho_0)(T - T_0) \frac{\partial^2 F}{\partial \rho T}(P_0, \rho_0, T_0) = 0 \] (4)

By a simple calculation, we have:

\[ \frac{\partial F}{\partial P} = \frac{1}{T} \] (5)

\[ \frac{\partial^2 F}{\partial P^2} = 0 \] (6)

\[ \frac{\partial F}{\partial \rho} = -\frac{1}{1 - \rho} + 1 + 2 \frac{\rho}{T} \] (7)

\[ \frac{\partial^2 F}{\partial \rho^2} = -\frac{1}{(1 - \rho)^2} + \frac{2}{T} \] (8)

\[ \frac{\partial F}{\partial T} = -\frac{P + \rho^2}{T^2} \] (9)

\[ \frac{\partial^2 F}{\partial T^2} = -\frac{2(P + \rho^2)}{T^3} \] (10)
Using Taylor expansion technology, we obtain an approximate pressure-density-temperature relationship up to second order. A higher order approximate relationship can be also easily obtained. The approximate formulation can be used for a fast prediction of pressure volume-temperature relationship to control thermophysical properties of cellulose.
Acknowledgment

The work is supported by Priority Academic Program Development of Jiangsu Higher Education Institutions (PAPD), National Natural Science Foundation of China under Grant No.11372205, Ningbo Science and Technology Innovation Team Foundation under Grant No. 2012B82014, Natural Science Foundation of Liaoning Province under Grant No. 20170540070 and Liaoning Provincial Education Department Project under Grant No. 2017J040.

References