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

by

***Ling LIN[a*], Ya LI[b*], Yongfang QIAN[c], and Yanping LIU[d]***

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

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*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]:

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

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

$$F(P,\rho,T)=\ln(1-\rho)+\rho+\frac{P}{T}+\frac{\rho^2}{T}=0 \tag{2}$$

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:

$$\begin{aligned}F(P,\rho,T)={}&\ln(1-\rho_0)+\rho_0+\frac{P_0}{T_0}+\frac{\rho_0^2}{T_0}+(P-P_0)\frac{\partial F}{\partial P}(P_0,\rho_0,T_0)+\\&+(\rho-\rho_0)\frac{\partial F}{\partial \rho}(P_0,\rho_0,T_0)+(T-T_0)\frac{\partial F}{\partial T}(P_0,\rho_0,T_0)=0\end{aligned} \tag{3}$$

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

$$\begin{aligned}F(P,\rho,T)={}&\ln(1-\rho_0)+\rho_0+\frac{P_0}{T_0}+\frac{\rho_0^2}{T_0}+(P-P_0)\frac{\partial F}{\partial P}(P_0,\rho_0,T_0)+\\&+(\rho-\rho_0)\frac{\partial F}{\partial \rho}(P_0,\rho_0,T_0)+(T-T_0)\frac{\partial F}{\partial T}(P_0,\rho_0,T_0)+\\&+\frac{1}{2}(P-P_0)^2\frac{\partial^2 F}{\partial P^2}(P_0,\rho_0,T_0)+\frac{1}{2}(\rho-\rho_0)^2\frac{\partial^2 F}{\partial \rho^2}(P_0,\rho_0,T_0)+\\&+\frac{1}{2}(T-T_0)^2\frac{\partial^2 F}{\partial T^2}(P_0,\rho_0,T_0)+(P-P_0)(\rho-\rho_0)\frac{\partial^2 F}{\partial P\partial \rho}(P_0,\rho_0,T_0)+\\&+(P-P_0)(T-T_0)\frac{\partial^2 F}{\partial P\partial T}(P_0,\rho_0,T_0)+(\rho-\rho_0)(T-T_0)\frac{\partial^2 F}{\partial \rho\partial T}(P_0,\rho_0,T_0)=0\end{aligned} \tag{4}$$

By a simple calculation, we have:

$$\frac{\partial F}{\partial P}=\frac{1}{T} \tag{5}$$

$$\frac{\partial^2 F}{\partial P^2}=0 \tag{6}$$

$$\frac{\partial F}{\partial \rho}=-\frac{1}{1-\rho}+1+2\frac{\rho}{T} \tag{7}$$

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

$$\frac{\partial F}{\partial T}=-\frac{P+\rho^2}{T^2} \tag{9}$$

$$\frac{\partial^2 F}{\partial T^2}=2\frac{P+\rho^2}{T^3} \tag{10}$$

$$\frac{\partial^2 F}{\partial \rho \partial P} = 0 \tag{11}$$

$$\frac{\partial^2 F}{\partial T \partial P} = -\frac{1}{T^2} \tag{12}$$

$$\frac{\partial^2 F}{\partial T \partial \rho} = -2\frac{\rho}{T^2} \tag{13}$$

Using the previous relationship, we have the following linear pressure-density-temperature relationship:

$$F(P,\rho,T) = \ln(1-\rho_0) + \rho_0 + \frac{P_0}{T_0} + \frac{\rho_0^2}{T_0} + (P-P_0)\frac{1}{T_0} +$$
$$+(\rho-\rho_0)\left(-\frac{1}{1-\rho_0} + 1 + 2\frac{\rho_0}{T_0}\right) + (T-T_0)\left(-\frac{P_0+\rho_0^2}{T_0^2}\right) = 0 \tag{14}$$

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

$$F(P,\rho,T) = \ln(1-\rho_0) + \rho_0 + \frac{P_0}{T_0} + \frac{\rho_0^2}{T_0} + (P-P_0)\frac{1}{T_0} + (\rho-\rho_0)\left(-\frac{1}{1-\rho_0} + 1 + 2\frac{\rho_0}{T_0}\right) +$$
$$+(T-T_0)\left(-\frac{P_0+\rho_0^2}{T_0^2}\right) + \frac{1}{2}(\rho-\rho_0)^2\left[-\frac{1}{(1-\rho_0)^2} + \frac{2}{T_0}\right] + (T-T_0)^2\frac{P_0+\rho_0^2}{T_0^3} -$$
$$-(P-P_0)(T-T_0)\frac{1}{T_0^2} - 2(\rho-\rho_0)(T-T_0)\frac{\rho_0}{T_0^2} = 0 \tag{15}$$

Equations (14) and (15) are valid when the predicted data ($P$, $\rho$, and $T$) are relatively closed to the reference ones ($P_0$, $\rho_0$, and $T_0$). We use the experimental data given in [1] to show the correctness of eq. (15). For a given pressure, $P$ = 20 MPa, 129.9 MPa, and 196.1 MPa, respectively, eq. (15) gives a simple density-temperature relationship or volume-temperature relationship, fig. 1.

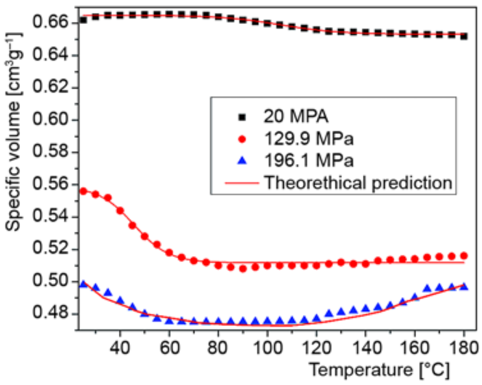


**Figure 1. Theoretical prediction at different pressure *vs.* experimental data**

## Conclusion

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.

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