Analysis on the Diffusion and Mechanical Properties of Eucalyptus Dried *via* Supercritical Carbon Dioxide

Ying Cao, Wei Wang,* and Wei Ma

Using the molecular dynamics software Materials Studio, a micro-level carbon dioxide - cellulose model was established to study the supercritical carbon dioxide drying of eucalyptus wood. The change of the primary components of the eucalyptus wood cellulose were also studied, by simulating various pressures, *i.e.*, 10, 15, 20, 25, and 30 Pa, and simulating a temperature of 323 K. Results showed that the diffusion coefficient of carbon dioxide decreases as the pressure increases, and it reaches the maximum at 20 Pa, which was confirmed by the number of hydrogen bonds in the carbon dioxide cellulose model. Combined with the comprehensive analysis of the mechanical parameters, the Poisson's ratio γ and the ratio of bulk modulus to shear modulus (K/G) values of cellulose first increased and then decreased as the pressure increased, and the Young's modulus increased as the pressure increased. From a microscopic point of view, the study shows that eucalyptus cellulose has good mechanical properties when dried by supercritical carbon dioxide under a pressure of 20 Pa. The simulation results of the dynamic model agreed well with the measured results, and the simulation results support the previous experimental data and the practical application results in production.

DOI: 10.15376/biores.17.3.4018-4029

Keywords: Wood drying; Molecular dynamics; Pressure; Cellulose; Mechanical properties

*Contact information: College of Engineering and Technology, Northeast Forestry University, Harbin 150040 China; *Corresponding authors: vickywong@nefu.edu.cn; cestlavie28@163.com*

INTRODUCTION

With the rapid development of the world, wood consumption has greatly increased. In order to alleviate the imbalance between the supply and demand of wood resources at the present stage, strengthening the efficient processing and utilization of plantation wood has become an important way to solve the contradiction between the ecological environment and wood demand. Eucalyptus is a type of high quality artificial fast-growing forest with a fine structure, hard texture, good mechanical structure, and beautiful patterns. Eucalyptus is an important raw material for furniture, wood structure building, and wood-based panels. However, eucalyptus is prone to cracking and deformation during its processing and drying due to its high growth stress, poor permeability, and low growth years. Wood drying is also one of the most important processes in wood processing and production (Dawson *et al*. 2015). In order to overcome the inherent defects of eucalyptus and improve its wood utilization value, it is important to carry out the functional improvement of eucalyptus. Therefore, research on wood drying has great potential and value.

Compared with chemical modification methods, physical methods provide a better optimized environment for wood. At present, the most commonly used wood drying method can be described as conventional drying, but this method has disadvantages such as long drying cycle and large drying stress. Compared with conventional drying methods, the emergence and application of supercritical fluid technology provides a new way for cellulose processing and modification. In particular, supercritical carbon dioxide is the most widely used supercritical fluid, because of its non-toxic, harmless, non-combustible, non-polluting, easy-to-recycle, and relatively low in cost (Gething *et al*. 2013; Franich *et al*. 2019).

Carbon dioxide has many excellent properties in the supercritical state, *e.g.*, a large diffusion coefficient, low viscosity, and no surface tension. Properties such as the solubility and dielectric constant can be rapidly changed with the adjustment of the pressure, and it has strong penetration and swelling capacity for natural polymers and synthetic polymers, as well as having antiseptic properties (Matsunaga *et al*. 2005; Cookson *et al*. 2009). Supercritical carbon dioxide is also an excellent heat transfer fluid, which is beneficial to speed up the heat transfer process in the drying process and improve the drying efficiency (Cabeza *et al*. 2017). Drying wood with supercritical carbon dioxide fluids can prevent wood cracking due to surface tension (Stahl and Bentz 2004). In addition, lower temperatures are required to dry wood with supercritical carbon dioxide The process can be controlled by changing the pressure and temperature, and the operation is simple. When the pressure is released, carbon dioxide escapes from the matrix. The carbon dioxide then can be recycled and reused. The whole process is simple and easy to operate and has good repeatability. It is a green and environmentally friendly method for processing modified polymers (Song *et al*. 2016).

When undergoing the drying process at a high temperature and high humidity, the wood undergoes internal compressive stress. Within the wood cell, capillary tension and water vapor partial pressure differences have a large combined effect. Due to the thermoplastic nature of the material, wrinkling phenomena can result. Studies have shown that the reason for the shrinkage of eucalyptus wood during drying is not only the compressive stress generated inside the wood, but also the capillary tension and water vapor partial pressure caused by the poor permeability of eucalyptus wood. These combined forces exceed those in high temperature and high humidity. When the transverse grain compressive strength of the wood cells in the state is exceeded, cell collapse occurs, resulting in the shrinkage of the wood (Stahl and Bentz 2004). Using supercritical carbon dioxide to treat wood can effectively improve the permeability of wood and greatly improve the quality of the subsequent wood drying process. Many studies have revealed the influence of the temperature and pressure on the drying effect and the caudate lobe eucalyptus wood moisture content distribution after drying *via* supercritical carbon dioxide (Oltean *et al*. 2007; Yang and Liu 2020). In addition, the transfer characteristics, permeability, and extracts were determined; these studies found that when the pressure was lower than 20 Pa, supercritical carbon dioxide has a high drying speed. However, as the pressure continues to increase, there is no positive correlation between the wood drying rate and the drying effect and pressure gauge (Yang and Liu 2020). The influence of other factors on the permeability has rarely been reported (Gething *et al*. 2013). It was found that the pressure in the drying process had a considerable effect on the speed, moisture content, and properties of the dried wood and improved the quality of the wood. However, too high of a temperature or pressure would destroy the structure of the wood, so it is very important to find the appropriate treatment environment.

Cellulose is the most important component of wood. It is a polymer comprised by D-glucopyranose units. Natural cellulose consists of crystalline and amorphous regions. The cellulose molecules in the crystalline region are arranged in a close and orderly order, and the bonds between the cellulose chains are difficult to be broken by small molecules, which can only be adsorbed on the surface of the cellulose. However, the cellulose molecules in the amorphous region are not regularly arranged. They are easily affected by the temperature and small gas molecules, and the adsorption capacity is also strong. During the drying process, the structure of cellulose is easy to change, which further affects the mechanical properties of cellulose (Khazraji and Robert 2013). Therefore, the amorphous region was selected as the research object in this paper.

Since the 1990s, with the rapid development of computer science and technology, simulation calculations have become one of the three primary methods of modern scientific research, along with theoretical analysis and experimental measurements. Materials Studio is a new generation of materials computing software developed by Accelrys company specifically for materials science. It can easily establish 3D molecular models and deeply analyze organic crystals, inorganic crystals, amorphous materials, and polymers (Hou *et al*. 2001). Materials Studio has been fully recognized as a promising molecular simulation software, and its application in the field of polymers is expanding. The design and modification of polymer materials *via* molecular simulation technology can shorten the experimental period, improve efficiency and save costs, and study the diffusion movement of small molecules from the microscopic level, thus reducing artificial data and analysis errors (Yin *et al*. 2006).

This paper investigates the changes in the mechanical properties of cellulose and the diffusion behaviour of carbon dioxide during supercritical carbon dioxide wood drying using molecular dynamics simulations. Through simulation, it was found that the change pattern of cellulose corresponds to the macroscopic property changes, with a view to providing theoretical support for the supercritical carbon dioxide drying method of wood.

EXPERIMENTAL

Modeling

Materials Studio 8.0 was used to simulate the Iβ amorphous region model of eucalyptus cellulose (Theodorou and Suter 1985). Studies have found that cellulose with different degrees of polymerization have little influence on the physical properties of materials (Mazeau and Heux 2008). In this paper, a cellulose chain with a degree of polymerization of 20 was established (Wang *et al*. 2020). Using the method proposed by Theodorou and Suter (1985), the amorphous cell tools (AC) module was used to build the model. The target density of the model was set to 1.5 g/cm^3 (Brandrup *et al*. 1999). The model was composed of one cellulose Iβ molecular chain and 20 carbon dioxide molecules, and the size of the model was 20.2 × 20.2 × 20.2 (A^3). The established model is shown in Fig. 1.

Dynamic Simulation

After building the model shown in Fig. 1, initial geometric structure optimization was firstly carried out. The Forcite module Calculation was used, with a smart algorithm to run the program, and one frame was output every 5000 steps, so that the free movement of the molecules in the mixed system tends to be balanced and energy minimization was achieved. In the macro canonical ensemble (NVT), the initial dynamic relaxation of the model was carried out at 323 K, the initial speed was set as then random, the time step was 1 fs, the total length of the simulation was 1000 ps, and one frame was output every 5000 steps until the system reached a relatively stable state. After the completion of the above steps, the initial frame of the dynamics simulation was obtained.

The pressure of the supercritical carbon dioxide drying wood process was set to 10 to 30 Pa as the simulation range, and the temperature spacing was 5 Pa. Five groups were set up in total. The Andersen method was used for temperature control (Andrea *et al*. 1983). The Berendsen method, as outlined by Berendsen *et al*. (1984), was used for pressure control, and the Ewald method was used for electronic addition, as outlined by Ewald (1921). At present, the Ewald summation method has become one of the standard algorithms for dealing with electrostatic interactions in simulated systems. The force field is the PCFF force field suitable for natural polymer materials, especially for organic compounds or molecular systems without transition metal elements (Maple *et al*. 2013).

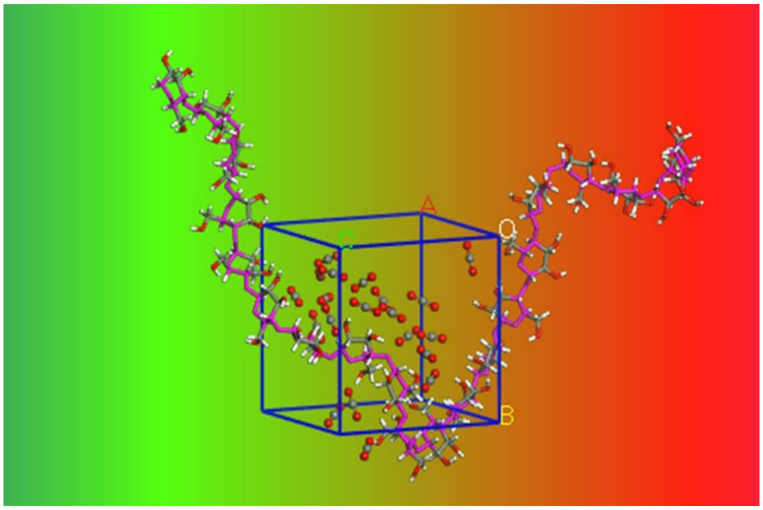

Fig. 1. The carbon dioxide-cellulose amorphous region model

RESULTS AND DISCUSSION

The Energy

In molecular dynamics (MD) simulations, energy and temperature stability are used to determine the equilibrium of the entire system (Allen and Tidesley 1989; Sangiovanni *et al*. 2016). When the fluctuation value is in the fluctuation range of 5% to 10%, the system is judged to be in equilibrium. Molecular dynamics simulation was carried out in the system, and the energy and temperature changes with the time of the system were obtained (Fig. 2). The energy fluctuation of the last 260 ps was relatively stable, and the fluctuation value is approximately 8.4%. It is judged that the system reached equilibrium at this time.

Figure 3 shows the temperature-time variation of the cellulose-carbon dioxide system in the simulation process. It can be seen from Fig. 3 that the temperature changes with time in a small range. In addition, it can be seen that the temperature fluctuates at around 320 K and is relatively stable, *i.e.*, basically controlled within a range of ± 20 K, which indicated that the system has reached an equilibrium state.

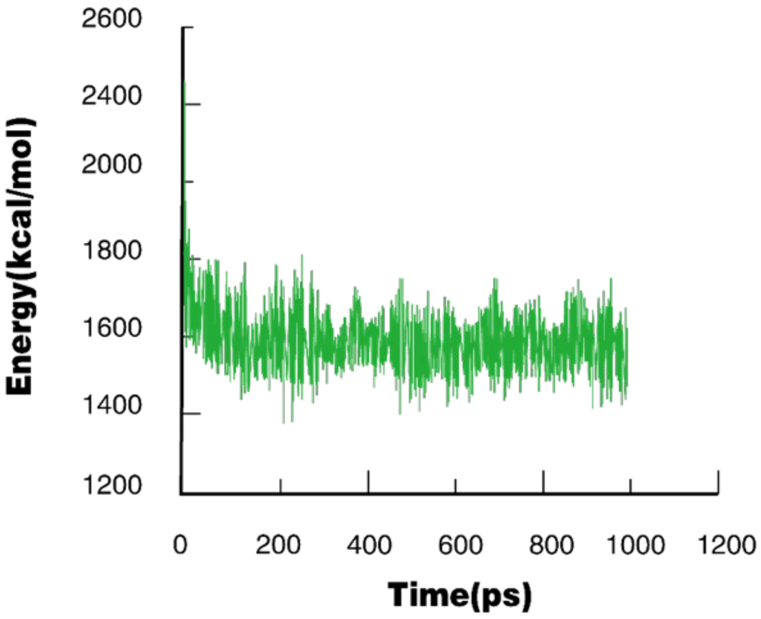

Fig. 2. Energy-time variation chart

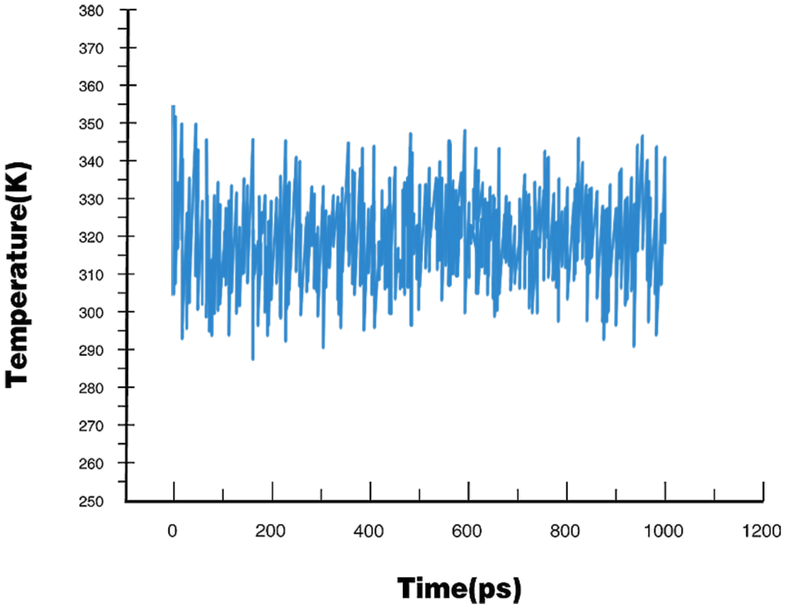

Fig. 3. Temperature-time variation chart

The accuracy of this simulation process can be expressed as a verification of the energy convergence parameter (δE), which is defined in Eq. 1,

$$\delta E = \frac{1}{N}\sum_{i-1}^{N}\left|\frac{E_i - E_0}{E_0}\right| \tag{1}$$

where N denotes the total number of steps of the simulation, the initial energy of the simulated system is expressed by E_0, and E_i denotes the energy of the system after *i* steps of the simulation. When δE is less than or equal to 0.001 to 0.003, the simulation results are reliable. It was calculated that $\delta E = 0.0025$, which also demonstrates that the energy convergence is reliable, and the interaction energy analysis can be performed.

Coefficient of Diffusion

The mean square displacement (MSD) can be used to observe the migration paths and behavior of the molecules in a microscopic system as the sum of squares of the molecular position vector increments of the gas molecules after a simulated period of time in the system. The specific values provide a more intuitive understanding of the diffusion changes of gas molecules, where < > denotes the average of the total number of particles, the displacement of the center of mass of the ith particle, and the initial moment after a certain simulation time, and *n* is the number of diffusing particles.

The expression is as presented in Eq. 2,

$$\mathrm{MSD} = \sum_{i=1}^{n}\langle|\vec{r_i}(t) - \vec{r_i}(0)|^2\rangle \tag{2}$$

The diffusion behavior of the small molecules of gases is generally expressed by the molecular diffusion coefficient, D, as shown in Eq. 3,

$$D = \frac{1}{6n}\lim_{t\to\infty}\frac{d}{dt}\sum_{i=1}^{n}\langle|\vec{r_i}(t) - \vec{r_i}(0)|^2\rangle \tag{3}$$

which can be simplified to Eq. 4,

$$D = m/6 \tag{4}$$

where *D* is the slope obtained by fitting the MSD curve using the least squares method (as shown in Fig. 4); the MSD value of carbon dioxide linearly increases with time during the simulation time from 0 to 1000 ps, which indicated that the diffusion coefficient of carbon dioxide was constant at 10 to 30 Pa.

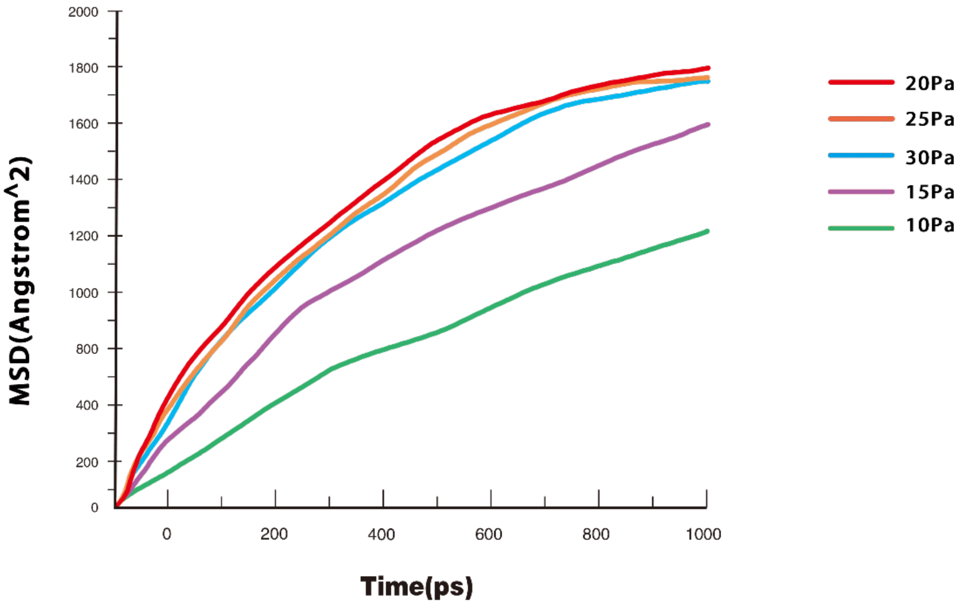

Fig. 4. MSD of gas molecules at different pressures

Goodness of fit refers to the degree to which the regression line fits the observed value. The statistic that measures goodness of fit is the square of the determinable coefficient (also known as the deterministic coefficient) R. R squared ranges from 0 to 1. The closer the value of R squared is to 1, the better the fitting degree of the regression line to the observed value is. The closer the value of R squared is to 0, the worse the regression line fits the observed value. Origin 8 software was used in this work to fit the obtained data and then calculated the goodness of fit by it (as shown in Table 1).

Table 1. Slope and Diffusion Coefficient of the Mean Square Displacement (MSD) Curve at Different Pressures

Pressure	10 Pa	15 Pa	20 Pa	25 Pa	30 Pa
Diffusion Coefficient (A^2/ps)	0.0378	0.0665	0.0799	0.0721	0.0784
Slope	0.22675	0.3994	0.47937	0.46256	0.47374
Goodness of Fitting	0.95018	0.970516	0.99365	0.97322	0.98372

As can be seen in Table 1, the fits of the data were all greater than 0.95, and the obtained diffusion coefficients were reliable and can be further analyzed. It can be seen from Fig. 4 that in the pressure range of 10 to 30 Pa, the overall trend of the diffusion coefficient of carbon dioxide molecules was increasing, and the carbon dioxide molecules move violently with the increase of pressure, and the diffusion coefficient reaches the maximum at the pressure of 20 Pa. When the bond force between cellulose and carbon dioxide is minimal, the mean square displacement increased, and the diffusion coefficient expanded. When the pressure reached between 20 and 30 Pa, the parameters remained stable, which was consistent with the experimental results of Yang and Liu (2020).

Supercritical carbon dioxide is always applied to dried wood, carbon dioxide molecules penetrate the wood and improve its permeability, thus reducing the barrier to water molecules flowing through the wood (Yang *et al*. 2020), but the pressure continues to increase. When the other parameters remain unchanged, increasing the pressure has little effect on the results of the dried wood, and any further increase will destroy the cellulose structure.

Hydrogen Bonding

Matter is composed of microscopic particles, *e.g.*, atoms, molecules, and ions, and the forces that bring the atoms, molecules, and ions together to form macroscopic matter. These forces include ionic bonds, covalent bonds, metal bonds, and various intermolecular forces. In addition, a special class of intermolecular forces is hydrogen bonds. Cellulose is the most abundant natural polymer in nature. There are a lot of hydroxyl groups on its molecular chain, and the hydroxyl groups make cellulose form a strong hydrogen bond network. Due to the presence of hydrogen bonds, substances can exhibit many special properties. Cellulose has excellent chemical stability, biocompatibility, non-toxicity, and lack of pollution and other characteristics (Matta *et al*. 2010). The hydrogen bonds between the cellulose chains play an important role in maintaining the stability of the cellulose structure and mechanical properties (Prins *et al*. 2010). The hydrogen bond calculation module in Material Studio software was used to count the number of hydrogen bonds between cellulose chains, as shown in Fig. 5.

Figure 5 shows the trend of the effect of different pressures on the hydrogen bonding in the amorphous region of carbon dioxide-cellulose; the number of hydrogen bonds between the cellulose chains first increased to a maximum number of 230 and then there was no considerable increase or decrease in the number. This shows that the pressure increase will enhance the hydrogen bonding interaction between the cellulose chain, to enhance the performance of cellulose, while too great a pressure cannot influence the experimental effect. The trend for the hydrogen bonds and diffusion coefficient is the same. The reason may be that with the increase in the pressure of the drying medium, the number of wood cells with shrinkage conditions increases, leading to an increase in the shrinkage degree of wood, and the original structure of the cellulose is destroyed. The diffusion degree of carbon dioxide is consistent with the number of hydrogen bonds between cellulose, and they are closely related.

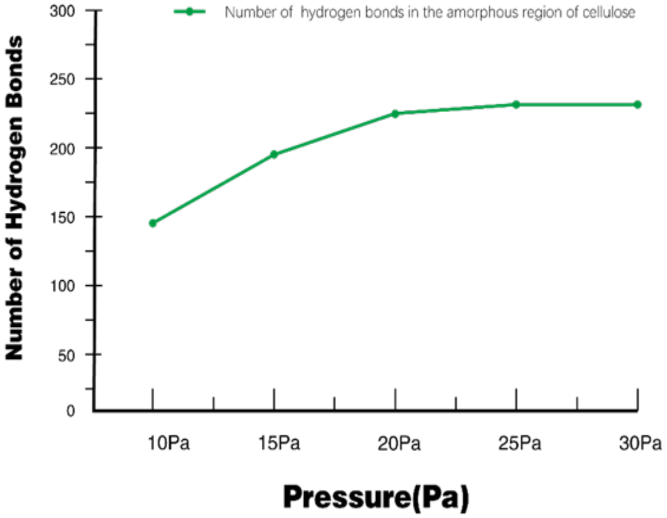

Fig. 5. Number of hydrogen bonds in the amorphous region of the cellulose at different pressures

Mechanical Property

The dynamics simulation results of the amorphous region of cellulose under different pressures were calculated, and the mechanical parameters which could characterize the mechanical properties of the wood were obtained. Since the amorphous region of cellulose can be considered isotropic, its mechanical properties can be calculated by C_{11} and C_{12}, with $C_{12} = \lambda$ and C_{11}-$C_{12} = \mu$; where λ and μ are called The Ramei constants, as shown in Eq. 5,

$$\left[C_{ij}\right] = \begin{bmatrix} \lambda+2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda+2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda+2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \tag{5}$$

(Wang *et al*. 2018).

Lamet's constant can be used to calculate mechanical properties, *e.g.*, Young's modulus (E), shear modulus (G), volume modulus (K), and Poisson's ratio (γ). The formulas are shown in Eqs. 6 through 9, respectively,

$$E = \frac{\mu(3\lambda+2\mu)}{\mu+\lambda} \quad (6)$$

$$G = \mu \quad (7)$$

$$K = \lambda + \frac{2}{3\mu} \quad (8)$$

$$\gamma = \frac{\lambda}{2(\lambda+\mu)} \quad (9)$$

The mechanical properties are expressed by Young's modulus (*E*), shear modulus (*G*), volume modulus (*K*), Poisson's ratio (*γ*), and *K*/*G* value (the ratio of the bulk modulus to shear modulus). Poisson's ratio (*γ*) is also known as the lateral deformation coefficient, which reflects the elastic coefficient of the lateral deformation of the material. The larger the Poisson's ratio, the stronger the plasticity of the material.

Young's modulus (*E*) is the longitudinal elastic modulus, which represents the rigidity of the material. The higher the value, the better the rigidity of the material. The ratio of the bulk modulus to shear modulus (*K*/*G*) reflects the toughness of the material, and the higher the value, the better the toughness. After the molecular dynamics simulation, the mechanical properties of the cellulose-carbon dioxide model under various pressures were calculated, as shown in Table 2.

Table 2. Mechanical Parameters of the Model at Different Pressures

Pressure (Pa)	*λ*	*μ*	Young's Modulus (*E*)	Poisson's Ratio (*γ*)	*K*/*G*	Shear Modulus (GPa)
10	8.4563	6.8732	17.5379	0.2758	1.2444	6.8732
15	9.1436	7.1829	18.3890	0.2801	1.2858	7.1829
20	8.7312	5.4634	24.6872	0.3108	1.6213	5.4634
25	7.4732	6.7521	17.0513	0.2627	1.2381	6.7521
30	10.9372	8.1436	20.9551	0.2866	1.3531	8.1436

From the data in Table 2, it can be seen that the Poisson's ratio and ratio of the bulk modulus to shear modulus (*K*/*G*) reach their maximum values at 20 Pa, so the mechanical properties of eucalyptus are at their best. The pressure has an effect on the flexibility of eucalyptus but has little effect on the wood after further increasing. With the increase of temperature, the value of Young's modulus increased, and the eucalyptus wood was not easily deformed. The value of the shear modulus was the lowest at 20 Pa, which indicated that the ductility of the eucalyptus wood gradually increased with the increase of pressure. With the increase in pressure, the active bond in cellulose became gradually stable, and the plasticity of the eucalyptus wood becomes high, which is not easy to break.

CONCLUSIONS

1. When the temperature is 320 K and the pressure increases from 10 to 30 Pa, the diffusion coefficient of the carbon dioxide in the cellulose is predicted to increase with the increase in pressure. High pressure can make the carbon dioxide molecules diffuse

more actively, but at a higher pressure of 20 Pa, the diffusion coefficient has no positive correlation with the pressure realization.

2. The mean square displacement of the eucalyptus cellulose chains increases with the increase of pressure, and the molecular motion in the system accelerates. The thermal stability of eucalyptus cellulose chain decreases, which indirectly affects the stability of eucalyptus cellulose. The variation trend of intercellulose hydrogen bonding is the same as the change of the mean square displacement, and the two are closely related.
3. In the pressure range of 10 to 30 Pa, the change in the mechanical parameters in the amorphous region of the cellulose with the pressure was calculated. The Poisson's ratio and ratio of the bulk modulus to shear modulus (K/G) value of cellulose showed an overall upward trend, and the two values increased first and then decreased, and reached the maximum at 20 Pa. These results indicate that the mechanical properties of eucalyptus may be the best at 20 Pa.

ACKNOWLEDGMENTS

The authors are grateful for the support by The Fundamental Research Funds for the Central Universities (Grant No. 41419020) and the Science Fund Project for Studying Abroad in Heilongjiang Province (Grant No. LC201407).

REFERENCES CITED

Allen, M. P., and Tidesley, D. J. (1989). *Computer Simulation of Liquids*, Oxford University Press, Oxford, United Kingdom.

Andrea, T. A., Swope, W. C., and Andersen, H. C. (1983). "The role of long ranged forces in determining the structure and properties of liquid water," *The Journal of Chemical Physics* 79(9), 4576-4584. DOI: 10.1063/1.446373

Berendsen, H. J. C. P., Postma, J. P. M., Gunsteren, W. F. v., Dinola, A., and Haak, J. R. (1984). "Molecular dynamics with coupling to an external bath," *The Journal of Chemical Physics* 81(8), 3684-3690. DOI: 10.1063/1.448118

Cabeza, L. F., Gracia, A. d., Fernández, A. I., and Farid, M. M. (2017). "Supercritical CO_2 as heat transfer fluid: A review," *Applied Thermal Engineering* 125, 799-810. DOI: 10.1016/j.applthermaleng.2017.07.049

Cookson, L. J., Qader, A., Creffield, J. W., and Scown, D. K. (2009). "Treatment of timber with permethrin in supercritical carbon dioxide to control termites," *Journal of Supercritical Fluids* 49(2), 203-208. DOI: 10.1016/j.supflu.2009.03.002

Dawson, B. S. W., Pearson, H., Kroese, H.W., and Sargent, R. (2015). "Effect of specimen dimension and pre-heating temperature on supercritical CO_2 dewatering of radiata pine sapwood," *Holzforschung* 69(4), 421-430. DOI: 10.1515/hf-2014-0055

Ewald, P. P. (1921). "Evaluation of optical and electrostatic lattice potentials," *Annals of Physics* 369(3), 253-287. DOI: 10.1002/andp.19213690304

Franich, R. A., Meder, R., Falge, M., Fuchs, J., and Behr, V. C. (2019). "Uncovering supercritical CO_2 wood dewatering *via* interleaved ^{1}H-imaging and ^{13}C-spectroscopy with real-time reconstruction," *Journal of Supercritical Fluids* 144, 56-62. DOI: 10.1016/j.supflu.2018.10.006

Gething, B. A., Janowiak, J. J., and Morrell, J. J. (2013). "Using computational modeling to enhance the understanding of the flow of supercritical carbon dioxide in wood materials," *Journal of Supercritical Fluids* 82, 27-33. DOI: 10.1016/j.supflu.2013.05.019

Hou, T. J., Zhang, W., and Xu, X. J. (2001). "Binding affinities for a series of selective inhibitors of gelatinasea using molecular dynamics with a linear interaction energy approach," *Journal of Physical Chemistry B* 105(22), 5304-5315. DOI: 10.1021/jp0044476

Khazraji, A. C., and Robert, S. (2013). "Interaction effects between cellulose and water in nanocrystalline and amorphous regions: A novel approach using molecular modeling," *Journal of Nanomaterials* 2013, 1-11. DOI: 10.1155/2013/409676

Maple, J. R., Hwang, M.-J., Stockfisch, T. P., and Hagler, A. T. (2013). "Derivation of class II force fields. III. Characterization of a quantum force field for alkanes," *Israel Journal of Chemistry* 34(2), 195-231. DOI: 10.1002/ijch.199400025

Matsunaga, M., Matsunaga, H., Kataoka, Y., and Matsui, H. (2005). "Improved water permeability of sugi heartwood by pretreatment with supercritical carbon dioxide," *Journal of Wood Science* 51(2), 195-197. DOI: 10.1007/s10086-005-0694-y

Matta, C. F., J Hernández-Trujillo, Tang, T.-H., and Bader, R. (2010). "Hydrogen-hydrogen bonding: A stabilizing interaction in molecules and crystals," *Chemistry - A European Journal* 9(9), 1940-1951. DOI: 10.1002/chem.200204626

Mazeau, K., and Heux, L. (2008). "Molecular dynamics simulations of bulk native crystalline and amorphous structures of cellulose," *Journal of Physical Chemistry B* 107(10), 2394-2403. DOI: 10.1021/jp0219395

Oltean, L., Teischinger, A., and Hansmann, C. (2007). "Influence of temperature on crac king and mechanical properties of wood during wood drying – A review," *BioResources* 2(4), 789-811. DOI:10.1007/s00226-007-0154-5

Prins, L. J., Reinhoudt, D. N., and Timmerman, P. (2010). "Noncovalent synthesis using hydrogen bonding," *Angewandte Chemie International Edition* 40(13), 2382-2426. DOI: 10.1002/1521-3773(20010702)40:13<2382:AID-ANIE2382>3.0.CO;2-G

Sangiovanni, D. G., Hellman, O., Alling, B., and Abrikosov, I. A. (2016). "Efficient and accurate determination of latticevacancy diffusion coefficients *via* non equilibrium *ab initio* molecular dynamics," *Physical Review B* 93(9), 1-5. DOI: 10.1103/PhysRevB.93.094305

Song, N., Jia, J., Wang, W., Gao, Y., Zhao, Y., and Chen, Y. (2016). "Green production of pristine graphene using fluid dynamic force in supercritical CO_2," *Chemical Engineering Journal* 298, 198-205. DOI: 10.1016/j.cej.2016.04.022

Stahl, M., and Bentz, M. (2004). "High-pressure treatment of wood – Combination of mechanical and thermal drying in the 'I/D process'," *Chemical Engineering & Technology* 27(11), 1216-1221. DOI: 10.1002/ceat.200406143

Theodorou, D. N, and Suter, U. W. (1985). "Detailed molecular structure of a vinyl polymer glass," *Macromolecules* 18(7), 1467-1478. DOI: 10.1021/ma00149a018

Wang, W., Wang, Y., and Li, X. (2018). "Molecular dynamics study on mechanical properties of cellulose with air/nitrogen diffusion behavior," *BioResources* 13(4), 7900-7910. DOI: 10.15376/biores.13.4.7900-7910

Wang, W., Sun, L., Wu, M., Li, X., and Song, W. (2020). "Molecular dynamics simulation of bamboo heat treatment with cellulose based on molecular different weight fractions of water," *BioResources* 15(3), 6766-6780. DOI: 10.15376/biores.15.3.6766-6780

Yang, L., and Liu, H. (2020). "Effect of supercritical CO_2 drying on moisture transfer and wood property of *Eucalyptus urophydis*," *Forests* 11(10), 1-11. DOI: 10.3390/f11101115

Yin, K., Zou, D., Yang, B., Zhang, X., and Xu, D. (2006). "Investigation of H-bonding for the related force fields in materials studio software," *Computers and Applied Chemistry* 23(12), 1335-1340.

Article submitted: March 25, 2022; Peer review completed: April 26, 2022; Revised version received and accepted: April 28, 2022; Published: May 10, 2022.
DOI: 10.15376/biores.17.3.4018-4029