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Modeling of Water Transport through Plasmodesmata in Plant Cell

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1. Introduction

Water is critically important for a live plant. Understanding the mechanism of the transport of water inside a plant is valuable for us to better foster the plant. There are extensively distributed micro/nano channels in a plant to transport the water which mainly comes from the root [1, 2]. In a human body, there are intracellular connexons by which water is transported through the nanotube with the diameter around 1.5 nm and with the axial length between 16 nm and 19 nm [3]. Water can smoothly flow through this very small nanotube to maintain the biological activity of a human being. However, such a fast flow is not explainable from the classical continuum fluid mechanics. It is believed that there is the special mechanism to govern such a water flow. In a plant, similarly there are a lot of plasmodesmata linking one cell to the neighboring cells [4, 5]; in each plasmodesmata there is a desmotubule with the cylindrical nanotube with the diameter ranging between 20 nm and 40 nm and with the axial length ranging between 12000 nm and 26000 nm [4, 5]; these nanotubes are functioned as transporting water to maintain the intracellular balance and exchange the nutrients between the neighboring cells. Classical continuum fluid mechanics shows that water hardly flows through such small and excessively long nanotubes. But, the fact is contrary. So, what is the mechanism of the water fast transport through the neighboring cells in a plant?

In calculating the water flow rate through the desmotubule, the classical Hagen-Poiseuille equation was ever used by considering the flow as the result of the pressure difference between the neighboring cells [6]. That belongs to classical continuum fluid mechanics. Nevertheless, the recent multiscale (nanoscale non-continuum and macroscopic continuum) calculation results show that if the wall slippage is ignored, the water flow rate through the nanotube in the human blood capillary wall with the diameter between 50 nm and 60 nm is much smaller than that calculated based on the wall slippage assumption [7]. It was concluded that the wall slippage should play a critically important role in the water fast transport through the blood capillary wall [7]. The nanochannel in a plant desmotubule should produce the far larger flow resistance to water according to the classical Hagen-Poiseuille equation as it possesses such specific geometrical sizes. Is the wall slippage still the fundamental mechanism for water transport through the neighboring plant cells?

Experiments have shown that when the diameter of a carbon nanotube, the wall of which is fairly hydrophobic, is no more than 7 nm, the water flow rate through the nanotube is much larger than that calculated from the classical Hagen-Poiseuille equation [8−10]; it was ascribed to the wall slippage effect. The carbon nanotube mimics the biological nanochannel in wall surface properties. In a plant, the nanochannel wall is also fairly hydrophobic and the wall slippage effect should also be incorporated when calculating the water flow rate. In a very small nanochannel, the water flow can be simulated by full molecular dynamics simulation (MDS) [11−13]. However, in simulating the water flow through the desmotubule, MDS should not be applicable because of the much larger diameter and the micrometer-scale axial length of the nanotube causing unaffordable computational costs. It is also suspected whether the continuum flow theory is applicable for simulating this water flow by incorporating the wall slippage [14].

Recent studies show that the water flow should be multiscale in the nanochannel with the diameter between 50 nm and 60 nm, consisting of both the adsorbed layer flow and the intermediate continuum water flow, though the adsorbed layer effect was found to be quite weak in such a nanochannel [7]. The water flow through the plant desmotubule should thus also be treated as multiscale. Classical multiscale approaches should not be applicable for simulating such a water flow because of too much cost of the computational storage and time by MDS in simulating the adsorbed layer flow [15, 16].

In the present study, another multiscale approach was used to calculate the water flow rate through the plant desmotubule. The nanoscale flow equation was used to calculate the adsorbed layer flow, and the Newtonian fluid model was used to simulate the intermediate continuum water flow [17]. The interfacial slippage was assumed to only occur on the water-nanotube wall interface. There are no available other simulation results for the water flow in a plant desmotubule by considering the multiscale flow. The present paper first attempts to study this multiscale flow. The advantage of the present multiscale approach is to give the fast solution without any computational burden on a current normal computer. The obtained calculation results are new, of physiological significance and important for us to more deeply understand the water flow through the plasmodesmata in a plant cell.

2. Studied object

A plant cell is typically shown in Fig. 1. The plasmodesmata links the neighboring plant cells, going through the primary and secondary walls of the plant cell respectively with the thicknesses 1000 nm-3000 nm and 5000 nm-10000 nm. It has the desmotubule with the nanotube the diameter of which ranges between 20 nm and 40 nm for transporting water and other nutrients. The plasmodesmata is highly permeable to solutes and the pressure difference between the neighboring plant cells drives the water flow through it [6]. It is the vital channel for exchanging the substances and information between plant cells. It is of significant interest to study the property of water transport through it to understand the physiological operation of a plant cell.

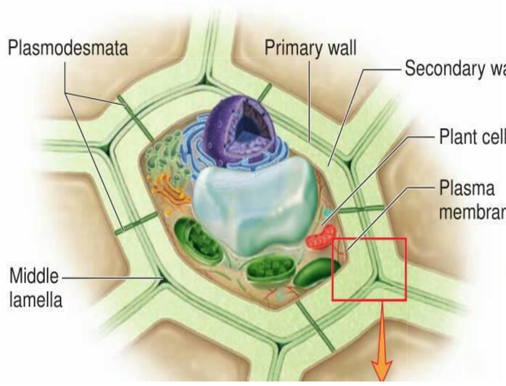
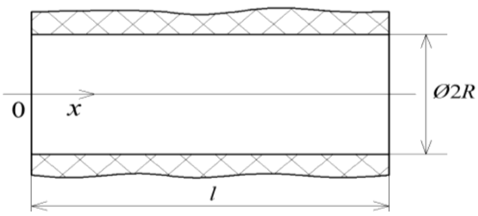
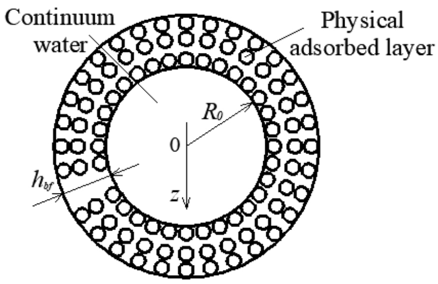


Fig. 1 A schematic picture of a plant cell



a



b

Fig. 2 The nanochannel in a plasmodesmata: a) profile of the nanotube, R =10 nm~20 nm, l =12000 nm-26000 nm; b) water contained in the nanotube

The single nanotube selected from a plasmodesmata is shown in Fig. 2, a. Its wall is essentially hydrophobic. When water flows through this nanochannel, there will be only a few molecular layers physically adsorbed to the channel wall with the thickness h_{bf} as shown in Fig. 2, b; the continuum water is surrounded by the physically adsorbed layer and covers the circular area with the radius R_0 on the cross-section of the channel. The flow in the channel is thus essentially multiscale consisting of both the non-continuum adsorbed layer flow and the intermediate continuum water flow.

3. Multiscale analysis of the water flow through the desmotubule channel

Due to the hydrophobicity of the wall of the desmotubule nanochannel, water easily slips on the channel wall. There should be no interfacial slippage on the adsorbed layer-continuum water interface. The water flow in the studied nanochannel is assumed as in the axial direction [2] and treated as isothermal because of the negligible water film viscous heating. The influences on the water density and viscosity of the pressure in the nanochannel are negligible because of low pressures.

By taking the adsorbed layer as the equivalently orientated molecule layers, Zhang [17] developed the mathematical equations respectively for calculating the volume flow rates of the adsorbed layer and the intermediate continuum fluid in a cylindrical micro/nano tube when the wall slippage only occurs on the adsorbed layer-channel wall interface. In the present study, we just used his analytical results and made further calculations for the water flow in the studied specific nanochannel based on the input parameter values.

For starting the wall slippage, the pressure difference between the neighboring cells should be [7, 17]:

$$DP = \frac{l\tau_s}{R_0 + D(n-1)}, \tag{1}$$

where: τ_s is the shear strength of the adsorbed layer-channel wall interface; D is the water molecule diameter; n is the equivalent number of the water molecules across the adsorbed layer thickness, and l is the axial length of the whole channel as shown in Fig. 2, a.

The critical power loss on a single channel for initiating the wall slippage is [7, 17]:

$$POW_{cr} = \frac{K_{cr} l (\tau_s h_{bf})^2}{\eta}, \tag{2}$$

where: η is the water bulk viscosity and

$$K_{cr} = \left[\frac{1}{2\lambda_{bf}\left(1+\frac{D(n-1)}{R_0}\right)}\right]^2 \left\{2\pi\frac{R_e}{R_0}\left\{\frac{4\varepsilon\lambda_{bf}^3}{C_y\left(1+\frac{\Delta x}{D}\right)}\left[1+\frac{1}{2\lambda_{bf}}-\frac{\Delta_{n-2}(q_0-q_0^n)}{h_{bf}(q_0^{n-1}-q_0^n)}\right]-\frac{2F_1\lambda_{bf}^3}{3C_y}\right\}+\frac{\pi}{4}-\right.$$

$$\left.-\frac{4\pi}{C_y}\left\{\frac{F_2\lambda_{bf}^2}{6}-\frac{\lambda_{bf}}{1+\frac{\Delta x}{D}}\left[\frac{1}{2}+\lambda_{bf}-\frac{\Delta_{n-2}(q_0-q_0^n)}{2R_0(q_0^{n-1}-q_0^n)}\right]\right\}\right\}, \tag{3}$$

where: $\lambda_{bf} = h_{bf}/(2R_0)$; R_e is an equivalent constant radius and often $R_e/R_0 = 1+\lambda_{bf}$; Δx is the separation between the neighboring water molecules in the axial direction in the adsorbed layer; $C_y = \eta_{bf}^{eff}/\eta$, η_{bf}^{eff} is the effective viscosity of the adsorbed layer and formulated as $\eta_{bf}^{eff} = Dh_{bf} / [(n-1)(D+\Delta_x)(\Delta_l / \eta_{line,l})_{avr,n-1}]$; $\varepsilon = (2DI + II)/[h_{bf}(n-1)(\Delta_l / \eta_{line,l})_{avr,n-1}]$; $q_0 = \Delta_{j+1} / \Delta_j$ and q_0 is constant; $F_1 = \eta_{bf}^{eff}(12D^2\psi + 6D\varphi)/h_{bf}^3$; $F_2 = 6\eta_{bf}^{eff} D(n-1)(l\Delta_{l-1} / \eta_{line,l-1})_{avr,n-1} / h_{bf}^2$;

$I = \sum_{i=1}^{n-1} i(\Delta_l / \eta_{line,l})_{avr,i}$;

$II = \sum_{i=0}^{n-2} [i(\Delta_l / \eta_{line,l})_{avr,i} + (i+1)(\Delta_l / \eta_{line,l})_{avr,i+1}]\Delta_i$;

$\psi = \sum_{i=1}^{n-1} i(l\Delta_{l-1} / \eta_{line,l-1})_{avr,i}$;

$\varphi = \sum_{i=0}^{n-2} [i(l\Delta_{l-1} / \eta_{line,l-1})_{avr,i} + (i+1)(l\Delta_{l-1} / \eta_{line,l-1})_{avr,i+1}]\Delta_i$;

$i(\Delta_l / \eta_{line,l})_{avr,i} = \sum_{j=1}^{i} \Delta_{j-1} / \eta_{line,j-1}$;

$i(l\Delta_{l-1} / \eta_{line,l-1})_{avr,i} = \sum_{j=1}^{i} j\Delta_{j-1} / \eta_{line,j-1}$; $\eta_{line,j-1}$ and Δ_{j-1} are respectively the local viscosity and the separation between the j^{th} and $(j-1)^{th}$ water molecules across the adsorbed layer thickness, and j and $(j-1)$ are respectively the order numbers of the water molecules across the adsorbed layer thickness.

When the wall slippage occurs, the total volume flow rate through the channel is [7, 17]:

$$q_v = \frac{C_1 POW}{\tau_s}, \text{ for } POW > POW_{cr}, \tag{4}$$

where: POW is the power loss on the channel and:

$$C_1 = \frac{h_{bf}}{l}\left[1 + \frac{1}{2\lambda_{bf}} - \frac{1 + \frac{\Delta_{n-2}(q_0 - q_0^n)}{D(q_0^{n-1} - q_0^n)}}{2\lambda_{bf}\frac{R_0}{D}}\right]. \tag{5}$$

When the wall slippage is absent, the total volume flow rate through the channel is [7, 17]:

$$q_v = C_2 h_{bf}^2 \sqrt{\frac{POW}{\eta l}}, \text{ for } POW \le POW_{cr}, \tag{6}$$

where:

$$C_2 = \frac{\sqrt{\pi}}{4\lambda_{bf}^2}\left\{8\frac{R_e}{R_0}\frac{\varepsilon\lambda_{bf}^3}{C_y\left(1+\frac{\Delta x}{D}\right)}\left[1 + \frac{1}{2\lambda_{bf}} - \frac{\Delta_{n-2}(q_0 - q_0^n)}{h_{bf}(q_0^{n-1} - q_0^n)}\right] - \frac{4R_e F_1 \lambda_{bf}^3}{3R_0 C_y} + \frac{1}{4} - \right.$$

$$\left. - \frac{4}{C_y}\left\{\frac{F_2\lambda_{bf}^2}{6} - \frac{\lambda_{bf}}{1+\frac{\Delta x}{D}}\left[\frac{1}{2} + \lambda_{bf} - \frac{\Delta_{n-2}(q_0 - q_0^n)}{2R_0(q_0^{n-1} - q_0^n)}\right]\right\}\right\}^{1/2}, \tag{7}$$

According to the classical (continuum) Hagen-Poiseuille equation, which neglects the existence of the adsorbed boundary layer, the total volume flow rate through the channel is [7]:

$$q_v = \frac{R^2}{2}\sqrt{\frac{\pi POW}{\eta l}}. \tag{8}$$

4. Input parameter values

The values of the important physiological parameters DP, POW_{cr} and q_v of the desmotubule nanochannel have been calculated for varying diameters and axial lengths of the channel. The values of the input parameters are as follows: $D = 0.28$ nm; $\eta = 0.001$ Pa·s; $\tau_s = 0.02$ kPa; $\Delta x/D = \Delta_{n-2}/D = 0.15$. It was taken that $\eta_{line,i} / \eta_{line,i+1} = q_0^m$, where q_0 and m are respectively positive constant [17].

For the weak water-channel wall interaction, the parameter C_y is given by [17]:

$$C_y(H_{bf}) = 0.9507 + \frac{0.0492}{H_{bf}} + \frac{1.6447E-4}{H_{bf}^2}, \tag{9}$$

where: $H_{bf} = h_{bf}/h_{cr,bf}$ and $h_{cr,bf}$ is the critical thickness and here taken as 1.4 nm.

The parameters ε, F_1 and F_2 are respectively [17]:

$$\varepsilon = 4.56E-6\left(\frac{\Delta_{n-2}}{D} + 31.419\right)(n + 133.8)\cdot$$
$$\cdot(q_0 + 0.188)(m + 41.62), \tag{10}$$

$$F_1 = 0.18\left(\frac{\Delta_{n-2}}{D} - 1.905\right)(\ln n - 7.897), \tag{11}$$

$$F_2 = -3.707E-4\left(\frac{\Delta_{n-2}}{D} - 1.99\right)(n + 64)\cdot$$
$$\cdot(q_0 + 0.19)(m + 42.43). \tag{12}$$

For the weak water-channel wall interaction, it was taken that $m = 0.2$; $n = 3$; $q_0 = 1.01$. The values of the parameters above give the very weak interaction between water and the channel wall of the desmotubule, indicating the high hydrophobicity of the channel wall.

5. Results

Fig. 3 shows the values of the dimensional pressure drop DP on the whole channel for initiating the wall slippage as functions of the radius R and the axial length l of the channel. DP is linearly increased with the increase of l. It is significantly increased with the reduction of R. It is on the scale of 10 kPa, which is normally achievable in a real plant. The wall slippage on the channel wall must therefore be taken into account.

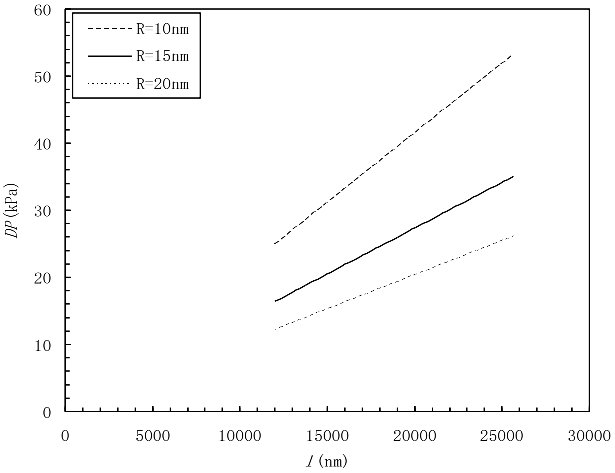


Fig. 3 Dimensional pressure drop *DP* on the whole single channel of the desmotubule for initiating the wall slippage

Fig. 4 shows the critical power loss POW_{cr} on the whole single channel of the desmotubule for initiating the wall slippage. It ranges between 3.0E-16 Watt and 3.3E-15 Watt, very small for maintaining the physiological function of a plant cell. When the power loss on the whole single channel is larger than POW_{cr}, the wall slippage occurs and it increases the water flow rate through the channel. The wall slippage is very important for water to smoothly flow through such narrow and long nanopores.

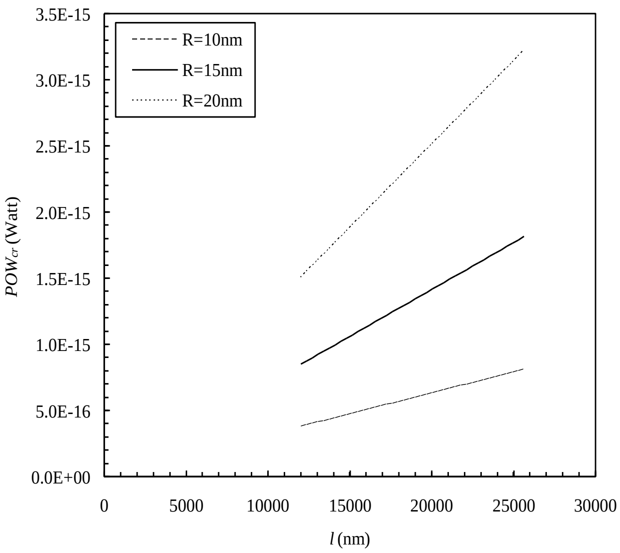
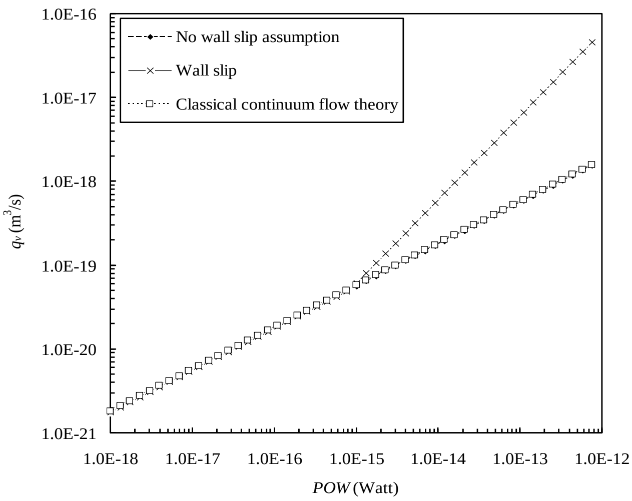
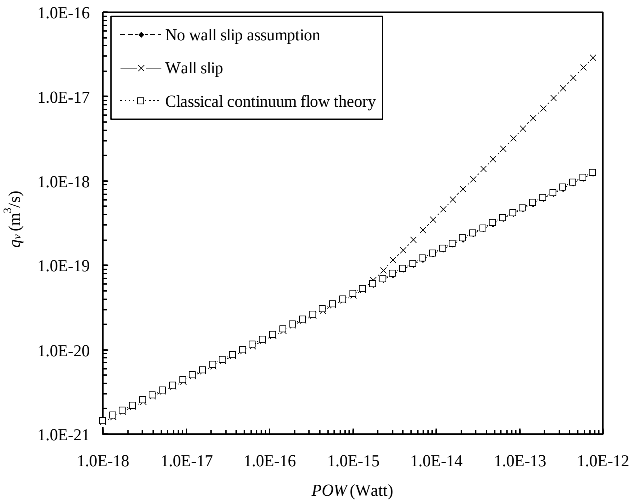


Fig. 4 The critical power loss POW_{cr} on the whole single channel of the desmotubule for initiating the wall slippage

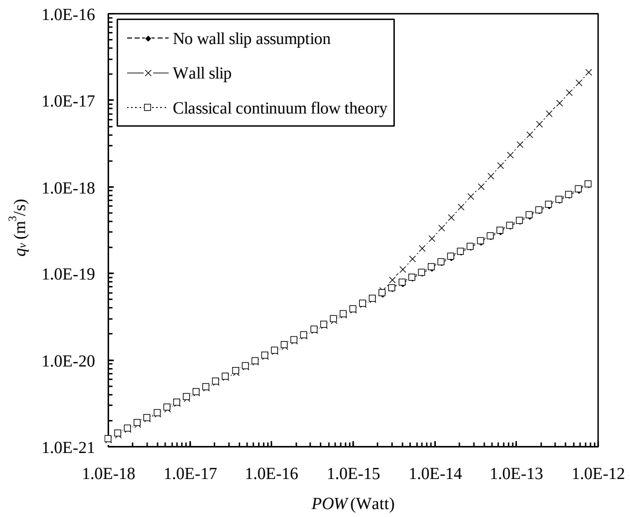
Figs. 5, a-c respectively representatively show the dimensional volume flow rate of water through the single channel of the desmotubule as function of the power loss on the whole channel when the wall slippage is taken into account or not; the calculation results from the classical continuum water flow model, which neglects the wall slippage, are also compared.



a) l = 12000 nm



b) l = 19000 nm



c) l = 26000 nm

Fig. 5 Volume flow rate of the water through the single nanotube of the desmotubule as function of the power loss on the whole channel based on the assumptions of the wall slippage or no wall slippage, R=15 nm

It is shown that when the wall slippage is ignored, the classical continuum water flow theory can well calculate the flow rate and the effect of the adsorbed layer is negligible; however, when the wall slippage is incorporated, the power loss on the channel which is large enough will increase the flow rate by several orders by generating the wall slippage as compared to the classical water flow theory calculation. When the wall slippage occurs, the water flow rate through the channel is linearly increased with the increase of the power loss on the channel with a significantly larger proportionality than the classical water flow model gives. For achieving a high flow rate, the required power loss on the whole channel is still very small. This is a very important function of a plant cell for maintaining the water transport. When no wall slippage occurs, both the flow rate through and the power loss on the channel are rather small; this is also the important function of a plant cell. It appears that the wall slippage is the critical mechanism for the water transport through the desmotubule channel in a plant cell; it is controlled by the pressure difference between the neighboringht cells.

6. Conclusions

1. The water transport through the nanotube in the plasmodesmata in a plant cell was analyzed. The diameter of the nanotube ranges between 20 nm and 40 nm; its axial length ranges between 12000 nm and 26000 nm. Classical continuum flow theory shows that the flow resistance of this nanotube is huge to water. However, actually this nanotube works well for the water to smoothly flow through.

2. The multiscale analysis was carried out for the water transport through this nanochannel. It incorporates the non-continuum adsorbed boundary layer flow and the intermediate continuum water flow. The nanoscale flow equation calculates the adsorbed boundary layer flow; the Newtonian fluid model describes the intermediate continuum water flow. Due to the high hydrophobicity of the nanochannel, the interfacial slippage was assumed on the adsorbed layer-channel wall interface.

3. The values of the important physiological parameters of the nanochannel have been calculated, such as the pressure drop and the critical power loss on the whole channel for initiating the wall slippage. The calculation results show that the wall slippage plays the critically important role in the water transport. Only a very small power loss on the whole single channel (less than 1.0E-12 Watt) is required to generate the wall slippage to increase the water flow rate by several orders. In the absence of the wall slippage, the volume flow rate through the nanochannel can be calculated from the classical continuum flow theory and it is very small and less than 1.0E-19 m^3/s for the radius of the channel equal to 15 nm.

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Z. Tang, Y. Zhang

MODELING OF WATER TRANSPORT THROUGH PLASMODESMATA IN PLANT CELL

S u m m a r y

The water transport property in the plasmodesmata in a plant cell is calculated from the multiscale flow equation by incorporating both the adsorbed boundary layer flow and the intermediate continuum water flow. The plasmodesmata has the desmotubule which is the cylindrical nanotube with the diameter ranging between 20 nm and 40 nm and the length from 12000 nm to 26000 nm. In the absence of the wall slippage, there is the large flow resistance in this nanochannel preventing the water from flowing through; for the easy transport of water through this nanochannel, the wall slippage must occur and it results in the water flow rate through the channel several orders higher than the classical continuum flow theory calculation, depending on the power loss on the transportation. The pressure drop and the critical power loss on a single desmotubule for initiating the wall slippage are calculated as functions of the diameter and the length of the desmotubule.

Keywords: flow, multiscale, plasmodesmata, transport, wall slippage, water.

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