Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting information

Delivery, Uptake, Fate, and Transport of Engineered Nanoparticles in Plants: A Critical Review and Data Analysis

Yiming Su[1], Vanessa Ashworth[2], Caroline Kim[1], Adeyemi S. Adeleye[3], Philippe Rolshausen[2], Caroline Roper[4], Jason White[5], David Jassby[1,]*
[1]Department of Civil and Environmental Engineering, University of California, Los Angeles
[2]Department of Botany and Plant Sciences, University of California, Riverside
[31]Department of Civil and Environmental Engineering, University of California, Irvine
[4]Department of Plant Pathology, University of California, Riverside
[5]Department of Analytical Chemistry, The Connecticut Agricultural Experiment Station

*Correspondence to:
David Jassby
University of California, Los Angeles, Los Angeles, CA 90095, USA
Tel: 310-825-1346
Email: jassby@ucla.edu

Description on the impact of Brownian diffusion on transport of NPs in plants

Based on typical sap velocity values, we quantitatively evaluated the impact of Brownian diffusion on NP transport by calculating the Pe number (Eqs. S1 and S2)[95]:

$$Pe = \frac{\rho v L}{\mu} = \quad \text{(S1)}$$

$$Re = \frac{\prime}{-} \quad \text{(S2)}$$

where Re is the Reynolds number[65,95], v is the velocity of sap (m/s), D_H is the hydraulic diameter of the xylem or phloem (m), and ρ is the density of sap (kg/m^3). Based on previous work[95], the diffusion coefficient (D) of NPs can be calculated using the Stokes-Einstein equation (Eq. S3):

$$D = \frac{k_d T}{3\pi u r} \qquad \text{(S3)}$$

where k_d, T, μ, and r are Boltzmann's constant (J/K), temperature (K), dynamic viscosity of the fluid (Pa·s), and radius of spherical NP (m), respectively. According to the literature, the viscosity of phloem sap ranges between 1.2×10^{-3} to 3.0×10^{-3} Pa·s (depending on the concentration of organics in the sap)[85]. As there are limited concentrations of organics in the xylem, μ is assumed to be 1.2×10^{-3} Pa·s, the lower limit of the phloem's viscosity. Thus, we derived D for NPs with different sizes under different μ (Figure S1). The D of NPs with r below 4 nm is comparable to that of sucrose (5.0×10^{-10} m^2/s)[95], which is one of the main sugars transported in the phloem. This implies that the diffusion of these small NPs in the phloem may need to be taken into consideration during NP formulation. The D of NPs with r over 7 nm is at least one order of magnitude lower than that of sucrose. D declines rapidly with increasing r, suggesting that the diffusion of larger NPs might not be crucial to their translocation in plants. To confirm this hypothesis, we calculated the Pe (Eq. S3). Based on the calculated D values, and the parameters provided in Table S3, the Re number for the phloem and the xylem are 0.002 and 0.05, respectively. The typical Pe number for NPs of different sizes in the phloem and the xylem can be seen in Figure S2.

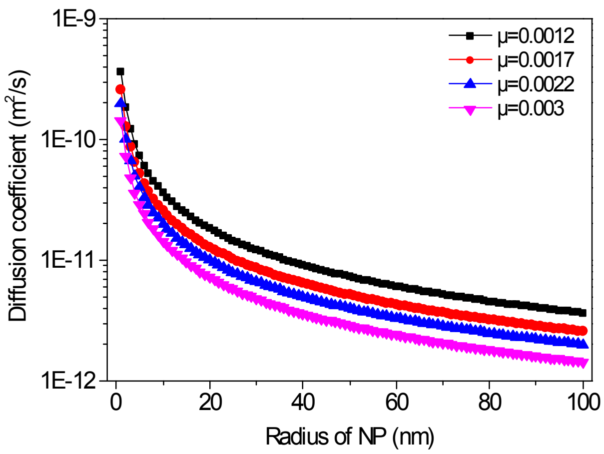

Figure S1. Diffusion coefficients of NPs with different sizes under different sap viscosity (T

= 298 K)

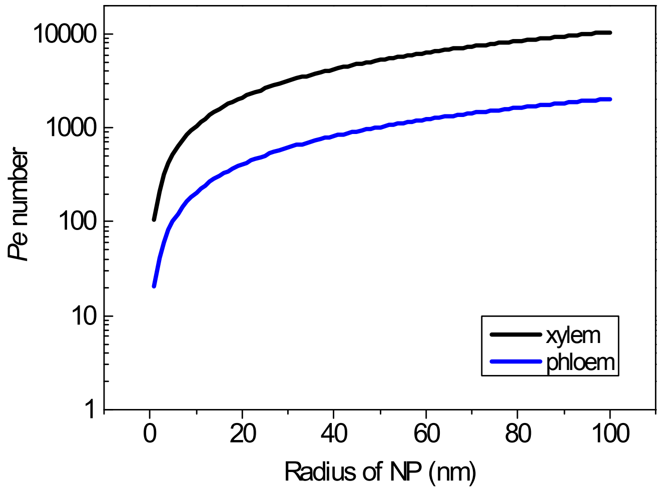

Figure S2. *Pe* numbers of NPs in phloem and xylem (T = 298 K, modeling parameters are provided in Table S3)

Table S1. Sap composition of rice

Component	Uppermost internode	Leaf sheath of seedling (7th- to 8th- leaf stage)
Sucrose	573.8 ±123.1	205.5 ±79.9
Total amino acids	124.8 ± 25.6	103.2 ±22.3
Potassium	40.4 ± 19.9	147.1 ±42.5
ATP	1.76± 0.16	1.63± 0.18

Table S2. Sap composition of tomato and soybean

component	Tomato			Soybean
	Apoplast (in fruit)	xylem	phloem	xylem
Glucose	13.4±2.3			
Fructose	18.2±2.5			
Malic acid	2.1±0.2	0.855 ±0.038		0.65+0.15
Citric acid	3.4±0.2	0.280 ±0.014		1.45+0.25
total Amino acid	14.4±1.7	1.5+0.02	395+49	2.7-0.75
Potassium	20.0±2.1	3.920 ±0.27		
Sodium	0.6± 0.4	0.080 ±0.01		
Magnesium	5.4±1.0	0.585 ± 0.03		1.17-0.04
Calcium	5.6±1.3	1.035 ±0.06		2.65+0.05
Phosphorus	2.9±0.6	0.340 ± 0.02		0.5-0.07
Chloride	8.6±0.1	0.610 ±0.03		
Ammonium	0.5±0.2			0.5-0.2
nitrate		5.240 ±0.38		
sulfate		0.420 ± 0.03		

Table S3. Related constants for DLVO and translocation model

	Density (ρ, kg/m^3)	ν (m/s)	D_h (m)	μ (Pa·s)	$Re=(\rho\nu D_h)/\mu$
Phloem	1000	$(1.5\sim4.8)\times10^{-4}$	$(1\sim30)\times10^{-6}$	$(1.2\sim3.0)\times10^{-3}$	$(0.05\sim6.25)\times10^{-3}$
Xylem	1000	$(1.5\sim48)\times10^{-4}$	$(1\sim40)\times10^{-6}$	1.02×10^{-3}	$(0.15\sim70.59)\times10^{-3}$

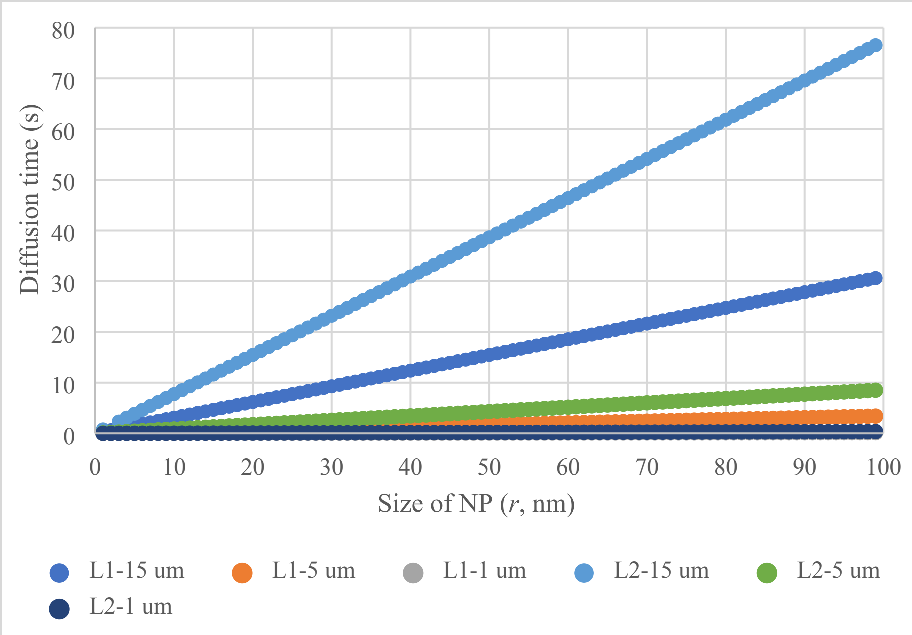

Figure S3. Diffusion time for NPs with different radius (r) to reach the surface of xylem/phloem (with different radius, L = 15, 5, 1 μm) from the center of lumen ($L1$, in phloem; $L2$, in xylem) estimated from equation, $L =$