

Modelling transport processes in tissues and organs at a mesoscopic scale

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Highlights: Three mesoscopic models of transport processes in plants are presented: water fluxes in tissues, zinc uptake in roots, and gas fluxes in leaves. The models aim at increasing our understanding of the interaction between physical and biological processes in plants. Besides giving ideas for derivation of other mesoscopic models, the presented results can be of use in functional-structural plant models.

Keywords: transport, uptake, transpiration, metals, zinc, nutrients, water, roots, leaves, genetic regulation

INTRODUCTION

Transport of water, nutrients and gases in tissues and organs takes place in highly structured domains with multifaceted paths: symplastic, apoplastic and transcellular (Steudle, 2000). While the apoplast is a porous medium in which Darcy's law applies, fluid movement in the symplast follows a viscous flow law (e.g. Stokes). In general, different physical processes have to be considered, in particular when these are coupled. To obtain mesoscopic mathematical models of sufficient physiological background, it is necessary to pose microscopic models, valid at e.g. the cell scale, to couple the microscopic domains by transmission conditions, and to derive mesoscopic/macroscopic models by “upscaling” for simulation and analysis. This approach is used widely in engineering (Hornung, 1997), but much less in biology (e.g. Marciniak-Czochra and Ptashnyk, 2008; Chavarría-Krauser and Ptashnyk, 2010). Regardless of the mathematical technicality, the ideas and steps carried out are intuitive: modelling of microscopic processes, determination of macroscopic models and simulation. Depending on the problem's scale, upscaling might be senseless as in discrete or semi-discrete models of auxin transport and morphogenesis (e.g. Goldsmith et al., 1981; Kramer, 2004; Chavarría-Krauser et al., 2005; Jönsson et al., 2012). Transport, deformation, flow, etc. are physical processes occurring in general independently of organisms yet tamed by cells to accomplish a specific function. For example, zinc uptake and transport in roots follow diffusion-advection-reaction laws modulated by expression of ZIP-transporters (Krämer and Sinclair, 2012; Claus et al., 2012). Regarding transport processes in plants, a duality between physical and biological processes is found. Understanding this duality is important to establishing functional-structural plant models (FSPM) and to plant physiology in general. We present three models to exemplify how mesoscopic integrative plant models can be obtained and elucidate further the interaction between physical and biological processes in plants. We focus on: water fluxes in tissues, regulated zinc uptake in roots, and gas fluxes in leaves.

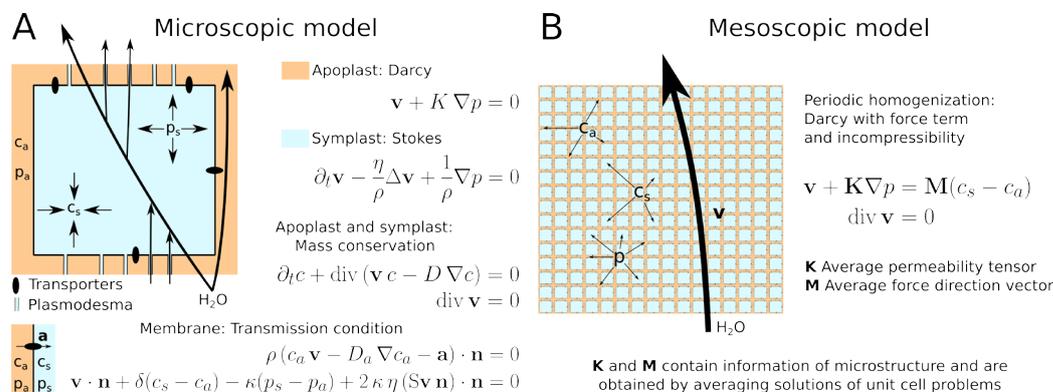


Fig. 1. A, Microscopic model based on conservation of mass and momentum. Transmission conditions account for transport over the membrane. B, Mesoscopic model obtained using periodic homogenization. The model is based on one pressure p , one velocity \mathbf{v} and two concentrations: c_a and c_s .

WATER FLUXES IN TISSUES

The existence of the apoplast and symplast in plant tissues opens diverse paths to water (Steudle, 2000). The contribution of the symplastic, apoplastic and transcellular paths is still unknown. We derive a model to analyse further these contributions by assuming an ideal tissue of perfect periodicity. The cells are assumed to have cell walls, plasma membranes and cytoplasm; plasmodesmata join their cytoplasms (Fig. 1A). The microscopic model consists of flow and transport equations for water and osmotic solutes. The flow is assumed to follow Darcy in the apoplast and plasmodesmata and Stokes in the symplast (Fig. 1A). We derive transmission conditions connecting the symplast and apoplast by balancing the fluxes at the interface. A regulation of transport is considered via ordinary differential equations describing the amount of free and bound transporters. Although the microscopic model is continuous, it could be reformulated as a discrete cellular model. Using homogenization techniques (Hornung, 1997), we obtain an average “upscaled” mesoscopic model (Fig. 1B). It is a Darcy law with a force term proportional to the local difference in solute concentration. Representations of the average transport coefficients are obtained from solutions of unit cell problems, which are posed for one cell and account for the microscopic structure. The mesoscopic model obtained is simple in structure, straightforward to solve numerically and can be applied in FSPM to describe water fluxes in tissues and organs.

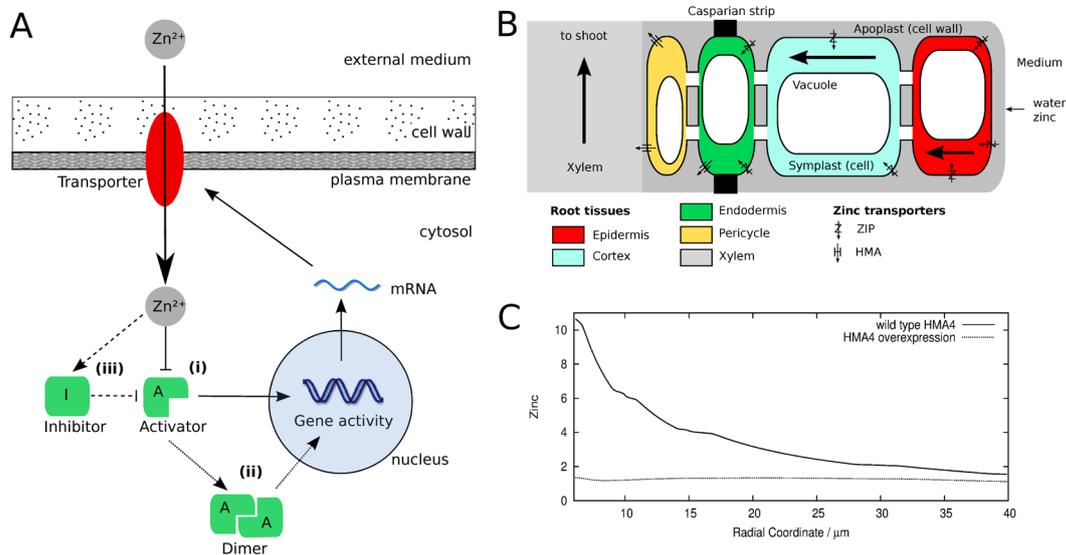


Fig. 2. Zinc and water uptake in roots. A, Schematic description of feasible zinc regulation models: (i) activator only, (ii) activator with dimerization, (iii) activator-inhibitor. B, Schematic description of radial transport of zinc. C, Simulation result showing zinc distributions under different levels of HMA4 (lower panel).

REGULATED ZINC UPTAKE IN ROOTS

The heavy metal zinc is an essential micronutrient yet potentially toxic for plants. Its uptake in roots needs to include mechanisms for the quick adaptation to a varying environment. Transport of zinc from the root epidermis to the central cylinder depends on three main processes: diffusion in the medium, advection with water, and cross-membrane transport. Modelling these processes allows analysing their relative impact and question biological hypotheses. Strict regulation of zinc uptake is presumably accomplished by modulation of zinc transporters in the membrane in response to changes of the cells' internal zinc concentration. Experimental measurements showed that the number of transporters is adjusted according to external concentrations by a still unknown system of transcription factors and activating and inhibiting agents (Talke et al., 2006; Assunção et al., 2010). We analysed the biological relevance of different simple scenarios comprising a simple activator, a dimerizing activator, and an additional inhibitor in an ordinary differential equations model (Fig. 2A). Our simulations suggest the existence of a dimerising activator and an inhibitor due to advantages in stability and robustness (Claus and Chavarria-Krauser, 2012a). Zinc uptake in roots depends also on passive diffusion and radial flow of water towards the xylem. To analyse the relative significance of these processes and the effect of geometry and microstructure, we posed a spatio-temporal transport model of the root of *Arabidopsis thaliana* (Fig. 2B; Claus et al., 2012b). The simulations show an inverse relation between accumulation and the level of the efflux transporter HMA4 (Fig. 2C), which is in accordance with measurements of HMA4 over expression (Hanikenne et al., 2008).

GAS FLUXES IN LEAVES

To gain insight in the physics and regulation of gas exchange (water vapour, carbon dioxide, and oxygen) in plant leaves we propose a dynamical first-principle model for a small disc-shaped section of a leaf around a single stoma (see Fig. 3). We focus on the mechanical interaction between epidermis cells and guard cells, coupled to water and solvent transport in the epidermis (symplastic and apoplastic compartments), as well as evaporation into and diffusion within the interstitial air space. Vapour exchange to the ambient air is controlled by the stomatal aperture which in turn is determined by the mechanics and the guard cell solute content. The underlying physical processes along with typical parameter values are described in standard literature (e.g. Nobel, 2005). The structure of the resulting model is a coupled system of ordinary and partial differential equations providing a more detailed description as compared to resistor network models. It also captures dynamic effects, and links microscopic physical properties to observable variables such as stomatal aperture and water loss. The model provides a physically accurate explanation to the inverse behaviour of stomatal aperture after sudden changes in ambient parameters, such as ambient moisture (Mott et al., 1997). This model is intended to serve as one building block for a future more comprehensive model of the leaf.

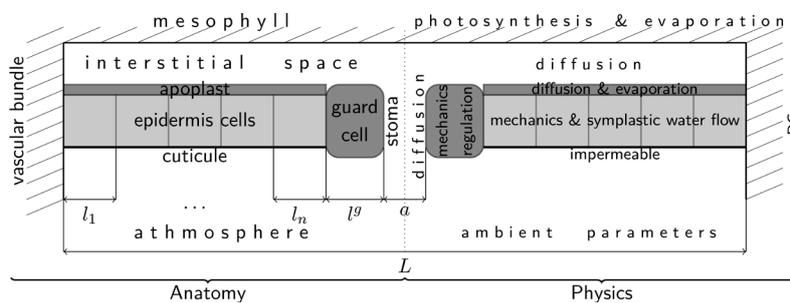


Fig. 3. Section through leaf epidermis centered around a single stoma.

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