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Stomatal transpiration and droplet evaporation on leaf surfaces by a microscale modelling approach

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ABSTRACT

Knowledge on convective water vapour exchange at leaf-air interfaces is required to assess transpiration of leaves via stomata and evaporation of droplets, which can both be considered as microscopic moisture sources, heterogeneously distributed across the leaf. An innovative modelling approach was proposed to investigate such convective mass transport from leaf surfaces, using computational fluid dynamics (shear-stress transport k–ω turbulence model with low-Reynolds number modelling). The main novelty lies in the fact that a large range of spatial scales (10^{-5}–10^{-1} m) was included and that the individual microscopic sources were modelled discretely. The convective exchange from the leaf model was strongly dependent on three parameters: surface coverage, air speed and source size. The relation between the convective flow rate and both the coverage ratio (CR) and the microscopic Sherwood number, i.e., the ratio of the source size to the viscous sublayer thickness, was quantified. It was shown that well-established convective transfer coefficients, obtained from plates or leaf models for a CR of 100%, can result in a significant overprediction of the convective exchange, compared to more realistic, lower CR. Furthermore, small variations in stomatal density (CR), e.g., due to biological variability, were shown to have a large impact on the convective exchange and droplets were found to evaporate more rapidly at low CR. The decrease in mass transfer rate due to stomatal closure was quantified as well. The proposed numerical modelling approach can be applied to increase our understanding of leaf transpiration and droplet evaporation, but also of the leaf boundary-layer microclimate and the transport processes therein. A critical discussion of the modelling assumptions allowed to identify focus points for future model refinement as well as future research.

1. Introduction

Accurate predictions of evapotranspiration processes from leaves, via stomata and droplets, are of interest for plant physiology, hydrology, agricultural production, boundary-layer meteorology and biosystems engineering. Stomata and small droplets on leaves are both distributed heterogeneously across the leaf surface and are of a small (microscopic) scale. They can be considered as discrete moisture sources at the leaf surface: leaf transpiration occurs predominantly via stomata, and evaporation occurs at droplet surfaces. The aim of this study is to increase our understanding of the convective water vapour exchange via these microscopic sources at the leaf-air interface, and its impact on the average moisture transfer from the leaf surface to the environment. For this purpose, we investigate the hypothesis that the exchange rate has a complex dependency on the size of the stomata/droplets, their surface coverage and the air speed. Such dependencies have not yet been identified in detail.

Stomata are local elliptical perforations in the epidermis and have sizes of a few tens of micron. They occupy one to a few percent of the leaf surface area, with a density of 10^1–10^2 stomata per mm^2 (e.g., [1]). The density can differ for upper (adaxial) and lower (abaxial) leaf surfaces. The bulk of the leaf moisture loss occurs via transpiration through the stomata, as the cuticle is quasi impermeable. Stomata thus play an important role in the plant hydrological cycle [2] and influence plant water uptake and water stress, which is the single most important problem in agricultural production [3]. The transpiration rate is mainly determined by the stomatal resistance, which is predominantly dependent on the stomatal aperture. The complex regulatory mechanism of opening and closing of the stomata is not fully understood yet [1,2]. The transpiration rate is however also dependent on the air flow conditions above the leaf surface, and thus the convective mass exchange between stomata and the environment – the resistance offered by the boundary layer [4–7]. This convective vapour exchange has been

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found to be mainly dependent on the stomatal aperture and density, and on the boundary-layer microclimatic conditions around the stomata, and is a subject of active research [8–9].

Droplets are deposited on leaves by rain, dew, or artificially, e.g., from pesticide spraying, and have sizes ranging from very small (10^{-4} m) to a few millimetres [10–14]. Knowledge on droplet evaporation from leaf surfaces is required to assess evapotranspiration processes and plant/tree leaf water budgets. Water availability at leaf surfaces also determines the boundary-layer microclimate, and the risk of contamination by pathogens or other infections. Furthermore, the evaporation kinetics of pesticide droplets, thus the droplet lifetime, determine pesticide efficacy [15–17]: fast evaporation can result in insufficient droplet spreading, reduced absorption of active chemical components or formation of crystals, whereas slow evaporation may induce germination of pathogens. An understanding of the convective exchange at the air-droplet interface is critical here, as it governs the droplet evaporation kinetics.

As stomata and droplets are distributed discretely over the leaf surface, they both lead to a very heterogeneous (non-uniform) mass exchange over the leaf surface, predominantly at the microscale level (10^{-5}–10^{-3} m). The impact of these point sources on the convective exchange is usually not considered by conventional convective transfer studies on leaves [9]: for real leaves, measurements of individual droplet evaporation/stomatal transpiration rate and stomatal aperture are not straightforward, which explains why usually only leaf-averaged transfer is assessed; for numerical studies or experimental studies using artificial leaves, homogeneous mass boundary conditions are usually imposed at the leaf surface, such as a uniform distribution of water vapour pressure over the entire surface. Although the mass transfer from a leaf can be up to 2.5 times higher than from a flat plate [9], the impact of the discrete distribution of the stomata (or droplets) on the transfer rate has not yet been isolated, as other influence factors, such as surface roughness, edge effects, leaf curvature, leaf orientation or flutter, inherently contribute as well [18,19].

Only a few researchers investigated in detail the effect of such discretely-distributed moisture sources on mass transfer, mainly for applications related to droplet evaporation. An analytical study by Schlünder [20] showed that for laminar boundary-layer flow over a flat surface, a high mass transfer rate could be obtained for a partially-wetted surface under specific conditions, by which the surface behaved very similar to a uniformly-wetted surface. Cannon et al. [21] developed an analytical model to describe transpiration from leaf stomata into the boundary layer, including transport in the substomatal cavities. This model was used to investigate boundary-layer interference effects between stomata. Such analytical considerations are, however, limited to simple air flow configurations, (usually laminar and two-dimensional). A few experimental studies were also performed, as detailed in Table 1. These studies looked only at air-side transfer, except Cannon et al. [21], which in addition mimicked the transport from the substomatal cavity through the stomata by using microscopically perforated plates.

The aforementioned experimental studies mainly considered macroscale moisture sources (>10^{-3} m). Furthermore, only the total convective transfer rate was determined. An experimental assessment of the boundary-layer flow and the local exchange processes therein, which determine the microclimate around the droplets and stomata, was not performed as this is very challenging at such small scales. Numerical modelling would partially alleviate these limitations, which could provide new insights. This is the perspective of the present study. With computational fluid dynamics (CFD), (passive) convective mass exchange in the boundary layer will be modelled from leaf level (10^{-1} m) down to the stomatal scale (10^{-5} m), thus covering a very large spatial range for a numerical study. Apart from quantifying the mass flow from the sources at the interface, high spatial resolution information is obtained on the flow field and the mass transport therein. By such numerical modelling, a systematic study is undertaken to identify the effect of the size of the stomata or small droplets, their surface coverage and the air speed on their convective exchange. To the knowledge of the authors, the only numerical study undertaken to quantify transpiration via microscopic sources [8] only considered the microscale level, as it modelled stomata arranged in a single stomatal crypt and investigated their effect on the crypt conductance. The main novelty of the computational modelling approach presented in this study lies in the fact that a very large spatial range is covered and that individual microscopic sources are modelled discretely.

2. Materials and methods

2.1. Numerical model

2.1.1. Computational domain

A simplified configuration was used to investigate convective water vapour (i.e., scalar) transfer from microscopic sources at a leaf surface: a 2D flat plate representing a leaf (length $L = 0.1$ m) was placed flush in two-dimensional channel flow (channel height $H = 0.5\text{ m} = 5L$). The 2D computational domain is presented in Fig. 1b, together with the imposed boundary conditions. The domain dimensions and the computational grid were based on best practice guidelines [22] and grid sensitivity analysis. An upstream ($L/2$) and downstream channel section ($5L$) were provided to avoid an influence of the imposed boundary conditions at inlet and outlet on the momentum and scalar transfer in the vicinity of the leaf. The grid is composed out of quadrilateral cells and contains 2.26×10^5 cells. From grid sensitivity analysis, the spatial discretisation error was estimated by means of Richardson extrapolation [23–24], and is below 0.6% for both leaf drag force and scalar flux at the wall.

2.1.2. Computational grid

2.1.2.1. Microscopic sources on leaf surface. To model discretely-distributed microscopic scalar sources on the leaf surface, representative for stomata or small droplets, very small computational cells of uniform dimensions were used on this surface. Stomata typically have a diameter of a few tens of micron when fully open; droplets have sizes (diameter) of about 10^{-4} m to a few millimetres (see Section 1). Thereto, a cell size (d) of 10×10^{-6} m was used on the leaf surface in the computational model. By grouping several of these cells, larger sources could be created (see Section 2.1.4). Including such a large range of spatial scales in the same computational model (10^{-5}–10^{-1} m) is particularly challenging with respect to grid generation. The grid in the boundary-layer region is shown in Fig. 2, and more details are presented in Supplementary material. Several transition regions were applied away from the leaf surface to reduce the number of cells in the computational model and to avoid very elongated cells. Note that a 2D model was used whereas in reality stomata and droplets are elliptic and circular, respectively, and are distributed heterogeneously over the leaf surface which does not have a flat topology. Nevertheless, realistic coverage ratios and source sizes were evaluated in this study, which provides a first step in understanding the effect of such microscopic sources on convective transfer rates. To reduce the complexity of the computational model, the droplet thickness (volume) was not considered. In reality, the exposed surface area of a droplet can be larger than a flat area depending on the contact angle, and droplets obviously protrude into the laminar (viscous) sublayer, influencing the air flow in the boundary layer. This viscous sublayer is the lower part of the boundary layer, where laminar flow occurs. So, as a first approximation, the droplet is