

## Transpiration from stomata via the leaf boundary layer: a microscale modelling approach

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**Highlights:** Convective mass transport from entire leaf surfaces was investigated with computational fluid dynamics. A novel aspect is that the stomata were modelled discretely. The convective exchange rate was relatively large, even for the limited surface coverage by stomata, and had a complex dependency on surface coverage and air speed. In addition, insight into the boundary-layer transfer at microscale level was obtained.

**Keywords:** convective transfer, transpiration, leaf, computational fluid dynamics, stomata

### INTRODUCTION

Stomata are local elliptical perforations in the leaf's epidermis which have sizes of a few tens of micron and which occupy one to a few percent of the leaf surface. As the cuticle is quasi impermeable, leaf transpiration occurs predominantly via stomata. Hence, they play an important role in the plant hydrological cycle (Berry et al., 2010) and influence plant water uptake and water stress. Apart from the stomatal aperture and density, the transpiration rate is also dependent on the air flow in the boundary layer on the leaf surface, and the exchange processes therein (Nobel, 2005). This convective exchange between stomata and the environment is a subject of active research (Roth-Nebelsick et al., 2009).

As stomata are distributed discretely over the leaf surface, they lead to a very heterogeneous (non-uniform) mass exchange over the leaf surface, at a microscale level ( $10^{-5}$  m). The impact of these small mass sources on the convective exchange is usually not considered by conventional convective transfer studies on leaves: for real leaves, measurements of individual stomatal transpiration rate are not straightforward, and therefore only bulk transpiration of leaves 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.

Only a few researchers have investigated in detail the effect of discretely-distributed moisture sources on mass transfer, but mainly for applications related to droplet evaporation (Cannon et al., 1979; Leclerc et al., 1986). The aforementioned experimental studies often considered macroscale moisture sources ( $> 10^{-3}$  m) and only the total convective transfer rate was determined. An assessment of the local exchange processes in the boundary layer was not performed as this is very challenging at the microscale. Some of these limitations could be alleviated by numerical modelling, which is the perspective of the present study. To the knowledge of the authors, the only numerical study undertaken to quantify transpiration via microscopic sources (Roth-Nebelsick et al., 2009) considered stomata arranged in a single stomatal crypt and investigated their effect on the crypt conductance. In the present study, the convective exchange in the boundary layer is modelled with computational fluid dynamics (CFD, both 2D and 3D) from leaf level ( $10^{-1}$ - $10^{-2}$  m) down to the stomatal scale ( $10^{-5}$  m), thus covering a very large spatial range for a numerical study. This is particularly challenging with respect to numerical grid generation, which is required to accurately solve the governing equations in the boundary layer. A systematic study is undertaken to identify the effect of the stomatal surface coverage and the air speed on the convective exchange.

### SIMULATIONS

A 2D and 3D model of a leaf were constructed to study convective transfer from microscopic scalar sources, such as stomata. Both models represent a flat leaf, which was placed in low turbulent air flow with a free-stream speed  $U_b$ . The length of the leaf was 100 mm in 2D and 25 mm in 3D. The computational grids contained  $0.226 \times 10^6$  cells and  $5.88 \times 10^6$  cells, for 2D and 3D, respectively. In order to model the microscopic stomata discretely, very small computational cells ( $\sim 50 \mu\text{m}$ ) were required on the leaf surface.

Instead of modelling mass transfer from these sources, heat transfer (i.e., a passive scalar) was modelled since this led to a significant decrease of the computational cost: in this case, the flow field had to be solved only once at each air speed, since the air properties (e.g., density) could be taken constant. As such, only the scalar (heat) transfer, and not the flow field, had to be recalculated for the different imposed boundary conditions, i.e., stomatal coverage ratios. The resulting heat transfer data can easily be converted to mass transfer by means of the heat and mass transfer analogy, and is presented in dimensionless form anyway in the present study. The boundary-layer development is also similar since the Lewis number is almost equal to one ( $\approx 0.8$ ). As such, heat (or mass) will be referred to as a scalar from now on. Only air-side transfer was modelled. A constant scalar value (temperature) was imposed at the stomata and a no-flux condition was used on the rest of the leaf surface. Different coverage ratios (CR) were evaluated, representative for those of real stomata, which vary roughly between 0.2% and 5%. The coverage ratio is defined as the ratio of the area occupied by the stomata ( $A_{\text{eff}}$  [m<sup>2</sup>]), to the total leaf area ( $A$  [m<sup>2</sup>]), i.e.,  $\text{CR} = A_{\text{eff}}/A$ . The CFD simulations were performed with the commercial code ANSYS Fluent 13. Steady Reynolds-averaged Navier-Stokes (RANS) was used in combination with the shear stress transport (SST)  $k-\omega$  model (Menter, 1994). Low-Reynolds number modelling (LRNM) was applied to resolve the transport in the boundary-layer region. This RANS turbulence model, in combination with LRNM, has already been shown to be very accurate for similar complex flow problems (e.g., Defraeye et al., 2012).

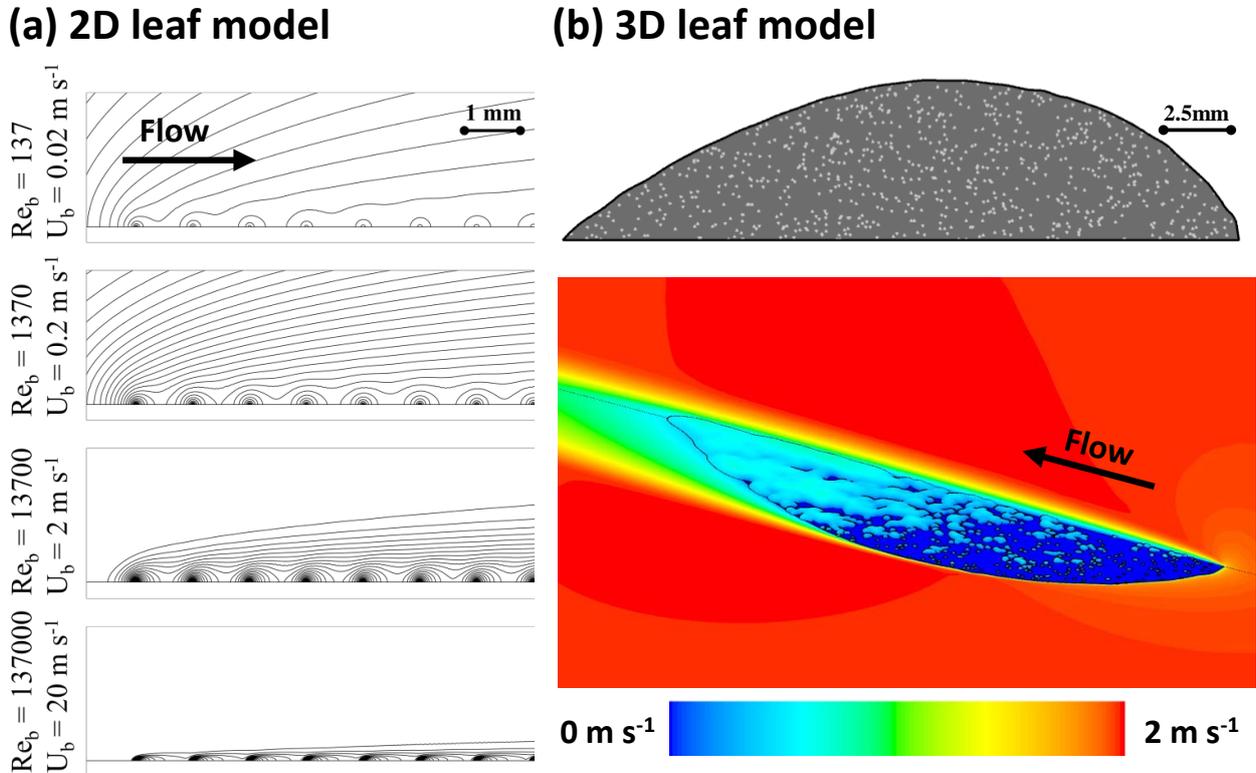


Fig. 1. (a) Scalar concentration contours (isocontours) in the boundary layer at the leading edge of the 2D leaf for a coverage ratio of 5% for different air speeds (Reynolds numbers) for a coverage ratio of 5%. (b) Top: distribution of stomata on 3D leaf surface (only one half shown) for a coverage ratio of 1%; Bottom: air speed on a scalar isosurface (i.e., a surface which represents a constant scalar concentration in the computational domain) in the boundary layer of the 3D leaf and on both vertical and horizontal symmetry planes for a coverage ratio of 1% for  $U_b = 2 \text{ m s}^{-1}$ .

## RESULTS AND DISCUSSION

In Fig. 1a, the scalar concentration contours are shown at the leading edge of the 2D leaf for different air speeds (Reynolds numbers) for a coverage ratio of 5%. The scalar boundary-layer thickness decreases with increasing air speed. At low speeds, the contours look more symmetrical on both sides of the sources, but at higher speeds, the scalar is convected more downstream and a wake zone is observed. In Fig. 1b, the air speed on a scalar isosurface in the boundary layer of the 3D leaf, and on both vertical and horizontal symmetry planes is shown for a coverage ratio of 1%. The boundary layer clearly becomes more saturated downstream of the leading edge, as the size of the volume occupied by the isocontour clearly increases.

The surface-averaged convective scalar flows ( $Q_{c,w,\text{avg}}$ ) from the 2D leaf are shown in Fig. 2a as a function

of the coverage ratio. The results at different air speeds ( $U_b$ ), thus  $d/\delta_{VSL}$  ratios, are presented. Here  $d$  is the size of the scalar sources ( $50\ \mu\text{m}$ ) and  $\delta_{VSL}$  is the average thickness of the viscous sublayer, i.e., the lower part of the boundary layer where laminar transport occurs and where large velocity and scalar gradients are found. These scalar flows are scaled with the surface-averaged scalar flow for a coverage ratio of 100% ( $Q_{c,w,avg,100\%}$ ). Note that these scalar flows are directly proportional to the leaf's convective transfer coefficient. Similar results are shown in Fig. 2b for the 3D leaf, but only for a single air speed ( $U_b = 2\ \text{m s}^{-1}$ ).

From Fig. 2, relatively high scalar flows at the surface are found at low coverage ratios (for all  $d/\delta_{VSL}$  ratios), thus they clearly do not vary linearly with the coverage ratio. This trend is predicted by both 2D and 3D modelling. This effect is more pronounced at low  $d/\delta_{VSL}$  (Fig. 2a), implying low air speeds (or small source sizes). These findings however also indicate that well-established convective transfer coefficients from plates or leaf models, obtained for a coverage ratio of 100%, can result in a significant overprediction of the convective exchange, compared to a more realistic, lower, stomatal coverage ratio, due to the discrete distribution of these microscopic sources. Furthermore, the largest decrease in scalar flows with coverage ratio was found at low coverage ratios (CR < 10%, i.e., the range shown in Fig. 2), which implies that small variations in the leaf's stomatal density (CR), e.g., due to biological variability, or a temporal variation of stomatal aperture have a large impact on the convective exchange as well.

In conclusion, the convective exchange from stomata was shown to be strongly dependent on surface coverage and air speed. The applied microscale modelling approach provided more insight in convective exchange processes at the stomatal level. Such a numerical modelling framework seems promising in contributing to the understanding of leaf transpiration, but also of microclimatic conditions in the boundary layer and the transport therein.

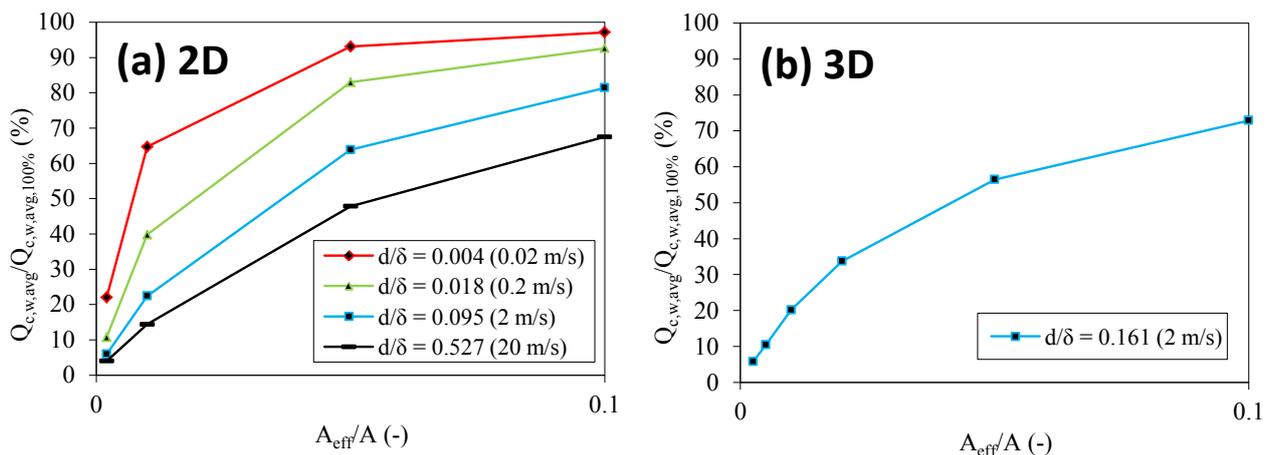


Fig. 2. Surface-averaged convective scalar flows at the leaf surface as a function of the coverage ratio, for CR up to 10%. The flows are scaled with the surface-averaged scalar flow for a coverage ratio of 100% ( $Q_{c,w,avg,100\%}$ ): (a) 2D model at different air speeds ( $U_b$ , i.e.,  $d/\delta_{VSL}$  ratios); (b) 3D model at a single air speed.

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