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COMPUTATIONAL INVERSE METHOD TO DETERMINE WETTING PARAMETERS OF PAPER-BASED MICROFLUIDIC SUBSTRATES

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Abstract.
Flow in unsaturated porous media can be described with the Richards equation, in which the microscopic interactions between the fluid and solid matrix are considered at a macroscopic level and expressed as nonlinear functions. Widely used porous media models provide expressions for these functions, with parameters that may be fit to the results of certain measurements. These models are usually already implemented in numerical tools—including our own software Fronts (https://github.com/gerlero/Fronts.jl). As a general equation for porous media, the Richards equation can also predict capillary flow on substrates used for microfluidic paper-based analytical devices, such as Whatman® -brand filter papers and nitrocellulose membranes. However, in the case of such materials, obtaining model parameters for the Richards equation can become a challenging task, due to practical limitations in measurements that cause a subsequent high uncertainty in the obtained parameters. In this context, using an inverse method can yield better results. In this work, we discuss different approaches for the inverse determination of model parameters for the Richards equation in microfluidic substrates, with the goal of selecting an appropriate computational scheme. We tested the scheme by performing our own wetting experiments and applying the inverse method on the experimental data. The necessary numerical support for the method was provided by Fronts, which has seen new features added to it since its introduction.