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Dynamics of water transport and swelling in human stratum corneum

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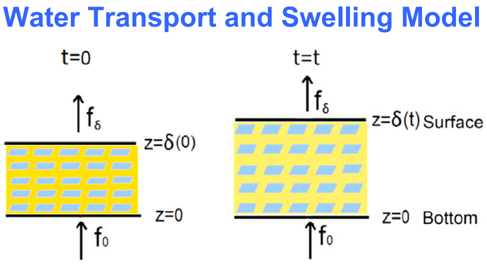
HIGHLIGHTS

- We developed a computational model describing water transport and swelling in skin.
- The model was calibrated using skin hydration data from the literature.
- The model predicts TEWL and and nonlinear water distribution profiles in skin.
- Dynamic calculation of stratum corneum hydration and dehydration rates is achieved.
- Dehydration occurs more rapidly than hydration due to variable water diffusivity.

GRAPHICAL ABSTRACT



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ABSTRACT

A computational model describing water transport and swelling in the stratum corneum layer of the skin has been developed. The model deals with varying water diffusion coefficient within the stratum corneum layer and a moving boundary with water entering or exiting the membrane under various boundary conditions. In steady state, the model can reasonably predict the transepidermal water loss (TEWL) and the membrane thickness as a function of surface relative humidity (RH) or water activity (a_w). The predicted TEWL is around 13 g/m^2 h in the relative humidity range of 0–70%. The model also successfully predicts nonlinear water distribution profiles within the stratum corneum at various relative humidities. In dynamic mode, the model is able to predict water distribution, membrane thickness, and water transport rate as a function of time for either hydration or dehydration under different surface boundary conditions including occlusion, exposure to air or exposure to gels. For the hydration process, the swelling rate of reaching a fully hydrated state under different surface boundary conditions is in this order: immersion in normal saline with $a_w = 0.996 >$ exposure to humid air with RH $= 0.996 >$ dry occlusive surface. For the dehydration process, the shrinking rate from the fully hydrated state is nearly the same under the surface boundary conditions of fixed surface $a_w = 0.05$ and exposure to air with RH $= 5\%$. The dehydration rate from the fully hydrated state is faster than the reverse hydration rate for reaching the fully hydrated state.

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1. Introduction

The water content of the skin's outer layer, the stratum corneum (SC), plays an important role in skin permeability and is a key element of skin condition. The SC swells to several times its normal thickness when exposed to liquid water or to high relative humidity (RH) either in vitro (Anderson et al., 1973b; El-Shimi and Princen, 1978; Kasting and Barai, 2003) or in vivo (Anderson et al., 1973a; Pirot et al., 1998; Warner et al., 2003). This swelling occurs primarily within the corneocyte phase (Bouwstra et al., 2003, 1991; Warner et al., 2003), but the intercellular lipids are also strained and their permeability is thought to increase as well (Kasting et al., 2003; Warner et al., 2003). Water pockets are seen within the lipid regions following extended hydration (Bouwstra et al., 2003; Warner et al., 2003). Low water content of the SC is associated with the appearance of dry skin (Rawlings and Matts, 2005) and is also a factor in more severe skin conditions including occupationally-damaged skin and atopic dermatitis. Prolonged high humidity or occluded environments also contribute to poor skin condition, e.g. diaper dermatitis (Warner et al., 2003). The water content of skin may be non-invasively assessed in vivo by conductance and capacitance measurements, e.g. corneometry (Rawlings and Matts, 2005), and by confocal Raman spectroscopy (Caspers et al., 2000, 2001), whereas water transport in vivo is assessed by transepidermal water loss (TEWL) (Roskos and Guy, 1989). Corresponding laboratory measurements include water adsorption isotherms in isolated SC (Anderson et al., 1973b; El-Shimi and Princen, 1978; Kasting and Barai, 2003), thermogravimetric measurements (Anderson et al., 1973a; Liron et al., 1994; Rauma et al., 2006) and tritiated water (^3H_2O) transport (Blank et al., 1984; Stockdale, 1978). A quantitative description of the water handling and transport properties of the SC may consequently be seen to be essential to a more complete understanding skin barrier homeostasis.

Quantitative observations regarding SC water handling properties date back many years (Anderson et al., 1973a; Blank, 1952; El-Shimi and Princen, 1978; Scheuplein and Morgan, 1967) and mathematical models for water sorption and transport in skin have been proposed periodically to tie together the many observations (Blank et al., 1984; El-Shimi and Princen, 1978; Kasting and Barai, 2003; Kasting et al., 2003; Liron et al., 1994; Pirot et al., 1998; Stockdale, 1978; Wang et al., 2006, 2007). Notably, the SC microtransport model developed by one of the investigators with collaborators in Buffalo (Wang et al., 2006, 2007) explicitly employs water content as a factor in the microstructure and permeability of the tissue. Yet this computational model is restricted to two static SC hydration states – partially hydrated (30% w/w) and fully hydrated (78% w/w). This restriction does not allow a realistic simulation of the transient swelling and subsequent dehydration of skin exposed transiently to an aqueous-based substance, such as a skin cream or urine under a diaper. The present development is aimed at removing this restriction. The model is constructed at the macrotransport level, with geometrical limits imposed by the static microscopic model and transport parameters fitted to experimental data.

2. Model development

2.1. Swelling model with moving boundary

The water transport swelling model is a one-dimensional, one-layer, homogeneous model, incorporating water transport across a membrane (the SC) with respect to both boundaries. The membrane will swell when the water influx exceeds the efflux. Conversely, the membrane will shrink when the efflux exceeds the influx. Water may enter or leave the SC from both the lower skin layers and the upper external environment. A schematic diagram is shown in Fig. 1.

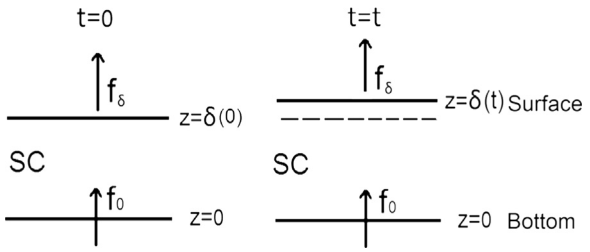

Fig. 1. Diagram of one-layer skin swelling model. The symbols of f_0 and f_δ represent combined water flux (the sum of diffusive and convective components) at the lower and upper boundaries of the SC membrane.

The model specifies a fixed lower boundary ($z=0$) and a moving upper boundary ($z=\delta(t)$). The thickness, δ, changes with time. With the assumption that the water partial molar volume in the SC is equal to the pure water molar volume, the rate of change of δ is:

$$\frac{d\delta}{dt} = \frac{f_0 - f_\delta}{\rho_w} \tag{1}$$

where f_0 and f_δ are combined water fluxes (g/cm^2 s) and ρ_w is the pure water density, 1.0 g/cm^3. The general water mass transport equation in the membrane is (Bird et al., 2007):

$$\frac{\partial C_w}{\partial t} = -\frac{\partial (vC_w)}{\partial z} - \frac{\partial j_w}{\partial z} \tag{2}$$

In Eq. (2), C_w is water concentration in g/cm^3, v is the convective velocity in cm/s, and j_w is the diffusive (or molecular) flux in g/cm^2 s. The quantity vC_w is the convective flux. Here v is defined as the volume-averaged velocity, thus j_w should be expressed as (Bird et al., 2007):

$$j_w = C_w(v_w - v) = f - C_w v = -D\frac{\partial C_w}{\partial z} \tag{3}$$

where v_w is the water velocity in cm/s, f is combined water flux at depth z in g/cm^2 s and D is observed diffusivity at depth z in cm^2/s.

Water flux at the fixed lower boundary, f_0, causes the convective velocity, v, which may vary with time, but is independent of depth since we assume that the water partial molar volume in the SC is equal to the pure water molar volume. Thus v is equivalent to the velocity at $z=0$,

$$v = \frac{f_0}{\rho_w} \tag{4}$$

Eq. (1) may then be transformed to yield:

$$\frac{\partial C_w}{\partial t} = -v\frac{\partial C_w}{\partial z} + \frac{\partial}{\partial z}\left(D\frac{\partial C_w}{\partial z}\right) \tag{5}$$

The boundary conditions are:

$$f_0 = -D\frac{\partial C_{w0}}{\partial z} + C_{w0}\frac{f_0}{\rho_w}\text{at } z = 0 \tag{6}$$

$$f_\delta = -D\frac{\partial C_{w\delta}}{\partial z} + C_{w\delta}\frac{f_\delta}{\rho_w}\text{at } z = \delta(t) \tag{7}$$

Note: (1) two additional boundary conditions should be provided based on the specific membrane environment in order to solve the partial differential equation, Eq. (5); and (2) the boundary conditions of Eqs. (6) and (7) have the same mathematical form, but different physical meanings. At the fixed boundary $z=0$,