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The impact of various drying kinetics models on the prediction of sample temperature–time and moisture content–time profiles during moisture removal from stratum corneum

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ABSTRACT

An attempt has been made here to model the moisture transport kinetics across porcine stratum corneum. Samples of porcine skin were dissected in the form of 'thin layers' (i.e. stratum corneum) of dimensions of 11.3 × 11.3 mm (70–200 μm thick). These layers were dried in a laboratory convection air dryer at 37 °C (normal human body temperature). The changes in weights of the samples were noted. The weight loss data was then converted in terms of moisture content (dry basis) and were monitored over time. Thereafter they were fitted against an empirical equation notably the Page model (Model 1) and the solution generated by the Fickian diffusion equation (Model 2). The current paper demonstrates the effectiveness of these two models in prediction of the sample temperature during drying. Furthermore, it also demonstrates the variation in spatial distribution of moisture content within the skin sample when moisture content and temperature dependency are introduced in the diffusivity. Such findings are important especially when developing skin multi-compartment physiologically based pharmacokinetic (PBPK) models to assess transdermal permeation of various hydrophilic penetrants.

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Keywords: Drying; Thin layer; Biomaterial; Effective liquid diffusivity; Optimisation; Porcine skin; Stratum corneum

1. Introduction

It has been demonstrated in the past that hydration of stratum corneum has an effect on the permeability of hydrophilic permeants through skin in transdermal drug delivery applications (Scheuplein, 1965; Michaels et al., 1975; Blank et al., 1984; Potts and Francoeur, 1991; Liron et al., 1994). It is therefore essential to have proper mathematical models that can accurately predict the moisture content at any position within the stratum corneum and skin as a whole. Such models would become the stepping stone to the development of more user-friendly skin multi-compartment physiologically based pharmacokinetic (PBPK) models. These models can then be used to assess transdermal permeability of various drugs and toxins.

Past studies conducted in this area mostly relied on studying the process of moisture absorption (Stockdale, 1978; Blank et al., 1984; Potts and Francoeur, 1991). These studies were mostly experimental. The primary purpose of these studies was to evaluate the moisture diffusivity. The common feature in all these investigations was that they were all carried out at steady state. The time scale of such a process can be very large (up to several days) (Blank et al., 1984). Therefore, such results are not of much significance especially for pharmacokinetic studies of hydrophilic drugs and transdermal toxicological assessment studies. Liron et al. (1994) recognised this problem and carried out unsteady

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Nomenclature

A	surface area (m^2)
A_2	constant used in latent heat evaluation
a_w	surface water activity
B	Page model constant
B_1	constant used in Eq. (A38)
C	Page model constant
C_1	constant used in equation (A38)
c	GAB equation constant
c_p	specific heat capacity ($J\,kg^{-1}\,K^{-1}$)
c_s	total solids concentration ($kg\,Solids/m^3$)
D_{aw}	diffusivity of water vapour in air ($m^2\,s^{-1}$)
$D_{l,eff}$	effective liquid diffusivity ($m^2\,s^{-1}$)
D_0	moisture content-dependent diffusivity ($m^2\,s^{-1}$)
D_{01}	apparent diffusion coefficient ($m^2\,s^{-1}$)
E_A	activation energy ($J\,mol^{-1}$)
$\dot{E}_v$	evaporation rate ($kg\,s^{-1}$)
F_1	absolute error (water content)
F_2	absolute error (temperature)
h_b	bottom face heat transfer coefficient ($W\,m^{-2}\,K^{-1}$)
h_m	mass transfer coefficient ($m\,s^{-1}$)
h_u	upper face heat transfer coefficient ($W\,m^{-2}\,K^{-1}$)
k	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
K	GAB equation constant
L	characteristic length (m)
Le	Lewis number $\left(\frac{\alpha_{mix}}{D_{aw}}\right)$
m_s	mass of dry solids (kg)
m_0	GAB monolayer water content ($kg\,H_2O/kg\,solids$)
N	number of observations in sampling space
Nu	Nusselt number (h_uL/k_{mix})
n	Lewis number exponent
P	number of fitting parameters used
Pr	Prandtl number ($\mu_{mix}c_{p,mix}/k_{mix}$)
p^{sat}	saturated vapour pressure (Pa)
R	universal gas constant ($J\,mol^{-1}\,K^{-1}$)
Re	Reynolds number ($\rho_{mix}v_{air}L/\mu_{mix}$)
RH	relative humidity
Sc	Schmidt number ($\mu_{mix}/\rho_{mix}D_{aw}$)
Sh	Sherwood number (h_mL/D_{aw})
T	temperature (°C, K)
t	time (s)
U	overall heat transfer coefficient ($W\,m^{-2}\,K^{-1}$)
u	power index used in latent heat evaluation
v_{air}	velocity of dry air ($m\,s^{-1}$)
V	volume (m^3)
w	weight fraction
x	length (m)
X	water content ($kg\,H_2O/kg\,solids$)
$\bar{X}$	spatial average water content ($kg\,H_2O/kg\,solids$)
X_∞	equilibrium water content ($kg\,H_2O/kg\,solids$)
X^V	volume fraction
z	exponential factor used in water content dependency function for effective liquid diffusivity

Greek letters

α	thermal diffusivity ($m^2\,s^{-1}$)
δ	thickness of skin sample (m)
δ_{dry}	thickness of bone dry skin sample (m)
ε	porosity of skin sample
λ_l	latent heat of vaporization ($J\,kg^{-1}$)
μ	viscosity (Pa s)
ρ	density ($kg\,m^{-3}$)

Subscripts

air	air
al	aluminium
cb	cardboard
exp	experimental
f	final condition
fat	fat
fibre	fibre
i	ith component
mix	air water vapour mixture
paper	paper
plastic	plastic
protein	protein
s	interfacial condition
sample	skin/paper sample
skin	skin
solids	dry solids
v	vapour
w	water
water	water
∞	dry gas phase
0	initial condition

state vapour sorption/desorption studies on porcine skin samples. Based on the mass gained/lost by the samples, the effective liquid diffusivity of moisture was estimated using Crank's analytical solution to diffusion equation (Crank, 1976). In all these studies the effective moisture diffusivity was considered to be a function of the skin moisture content.

The above attempts made for studying moisture transport across skin/stratum corneum had neglected the influence of temperature (ambient and skin sample) on moisture diffusivity. However, as will be shown later, temperature does play an important role, especially when predicting moisture content at any spatial location within the skin sample. This issue was later addressed by Kasting et al. (2003) when they attempted to correlate effective moisture diffusivity as a function of moisture content and temperature. The temperature dependency function was represented in the form of an Arrhenius relationship. The moisture content dependency on the other hand was dependent on the local water activity within the skin sample at any spatial location and certain micro-structural parameters such as pore radius within the skin sample and radius of water molecule.

While the approach of Kasting et al. (2003) did take into account the effect of temperature on effective moisture diffusivity, it did encounter problems, especially when the skin samples are completely saturated (occluded) with moisture (at saturation, $a_w = RH = 1$). In such cases the diffusive flux would be completely absent. Kasting et al. (2003) did not encounter this problem as none of their case studies involved the use of saturated stratum corneum samples.

In the present study, the effect of both skin temperature and skin moisture content on moisture transport across

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