Macro-scale Mathematical Model for Hydration and TEWL in intact Stratum Corneum

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The Plan

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Introduction

Skin properties are mostly the realm of the biosciences. However, some skin properties are accessible to physical modelling:-

Hydration
Sorption/desorption
Swelling
Transepidermal water loss
Skin stripping

Our aim is a better understanding of measurements such as TEWL and hydration.

Our approach is macro-scale modelling, where water binding effects and the *brick & mortar* structure of the stratum corneum (SC) etc are all subsumed into an effective diffusion coefficient D_{sc} that may change with SC hydration.

Method

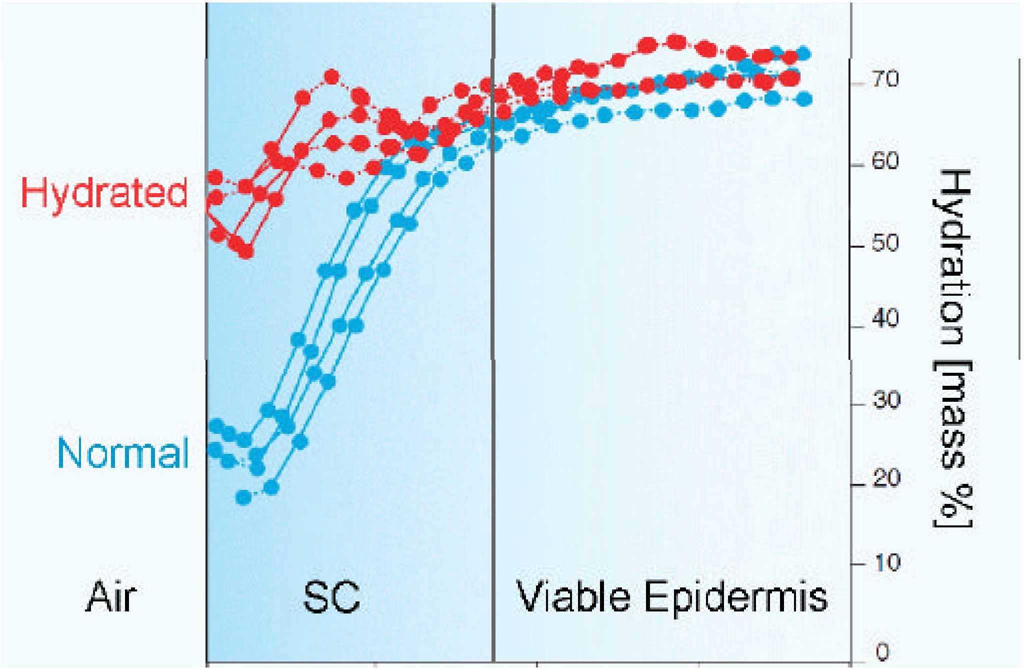
The method used is to calculate the steady-state flux of water diffusing from the viable epidermis, through the SC, into the ambient air. The following components are included in the model:-

1. Skin hydration profile
2. Water vapour transport in the adjacent air
3. Adsorption/desorption at the skin surface
4. SC swelling

In steady-state conditions, there is no skin surface water loss (SSWL) and the TEWL flux through the SC is equal to the water vapour flux in the adjacent air. This *conservation of flux* is one constraint used in the calculations. Another constraint is the relationship between SC surface hydration and the relative humidity (RH) of the adjacent air, which is determined by the *sorption isotherm*.

Component 1: Skin Hydration Profile

Steady-state hydration depth profiles measured using confocal Raman spectroscopy give information about water mobility in the SC and viable epidermis. Shown here are example profiles measured on untreated volar forearm skin in-vivo.



Hydration depth profiles relate to TEWL via **Fick's first law** of diffusion. The slope at any point is inversely proportional to the diffusion coefficient, $\boldsymbol{D_{SC}}$.

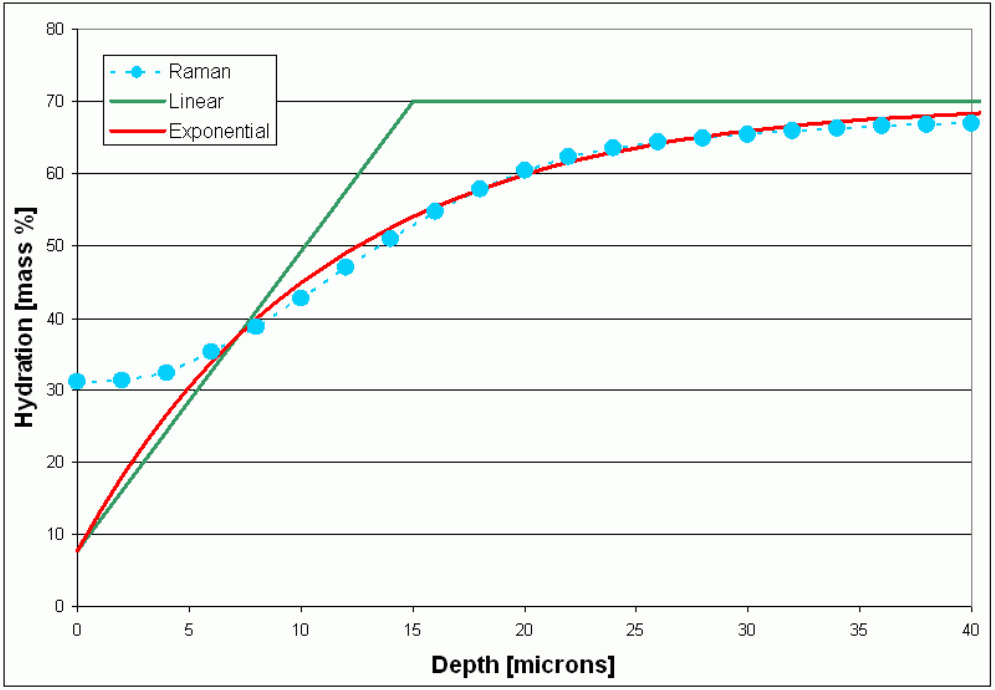
$$D_{SC} = \frac{-J}{dc/dz}$$

Figure adapted from:-

Gabard, B and Barel, AO: *Dynamique de l'hydratation cutanée*. In: Cosmétology et dermatologie esthétique, Elsevier Masson SAS, Paris (2008).

Hydration Depth Profile Representations

Two hydration depth profile representations are used in this work:-



1. A **linear profile** (ie constant D_{SC}).

2. An **exponential profile**

$$c(z) = c_{\max} - \Delta c \cdot \exp\left(\frac{-z}{z_0}\right)$$

for which

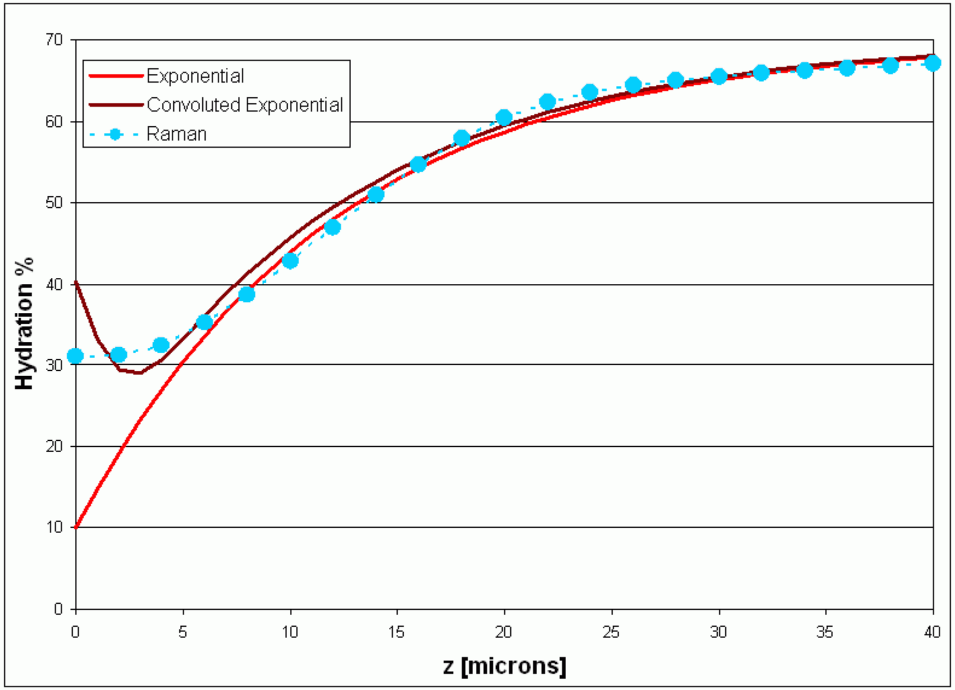
$$D_{SC}(c) = \frac{k}{(c_{\max} - c)}$$

These profiles are compared with a confocal Raman profile in the above figure. The deviation near the SC surface is attributable to the finite spacial resolution of the confocal optics, see next.

Raman data provided by River Diagnostics BV, Rotterdam, The Netherlands.

Spacial Resolution Effect

The spacial resolution of the confocal Raman optics can be represented by a Gaussian resolution function with a FWHM ~4.8 microns. This causes the true hydration profile to be distorted.



A comparable distortion can be simulated with the exponential hydration profile by convoluting it with the same resolution function. This comparison shows that the exponential profile is a reasonable representation of an in-vivo volar forearm hydration profile.

Raman data provided by River Diagnostics BV, Rotterdam, The Netherlands

Component 2: Air

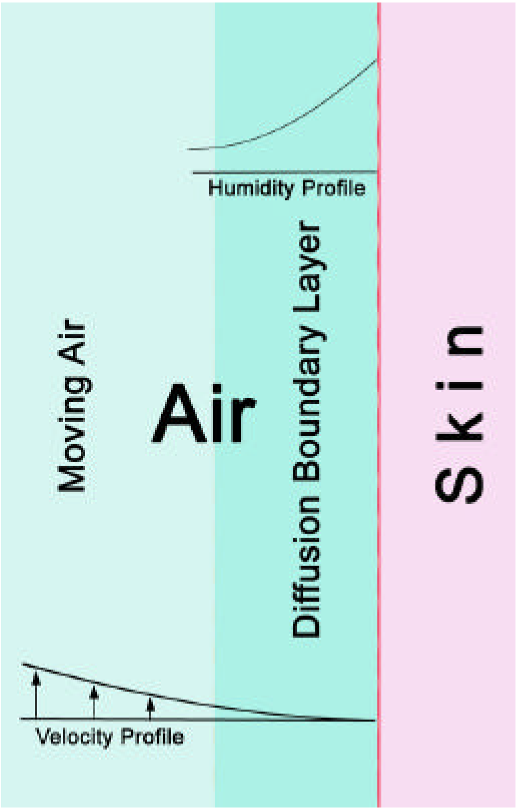
The model assumes that water from TEWL evaporates from the SC surface into the adjacent air. According to fluid dynamics theory, the air immediately adjacent to the SC surface is still, irrespective of air movements further away. This is the **diffusion boundary layer** of still air. The moving air beyond acts as a vapour sink of constant (ambient) humidity and temperature.

The thickness of the diffusion boundary layer depends on the geometry of the object and the properties of the moving air. For a horizontal volar forarm, for example:-

~5mm: Normal (uncovered) conditions indoors.

~12mm: Very still air (only natural convection).

~24mm: Open TEWL measurement chamber.



Relative Humidity at the SC surface

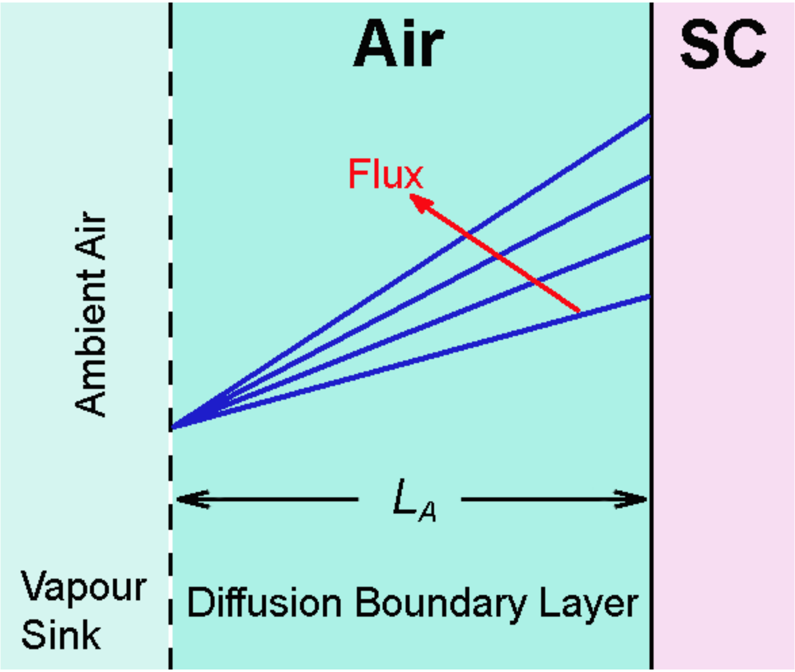
The relative humidity (RH) at the SC surface depends on:-

1. Ambient RH.

2. The flux of water vapour (TEWL).

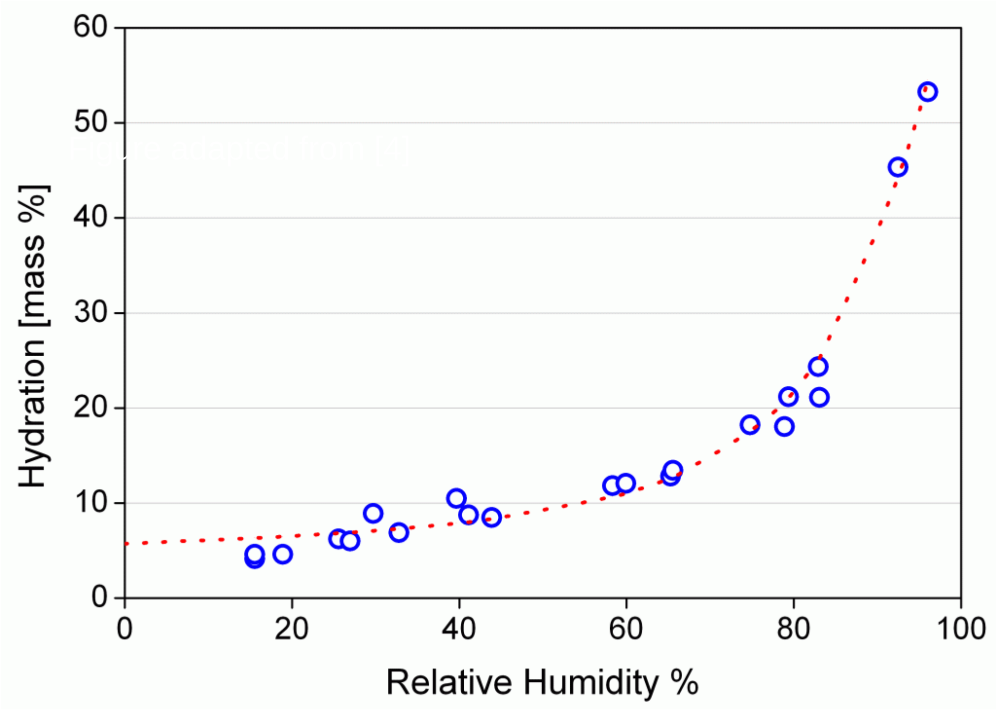
3. The temperature of the SC surface.

The model assumes that the SC & the air in contact with it are at the same temperature, typically 30°C.



Component 3: SC Surface adsorption/desorption

The connection between the skin & the adjacent air is the **sorption isotherm**.



Adsorption & desorption processes at the SC surface maintain a balance between the **hydration** of the SC surface and the RH of the adjacent air.

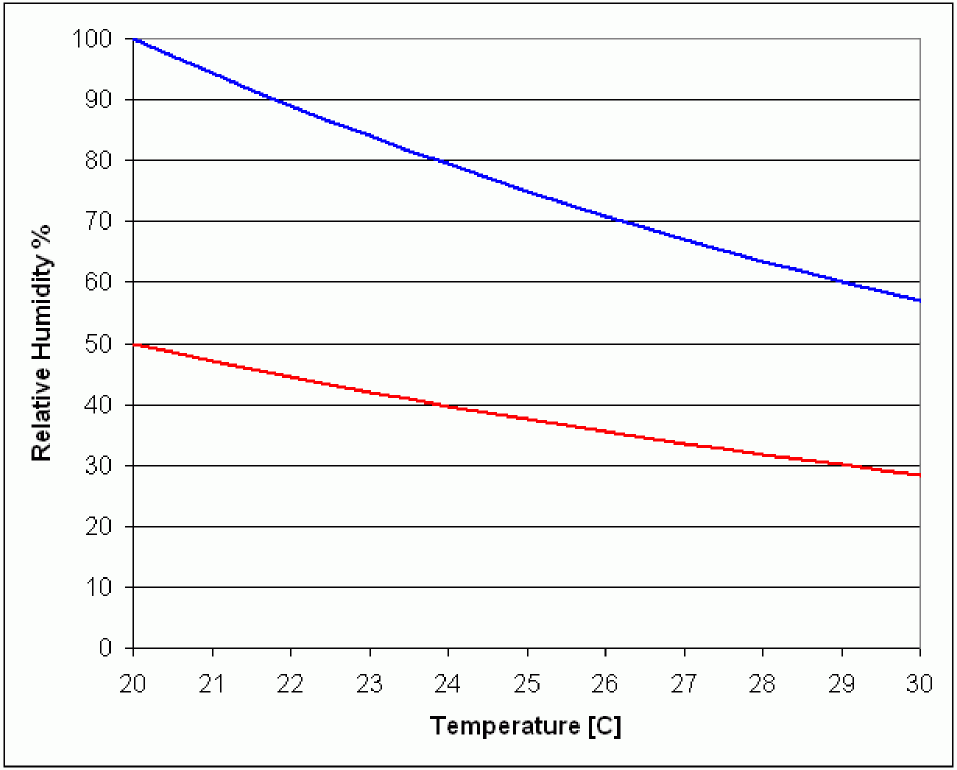
The SC surface adapts rapidly to RH changes, because only its top layer is exposed to air.

The bulk of the SC takes longer to adapt, because of the low mobility of water within the SC.

Figure adapted from:-

Lévêque, J-L: *Water-keratin interactions*. In: Bioengineering of the skin: Water and the stratum corneum. (Elsner, P, Berardesca, E, Maibach, HI, eds), pp. 13-22. CRC Press, Boca Raton (1994).

Relative Humidity at the SC Surface



The RH at the SC surface is substantially lower than ambient RH, because the SC surface is at a higher temperature than the ambient air. In the above figure, The SC (and the air in immediate contact with it) is at 30°C whereas the ambient air is at 20°C.

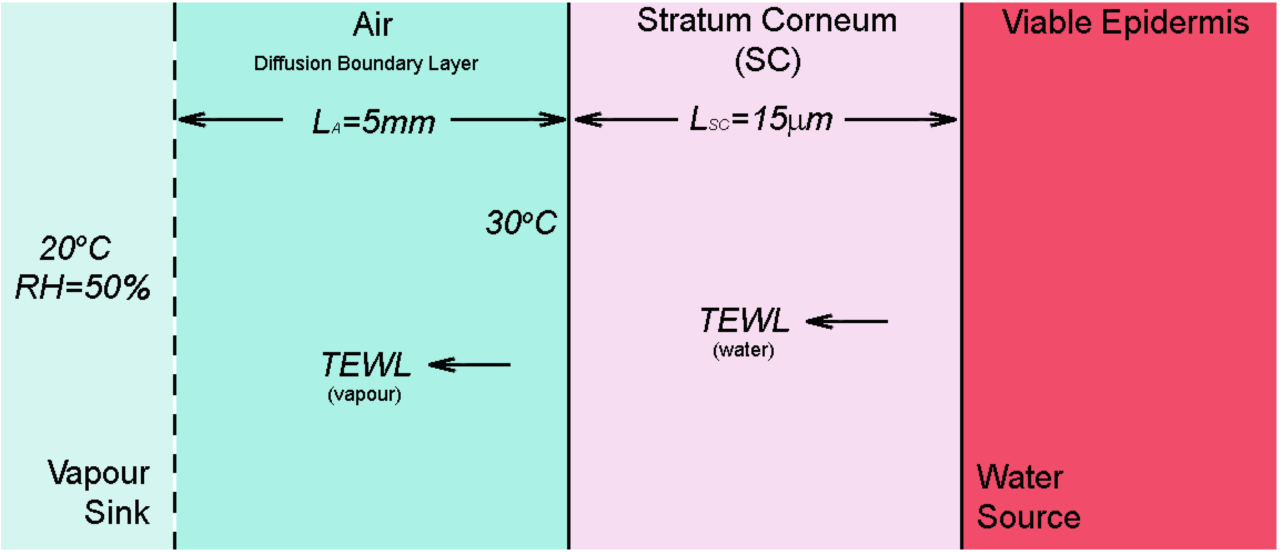
Component 4: SC Swelling

SC swelling is assumed to be isotropic and additive, where the volume of hydrated SC is given by the sum of the volumes of dry SC and water of hydration. With this assumption,

$$\frac{\Delta L}{L_{DRY}} = \frac{c}{3(r_W - c)}$$

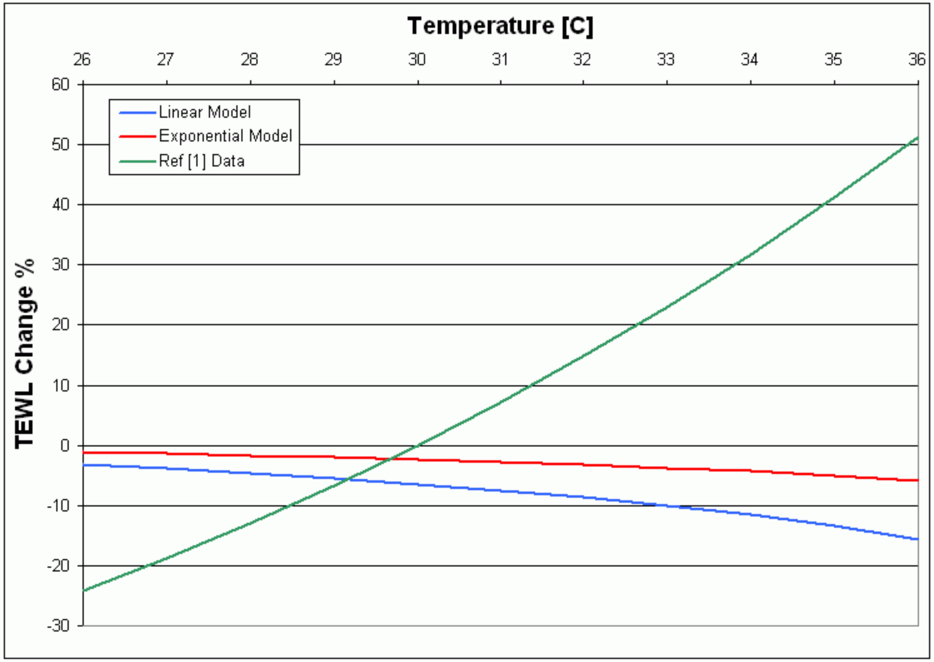
where ***?L*** is the hydration-dependent swelling, L_{DRY} is the thickness of dry SC, $?_W$ is the density of water and ***c*** is the concentration of water in the SC. Unidirectional swelling (in thickness only) would be three times larger.

Example Calculations



This diagram represents the model, together with some of the values used in the calculations that follow. These were performed using the Excel 2003 spreadsheet and its VBA (Visual Basic for Applications) feature. Properties were calculated layer by layer, dividing the SC into 1000 layers. A typical diffusion coefficient was found to be 0.15% smaller with 500 layers and 0.07% larger with 2000 layers.

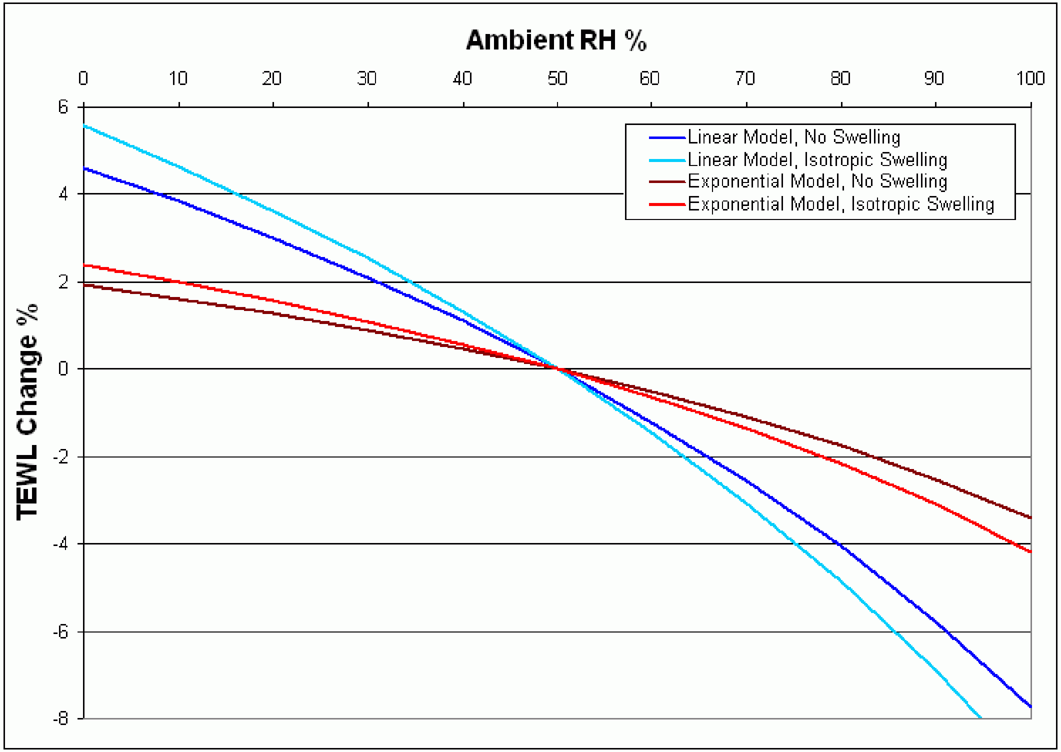
Calculation 1: Baseline TEWL vs SC Surface Temperature



The change of TEWL with temperature is smaller and in the opposite sense to the measurements of [1]. This is because the model parameters are currently independent of temperature. The small TEWL decrease is caused by a decrease of RH of the air in contact with the SC. A coupled thermal model is needed to calculate such temperature dependences. This is under development.

[1] Halkier-Sorensen, L, Thestrup-Pedersen, K and Maibach, HI: *Equation for conversion of transepidermal water loss (TEWL) to a common reference temperature: what is the slope?* Contact Dermatitis. **29**: 280-1 (1993).

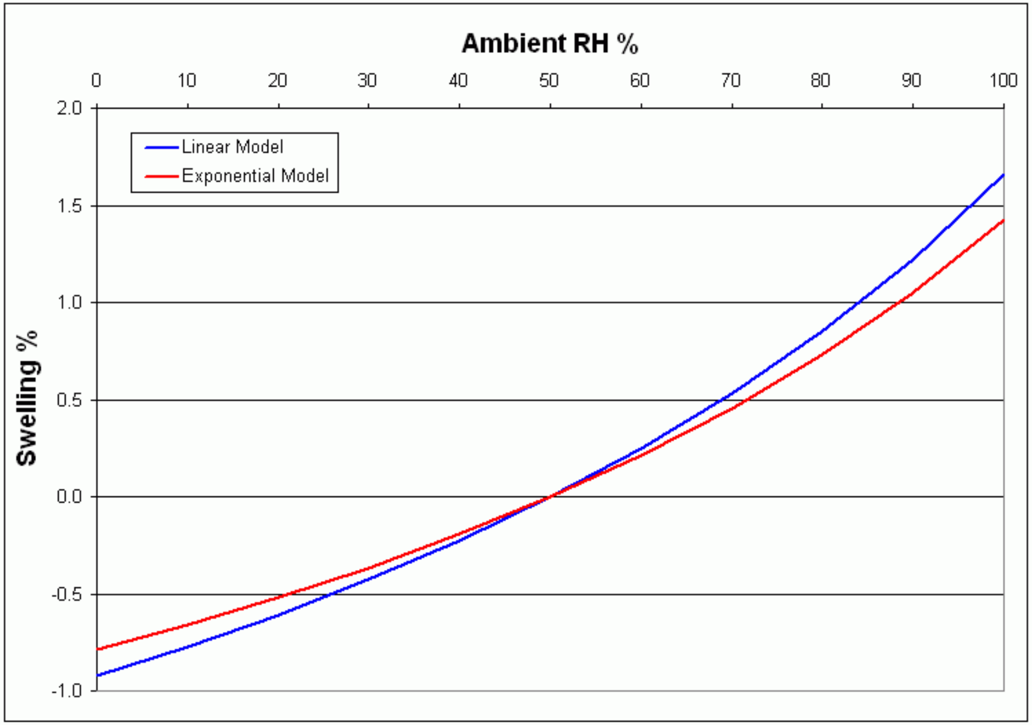
Calculation 2: Baseline TEWL vs Ambient RH



The calculated trend of increasing TEWL with decreasing ambient RH is contradicted by the experimental evidence of [1], for example. This is a well known problem with models using a constant diffusion coefficient. The inclusion of a hydration-dependent diffusion coefficient in the exponential model goes some way towards solving this problem, but currently not far enough.

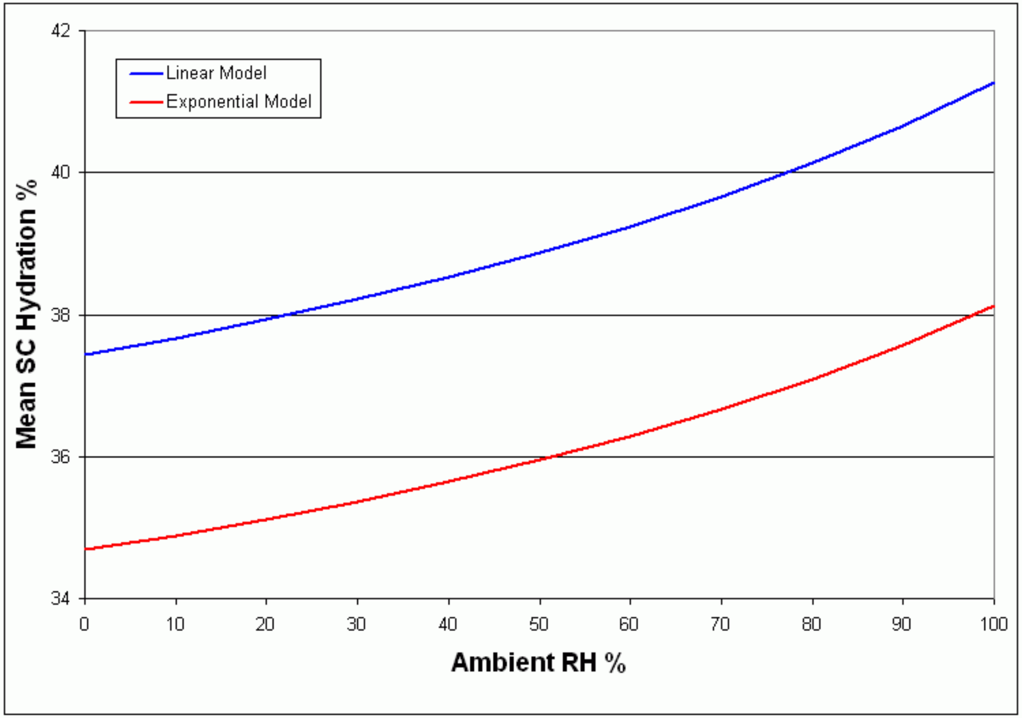
[1] Egawa, M, Oguri, M, Kuwahara, T and Takahashi, M: *Effect of exposure of human skin to a dry environment*. Skin Res Tech. **8**: 212-8 (2002).

Calculation 3: Swelling vs Ambient RH



The calculated thickness change with ambient RH looks plausible. Note that the swelling depends on the RH at the SC surface, which is lower than ambient RH. Comparisons with experiment should be used to improve the swelling model.

Calculation 4: Mean Hydration vs Ambient RH



The calculated dependence of mean hydration on ambient RH looks plausible.

Conclusions

The model needs to be developed further:-

1. Improve the hydration profile representation (TEWL vs RH)
2. Include temperature effects (TEWL vs T).
3. Extend to tape stripping (SC thickness measurement).
4. Extend to non-steady-state conditions (recovery from perturbations).