**Introduction**

Water within stratum corneum (SC) plays a key role for stratum corneum’s barrier function as well as its cosmetic properties [1-3]. Stratum corneum is dry outside and wet inside and there must exist a water concentration gradient. This water concentration gradient will cause water to diffuse from deeper part of stratum corneum toward stratum corneum surface, and forms the trans-epidermal water loss (TEWL). TEWL is an important index for time-serial drug delivery studies and there are many factors that might affect the TEWL. The purpose of this study is to simulate three dimensional dynamic water diffusion processes through in-vivo human stratum corneum based on brick-and-mortar [1,2,4] model using finite element methods, and to study the factors that might influence TEWL.

**Methodology**

The three-dimensional water diffusion through in-vivo stratum corneum can be described by following diffusion equation:

\[
\frac{\partial H}{\partial t} = D \nabla^2 H + J
\]

Where \(x\) and \(y\) are the lateral axes that are within the SC surface, \(z\) is the vertical axis that is going from the SC surface (\(z=0\)) to the bottom of the SC (\(z=L\)), \(L\) is the SC thickness, \(H(x,y,z)\) is the SC hydration, \(D\) is its water diffusion coefficient, \(J\) is just outside the corneocyte, and \(0\) is just inside the corneocyte. Based on this description, a 3D brick-and-mortar model was built to simulate in-vivo human stratum corneum in order to have a better understanding on the effects of corneocyte size, stratum corneum thickness, external conditions and non-homogeneous diffusion coefficients on TEWL, see Figure 1. In this model, stratum corneum has two external boundaries: SC-air boundary and SC-epidermis boundary, it also has one internal boundary, corneocytes and lipids boundary. We set the initial conditions and boundary conditions, use literatures for water diffusion coefficients of corneocytes and lipids (i.e. Weak and months), and use finite element methods to simulate the dynamic water diffusion processes over a period of time within stratum corneum. Following values are used in the simulation:

- Corneocyte size (12x12x12 µm³), SC thickness L=100µm
- \(D_{\text{corneocyte}}=10^{-13} m^2/s\)
- \(D_{\text{lipids}}=10^{-13} m^2/s\)
- \(H_{\text{corneocyte}}=100\%\) or \(44.44\ mol/m^3\)
- \(H_{\text{lipids}}=30\%\) or \(16.67\ mol/m^3\)

**Results and Discussion**

Figure 2 shows the 3D water dynamic distribution within SC at different times. In the beginning, water concentration is much higher in lipids, due to the relatively high diffusion coefficients of lipids, but as time goes on, the difference between water concentration distributions and corresponding water flux distributions at different times. The results show that the water concentration distribution within corneocytes and lipids tends to become linear as time goes on, and the difference between water flux within corneocytes and lipids is also getting smaller.

![Figure 2. Water concentration distributions within stratum corneum at time 0, 100, 200, 500, 1000 and 1600 seconds.](image)

**Conclusions**

Finite element simulation is a powerful tool for studying dynamic water diffusion processes within a sample with complicated geometry, like 3D stratum corneum. For water diffusing through SC, both transcellular routes and intercellular route are important; however, the majority amount of water still diffuses through transcellular routes due to the high corneocyte to lipids cross area ratio. The results show that water diffusion flux, i.e. TEWL, is inversely proportional to corneocyte size, i.e. the smaller the corneocyte size, the higher the TEWL. The results also show that the SC model with smaller corneocytes has a quicker diffusion process.

**Acknowledgement**

We thank Drs. J Cycle, JID, 124, 1099-1110, (2005).

**References**


