2D Modelling of subcellular molecular transfer in skin

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**BACKGROUND**

- Mathematical models of skin permeation are essential to fields as diverse as skin care, transdermal drug delivery, exposure to hazards assessment and toxicity assessment.
- The research and studies regarding skin (mathematical) modelling emerged in the past decades and many different approaches have been proposed.
- The main deficiency in these approaches is that they neglect many important aspects and effects such as the follicular pathway and the structural details of the epidermal layer.

**AIM**

Develop a 2D multiscale model of molecular transfer in skin including the follicular pathway.

**OBJECTIVES**

- To develop a 2D model that integrates the physiochemical attributes and structural details of the three different skin layers and the hair follicle.
- To test and validate the model against experimental data.
- To deliver a user-friendly computational tool to be evaluated by end-users.

**METHODOLOGY - PROGRESS**

- The first part of the model assembled is the stratum corneum (SC).
- SC is represented as a heterogeneous material with the widely accepted “brick and mortar” structure.
- Corneocytes (bricks) are filled with keratin and water surrounded by an intercellular lipid matrix (mortar).
- The model requires the molecular weight (MW) and octanol-water partition coefficient (Kow) of the chemical to be tested in order to produce results.
- The mass transfer properties of solutes in both the lipid matrix and the corneocytes are directly calculated from fundamental physical and chemical properties [1].

For the calculation of the concentration of the applied chemical a mass balance calculation took place. The governing equation for the interfacial mass transfer between two neighbouring grids A and B is:

\[
\frac{dC_a}{dt} = \frac{1}{\rho_a \eta_a} \left( \frac{A_b C_b}{\Delta x} - \frac{A_a C_a}{\Delta x} \right)
\]

**PRELIMINARY RESULTS**

- The images below represent the SC structure at different times after the application of 4-cyanophenol (4-CP).
- The concentration at the application layer is constant at 0.11 mol/L (infinite source).

Model prediction (lines) compared with in vivo tape striping data of 4-CP permeation into the forearm of a healthy volunteer after exposure times of 1 (x), 5 (o) and 15 (•) minutes. In vivo data obtained from Stinchcomb et al. [2]

**CONCLUSIONS**

- A precise model of transdermal permeation of SC has been developed.
- The model has been proved accurate compared to other published models and experimental data.
- The framework for the next updated version of this model has been set.

**REFERENCES**