Development and Initial Results from the Inclusion of Evaporation into a 2D dermal absorption model

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1. Introduction

In experimental scenarios, diffusion into the skin is affected by skin and chemical properties; however, in real life scenarios the vehicles' ability to deliver the active into the skin is impacted by the environment. As such evaporation of the vehicle will occur. Where evaporation will depend on the molecular weight, boiling point, vapour pressure and solubility of the solute and the temperature.

The main aim is to develop an evaporation code which will be integrated into the Surrey model to improve the finite dose application.

2. Evaporation

We simulate evaporation of up to three ingredients under ideal and non-ideal conditions. Non-ideal evaporation allows ingredients in the vehicle to interact and this impacts evaporation.

The main equations for evaporation of the active ingredients are given below, including calculation of diffusion coefficient and Fick's law of diffusion:

$$D_{Active} = \frac{Boltzmann\ Constant * T}{6\pi\eta r}$$

$$Conc_{Active} = P_{active} \times \frac{Mole\ Fraction\ Active}{Rg \times T}$$

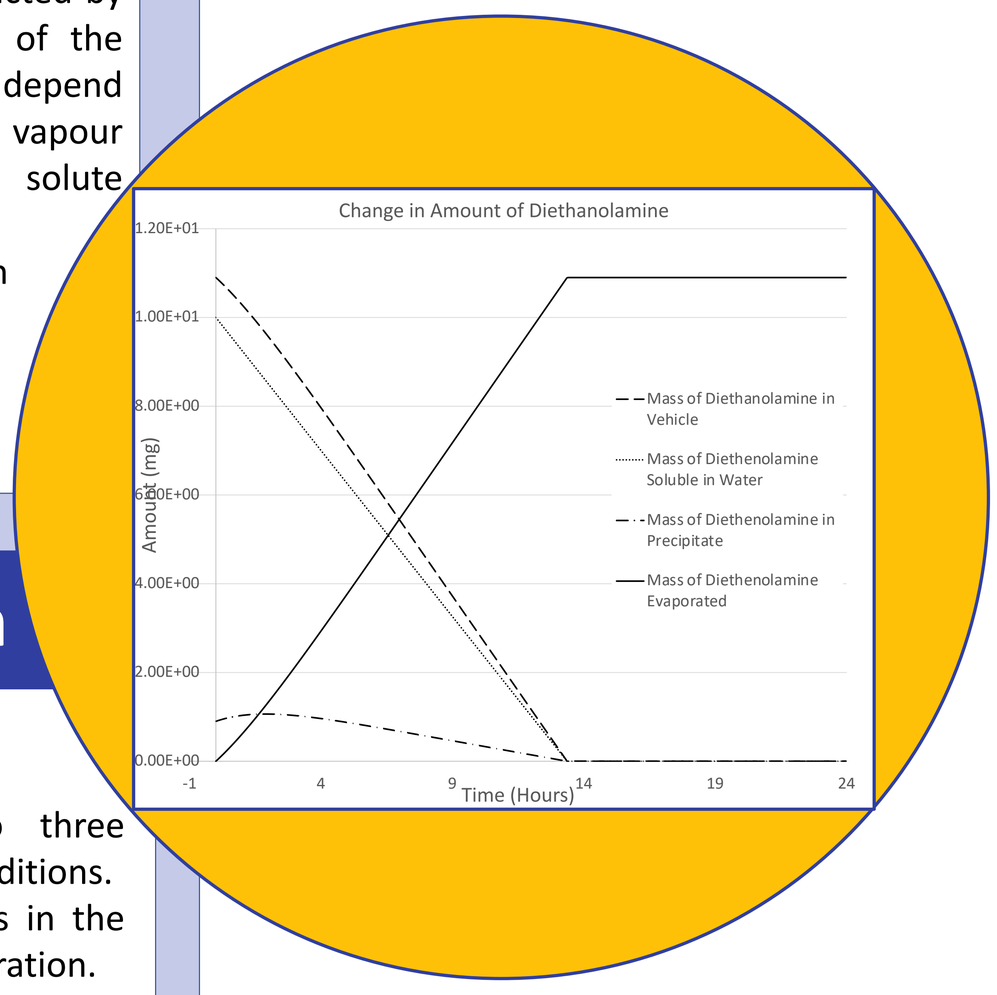
$$J_{Active} = D_{active} \times \frac{Conc - 0}{h}$$

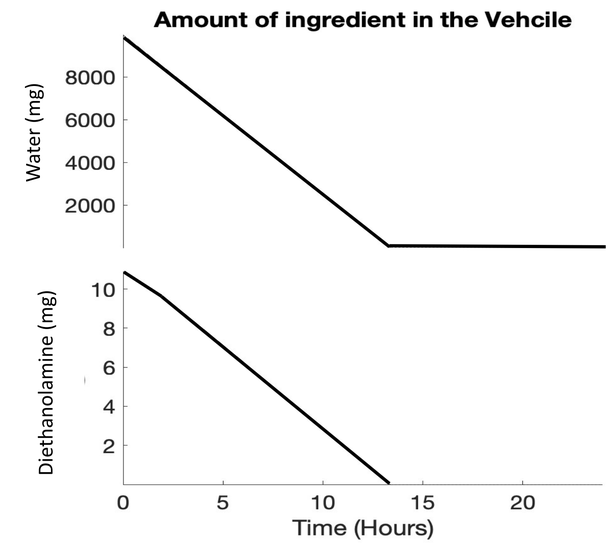
$$\frac{dy}{dt}_{active} = -J_{active} \times A$$

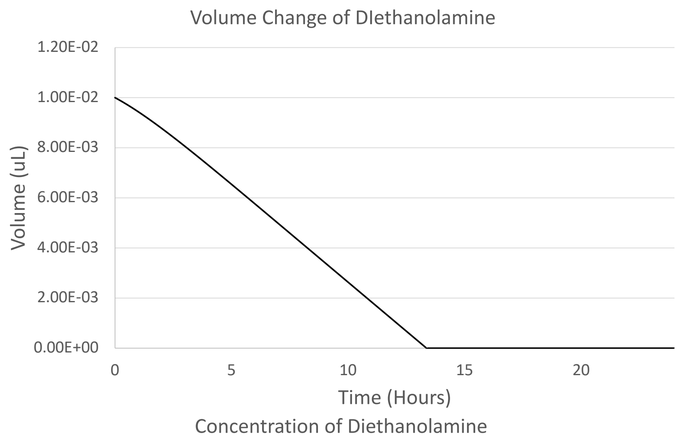
The choice of chemicals and the experimental conditions (skin thickness and dosage) have been informed from Hewitt et al., 2020. This poster has shown evaporation for Water: Diethanolamine (MW 105, Solubility 100 g/100ml, Vapour Pressure 0.03 Pa).

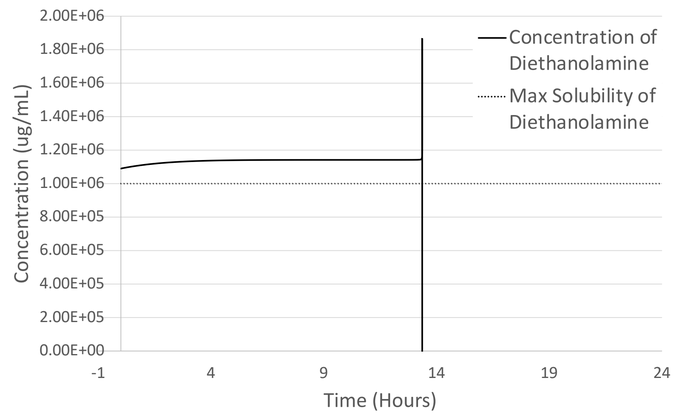
3. Model Results

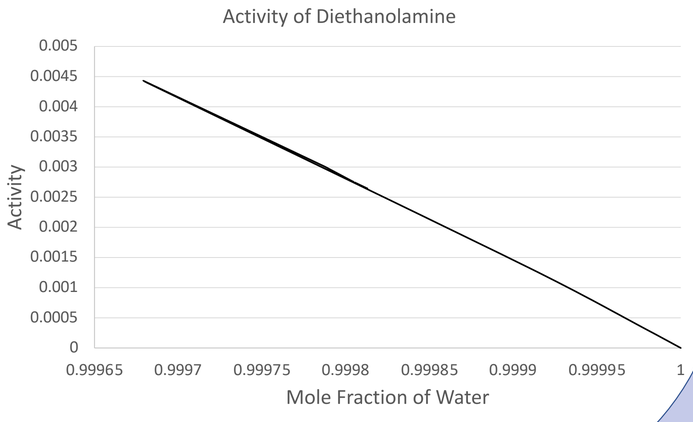
The results shown below have considered a two ingredients vehicle of Water: Diethanolamine at a starting dose of 10.6 ug/L. This dosage is inline with Hewitt et al, 2020. All simulations here have been performed at 32 °c for 24 hours.











This model makes the following assumptions:

- Condensation has not been considered.
- Wind has not been considered
- There are no traces of the active present in the atmosphere at t = 0.
- The simulation occurs at standard pressure.

4. Conclusion

Main conclusions:

- The model simulated evaporation time course
- The model can be applied to a wide range of chemicals
- Needs further validation with experimental data

Future work includes:

- Further application of the model
- Experimental work for validation of the model

References

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