Dermal Absorption

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SAMBa ITT5

Outline

The problem: a recap

Approach 1: compartment-based modelling

Approach 2: a random walk

The future

The problem: a recap

The problem

MAIN QUESTION: How do co-formulants change the absorption of the active ingredient (AI) through the skin?

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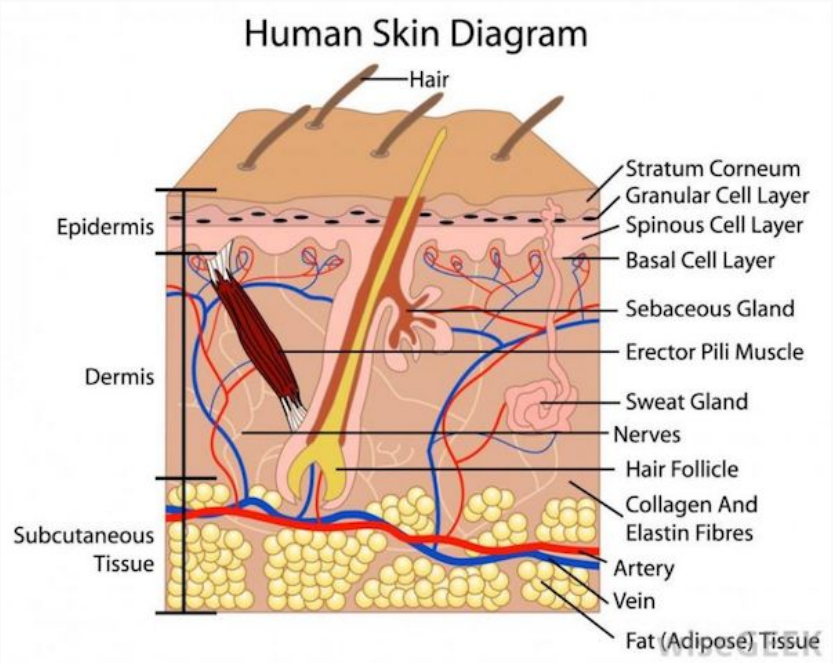
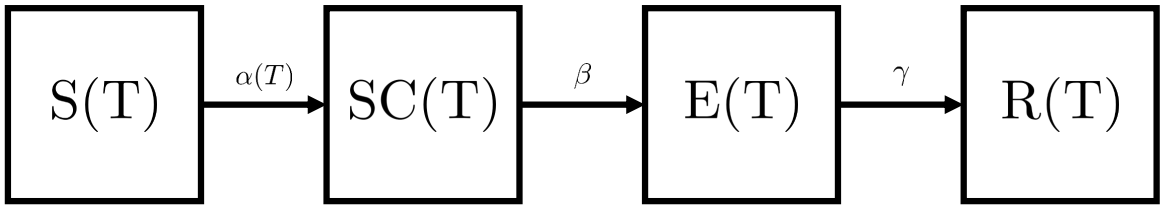


Why is this important?

- AI is generally toxic to humans.
- Don't want the co-formulant to increase the rate of absorption into the blood stream.
- If co-formulant reduces the rate, this would be desirable.

Approach 1: compartment-based modelling

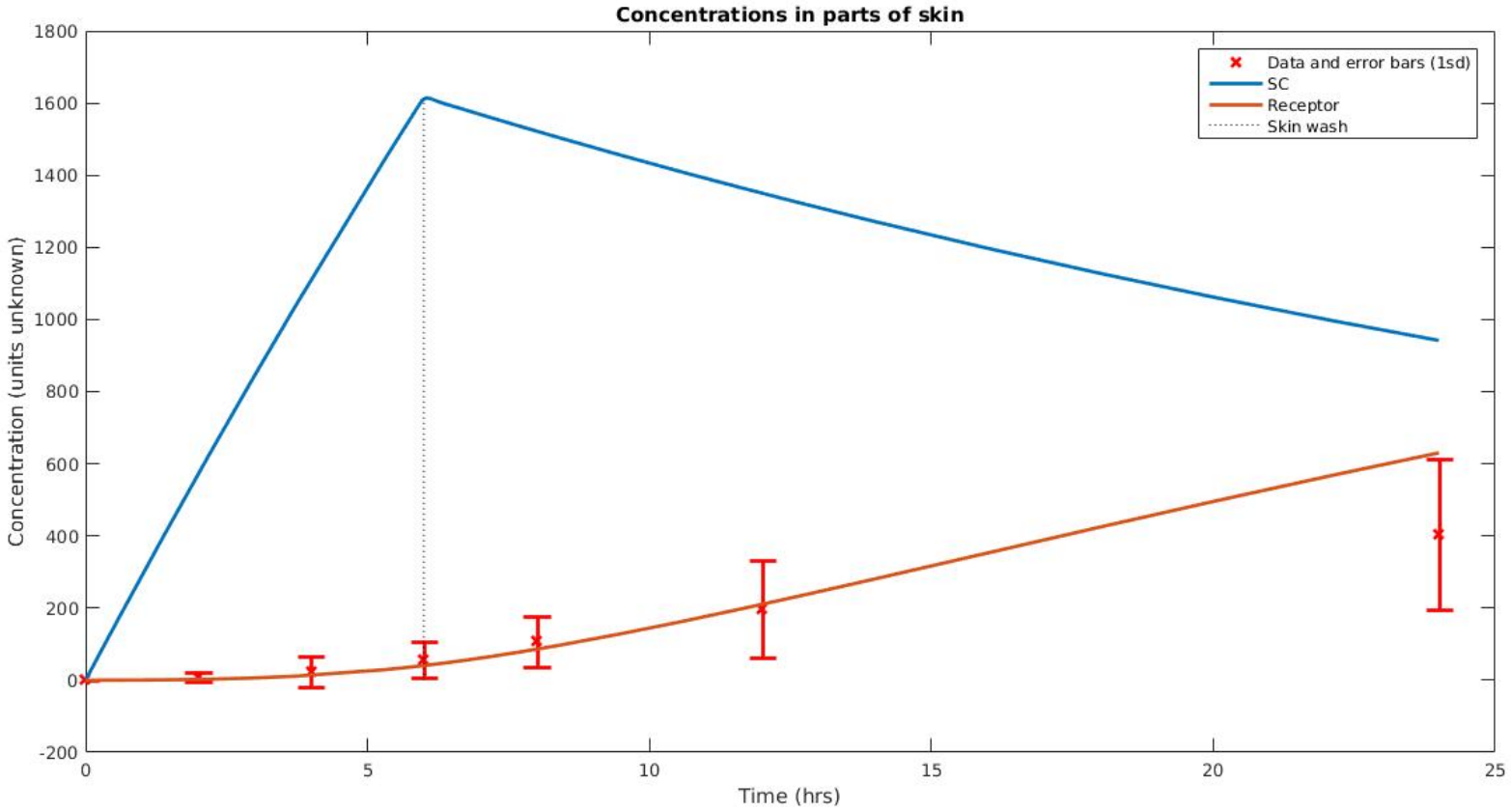
Compartment-based ODEs



The law of mass action:

$$\frac{dS}{dT}(T) = -\alpha(T)S(T)$$
$$\frac{dSC}{dT}(T) = \alpha(T)S(T) - \beta SC(T)$$
$$\frac{dE}{dT}(T) = \beta SC(T) - \gamma E(T)$$
$$\frac{dR}{dT}(T) = \gamma E(T)$$

Compartment-based ODEs

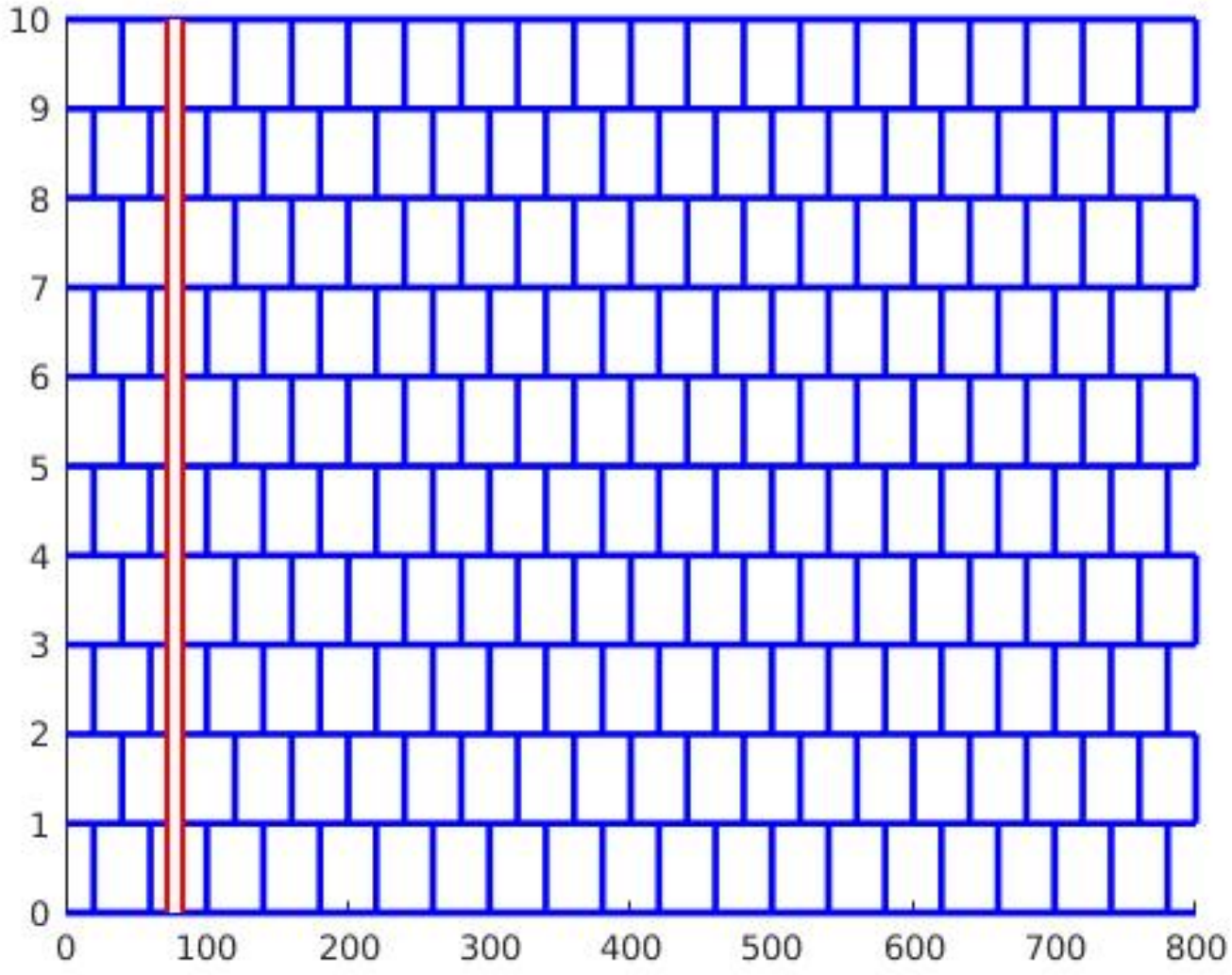


Extensions

- Include the co-formulant in the model to determine the effects.
- More realistic α function (rate of absorption through skin).
- Can we match experimental data. Classification problem?
- Add in more compartments to simulate different layers of skin.

Approach 2: a random walk

The stratum corneum (SC) (according to MatLab)



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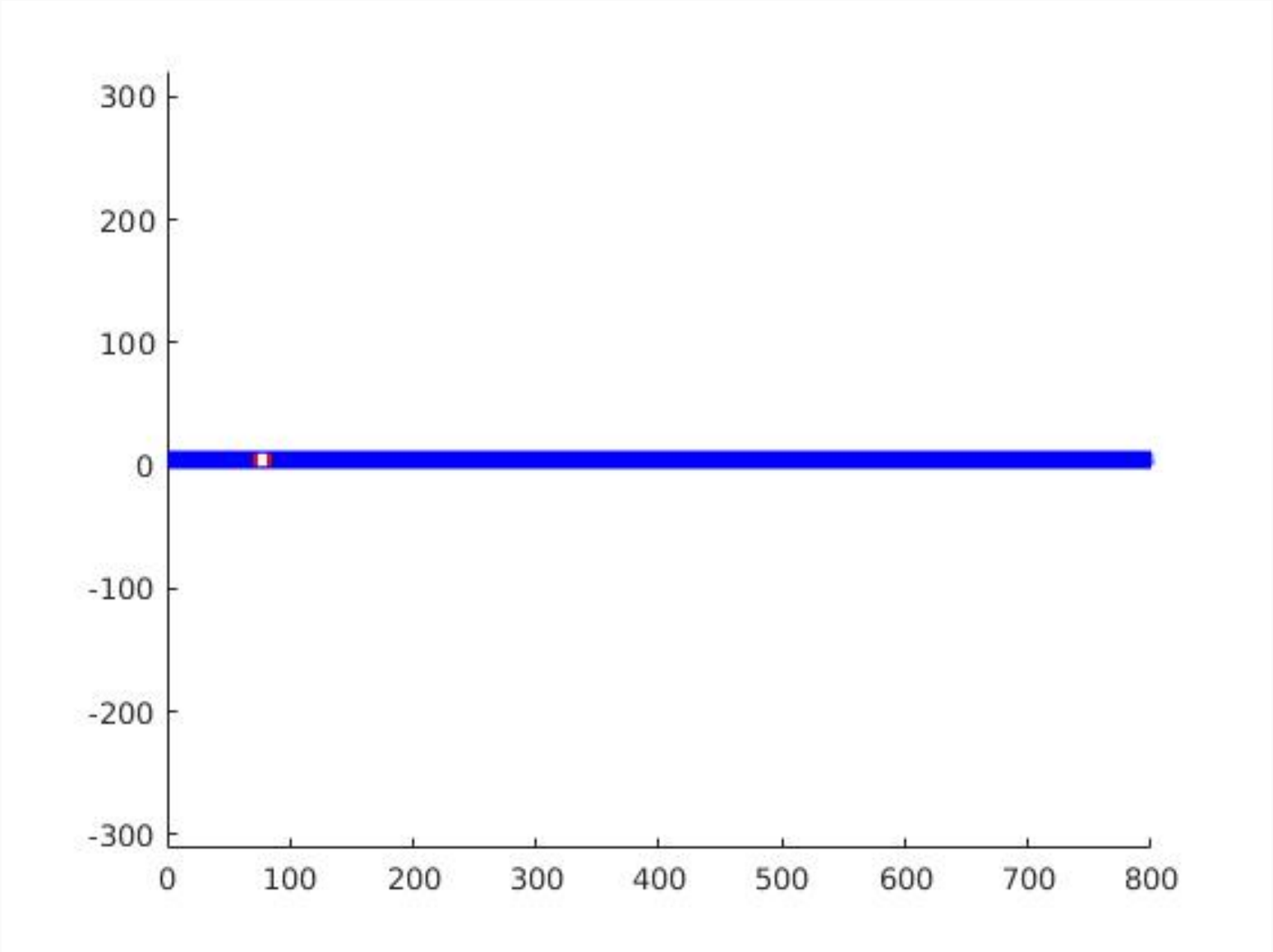

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- Simulated using the Gillespie algorithm:
  1. Calculate the time until the next particle jumps.
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- **Inner boundary**: Can move downwards at a different rate.

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Why a random walk model

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Extension of random walk model

- Addition of hairs.
- Model the co-formulants as separate particles which affect the diffusivity of AI.
- Vary the regularity of SC with possible dependence on co-formulants.

The future

Questions, questions, questions...

- Can we reproduce experimental results using our random walk approach?
- Can we measure the effect of the blocks (effective diffusivity)?
- Given data, can we pick out the effects of different co-formulants?
- Can we produce a PDE from the random walk model?
- Similar model for leaf. Can we balance the effectiveness as a pesticide with impermeability of the skin?

Thanks for listening

Any questions?