Affinity-Based Computational Model for Hydrogel Drug Delivery

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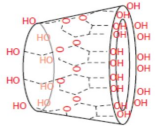
Need: Rapid release of drugs leads to **toxicity**

- Use Cyclodextrin (CD) to ↓ toxicity
- Researchers are **unable to predict release** from CD affinity-based hydrogels



CD

Objective: Develop a model to accurately **predict drug release** from a CD hydrogel

Constraints:

- **Existing literature** for model verification
- **Computational power** of a laptop (8 GB RAM)

Requirements for Predicted Release:

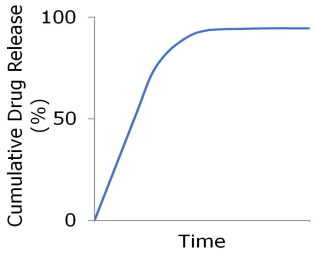
- Must **match** data in literature ($R^2 \geq 0.85$)
- Must be dependent on **affinity** and **[CD]:[drug]**

Solution – Design:

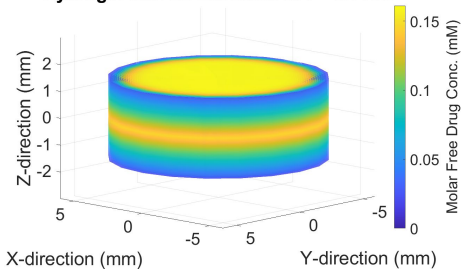
Fick's 2nd Law of Diffusion

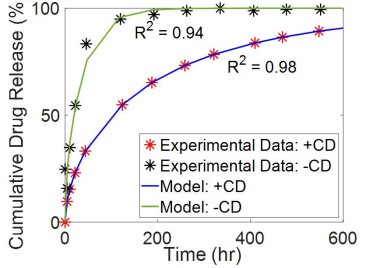
Michaelis Menten Enzyme Kinetics

MATLAB ODE Solver



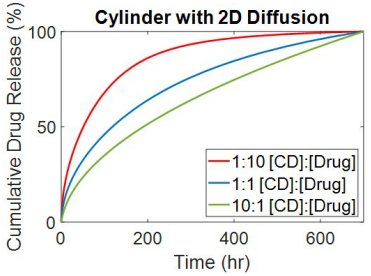
Solution: HydroSim - a user friendly model for hydrogels





Results:

- ✔ Matches experimental data
- ✔ Dependent on affinity
- ✔ Dependent on [CD]:[drug]
- ✔ GUI enables sensitivity analysis



Revisions:

- Expansion into 3D diffusion mechanisms
- Verification with new studies

Impact:

- Save time and ↓ drug delivery research costs
- Hydrogel educational tool for students