Modeling and Uncertainty of Restrictive Parylene-C (PPX) Deposition for Enhanced Drug Delivery Applications

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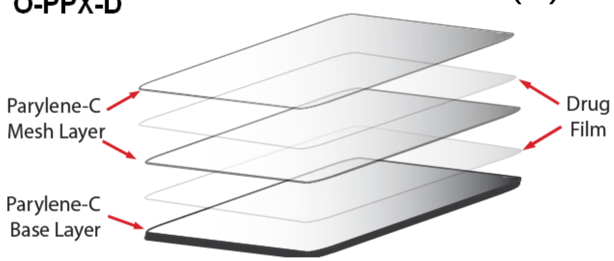
RESEARCH OBJECTIVE

Previous work has highlighted the capacity for PPX derived films to act as a drug release platform. A wide number of therapeutics can be integrated into the film, which is incorporated in alternating layers of deposited PPX. However, identification of the specific imperfections present in the elution or topmost PPX layer has remained elusive. The aim of this project is to develop a computational model that can shed light on the underlying mechanism governing the release mechanism in sub-monolayer PPX thin films and to validate the model through comparison with experiments.

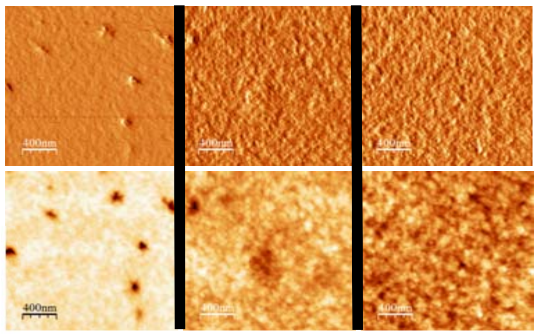
•Oxidized (**O**) Parylene-C (**PPX**) Drug Elution Device (**D**)

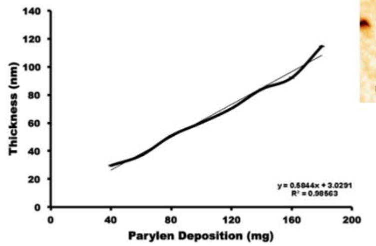


•Experiments

•60mg •100mg •140mg

Film properties such as thickness and RMS roughness are measured using ellipsometry and atomic force microscopy.



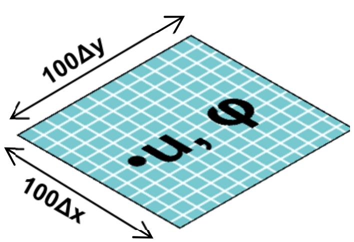


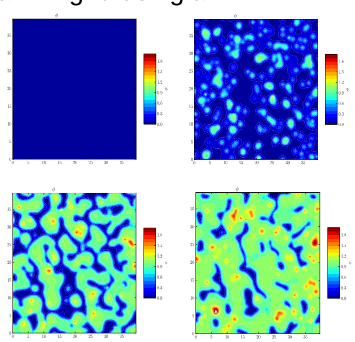
•Phase Field Model:

$$\frac{\partial u}{\partial t} = \nabla \cdot D \nabla u - \frac{\partial \phi}{\partial t} + \delta(r - r')\delta(t - t') \qquad t' = \frac{1}{Fl^2}$$

$$\frac{\partial \phi}{\partial t} = -\frac{1}{\tau}\frac{\delta H}{\delta \phi} = \frac{1}{\tau}\left\{W^2 \nabla^2 \phi - 2\sin(2\pi\phi) - \lambda(u - u_{eq})[2\cos(2\pi\phi) - 2]\right\} + \lambda_n D u^2$$

Two coupled equations govern the interaction between the monomers diffusing on the substrate and the polymerized islands. The system of nonlinear PDEs are solved on a 2-D grid using a finite difference scheme.

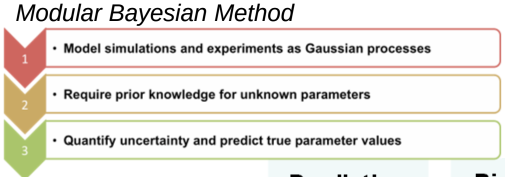




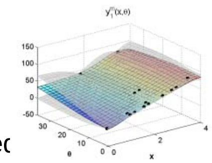
•Uncertainty Quantification

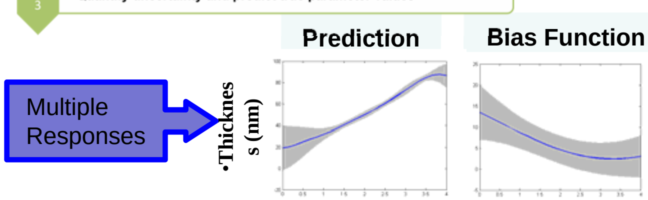
The phase field model for film growth is compared with the experimental data in order to validate the model. Due to the numerous sources of uncertainty in the experiments and modeling, a modular Bayesian approach is needed to fully account for the possible error.

Modular Bayesian Method



Metamodel for computer simulation





With the model validatec simulations can be used to tune the deposition parameters to optimize the drug release capabilities of the thin films.

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