

## **Mathematical Modeling of Pharmaceuticals:**

### **Predictive Design for Better Medicines**

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Smart designs of drug molecules and pharmaceutical formulations can target treatments to specific tissues, reduce side effects, and improve patient quality of care. Computational models for evaluating pharmaceutical formulations can narrow the range of experiments needed to identify successful designs by predicting performance and thus reducing the development time and driving down costs. Models coupled with sophisticated process control strategies allow for careful monitoring of manufacturing to reduce wasted materials and energy and to adhere to quality standards. I will overview mathematical modeling efforts in several pharmaceutical domains and will highlight work related to predicting drug release from controlled-release formulations that administer medicine over extended periods with a single dosage. I will show how coupled, nonlinear partial differential equations can be used to capture the complex dynamic interactions between simultaneous chemical reactions and mass transfer. I will describe mathematical techniques that can be used to reduce the system size from thousands of equations to just a few while retaining resolution of the biodegradation of the pharmaceutical formulation that strongly influences the drug release dynamics. These techniques can aid in the design of improved controlled-release formulations. I will conclude with a brief discussion of my proposed research in systems biomedicine and pharmaceuticals.