

(54) Title of the invention : AI AND PARTIAL DIFFERENTIAL EQUATION BASED PK-PD MODEL FOR DRUG FORMULATION & DOSAGE OPTIMIZATION

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(57) Abstract :
The integration of Artificial Intelligence (AI) with Partial Differential Equations (PDEs) in pharmacokinetics-pharmacodynamics (PK-PD) modeling offers a transformative approach to drug formulation and dosage optimization. Traditional PK-PD models rely on PDEs to describe drug absorption, distribution, metabolism, and excretion (ADME), but they often struggle with parameter estimation and patient variability. AI techniques such as Physics-Informed Neural Networks (PINNs) enhance PDE-based models by improving predictive accuracy while maintaining physiological consistency. Additionally, Gaussian Processes (GPs) aid in uncertainty quantification, while Bayesian Optimization refines drug dosage dynamically based on real-time data. Reinforcement Learning (RL) further personalizes treatment by continuously learning optimal dosage regimens from patient responses, and Deep Neural Networks (DNNs) model complex drug interactions more effectively. This AI-driven PK-PD framework enhances treatment precision, minimizes adverse effects, and accelerates drug development by adapting dosages in real time. The proposed approach significantly outperforms conventional models, offering a robust solution for personalized medicine and optimized therapeutic outcomes.

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