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Computational Studies of Drug Release, Transport and Absorption in the Human Intestines FARHAD BEHAFARID, J. G. BRASSEUR, U Colorado, G. VIJAYAKUMAR, NREL, B. JAYARAMAN, Oklahoma State U, Y. WANG, Georgia Tech — Following disintegration of a drug tablet, a cloud of particles 10-200 μm in diameter enters the small intestine where drug molecules are absorbed into the blood. Drug release rate depends on particle size, solubility and hydrodynamic enhancements driven by gut motility. To quantify the interrelationships among dissolution, transport and wall permeability, we apply lattice Boltzmann method to simulate the drug concentration field in the 3D gut released from polydisperse distributions of drug particles in the "fasting" vs. "fed" motility states. Generalized boundary conditions allow for both solubility and gut wall permeability to be systematically varied. We apply a local 'quasi-steady state' approximation for drug dissolution using a mathematical model generalized for hydrodynamic enhancements and heterogeneity in drug release rate. We observe fundamental differences resulting from the interplay among release, transport and absorption in relationship to particle size distribution, luminal volume, motility, solubility and permeability. For example, whereas smaller volume encourages higher bulk concentrations and reduced release rate, it also encourages higher absorption rate, making it difficult to generalize predictions. *Supported by FDA.*

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