

COUPLED DEFORMATION AND SOLUTE DIFFUSION IN SWELLING MOLECULAR SOLIDS

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Abstract. Precision of dosage, mechanical and chemical stability and ease of storage and distribution make tablets the most popular drug delivery dosage form currently in use. A typical pharmaceutical tablet consists of several different powders, (such as actives, excipients, lubricants, glidants, disintegrants, etc.) compressed into a solid body. Usually administered orally, tablets disintegrate and dissolve in the gastro-intestinal tract, allowing for the pharmaceutical active to be absorbed in the body. It is the properties of this dissolution, which govern a tablet's performance as a drug delivery form. Despite its importance for the process of time-controlled delivery, the complexity of the phenomena and the multiple scales involved cause drug dissolution to remain poorly understood. In this talk we present modeling, simulation and experimental data concerning the coupled deformation and solute diffusion in swelling molecular solids. A key experimental feature is that the concentration profiles, which are tracked in time and space via image processing, show a wave-like behavior with a relatively sharp but not discontinuous interface between the rubbery and glassy phase. A computational model that describes solvent penetration through deformable polymeric solid is also presented and compared with the experimental data, showing a good overall agreement. In particular, about the linear motion of the interface indicating the stress-diffusion coupling.