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Multi-physics problems in particulate engineering – 3 case studies

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Industries such as food, pharmaceuticals, chemicals, consumer goods, agriculture, mineral processing as well as advanced materials for healthcare, energy and environment, rely extensively on particle science and engineering. We present 3 case studies that involve coupling the equations of heat transfer, mass transport, chemical reaction, incorporating also the mechanical behaviour in process modelling.

1. Droplet drying is traditionally modelled using different sets of equations describing heat and mass transfer for successive stages of drying, separated by pre-defined end conditions. By incorporating the mechanical behaviour of the particulate phase with appropriate evolution laws, we solve a single set of governing equations. Different granule microstructures are obtained (e.g. dense granule, loose granule, hollow shell, expanded hollow shell, etc.) depending on the evolving strength and permeability of the granular skeleton, evaporation rate, heat and mass transfer rates withing the droplet and with the surrounding atmosphere.
2. Swelling and disintegration of multi-component polymeric structures is modelled considering mass transfer and transformations in the solid phase. By incorporating the mechanical response (through a swelling stress) and material properties such as elastic parameters and failure models which evolve with fluid ingress, it is possible to describe 1) drug release profiles for controlled release tablets or 2) breakup of immediate release tablets. Similar to droplet drying, the behaviour can be modelled using a single set of governing equations with suitable parameter evolution laws.
3. Fungi growth on grain storage silos has significant quality, safety and economic implications. Fungi growth is modelled using a rate equation which can incorporate moisture content, temperature, oxygen content, and other parameters. For example, fungi growth rate is affected by temperature, which is determined by solving heat transfer equations, considering silo size and outside temperature fluctuations during day/night or over longer timescales, as well as the metabolic heat generation due to fungi growth. Relative humidity depends on the temperature of the air and moisture migration is described by diffusion. The local oxygen content is also described using diffusion. The mechanical contact areas between two individual grains arising due to self weight affects and is affected by the heat and mass transfer processes.

The application examples discussed above demonstrated that coupling mechanical behaviour with chemical reactions and heat and mass transfer offers a unified framework that provides greater insight and enables more accurate modelling for better material and process design. While solving coupled equations no longer presents technical difficulties, the experimental data requirements for model calibration have increased.

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