

Expanding Frontiers in Particulate Product Development – Bridging Mechanistic Models and Cognitive AI –

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Virtual product and process development has traditionally relied on mechanistic, physics-based models. Across fields ranging from energy technologies and battery research to chemical engineering and pharmaceutical process development, approaches such as continuum modelling, computational fluid dynamics, population balance models and discrete element methods have enabled the quantitative description of complex systems.

These methods provide valuable physical insight and support systematic design decisions. However, their predictive power may decrease as process complexity, material heterogeneity, and the number of interacting phenomena increase. In addition, high-fidelity simulations are often computationally demanding and difficult to integrate into fast, iterative development workflows. Data-driven methods and narrow artificial intelligence (AI) have therefore gained increasing importance. They are commonly applied in the form of surrogate models, parameter optimisation, virtual sensors, digital twins, and predictive decision-support tools. Although these approaches can significantly accelerate development, they are often application-specific and show limited transferability across products, processes, and domains. The emergence of transformer architectures and large language models marks a further step towards more general virtual product development. Originally developed for language processing, these models can combine numerical data, images, experimental results, simulation outputs, technical documents, and domain knowledge. They thus provide a flexible interface between data, models, human expertise, and engineering workflows. When trained and adapted at scale, such systems can support contextual reasoning, knowledge integration, design-space exploration, and increasingly autonomous action. This talk places these developments within the broader evolution of modelling and simulation in engineering. It introduces the principles of transformer-based models and discusses their potential in virtual product development through fine-tuning, retrieval-augmented generation, mixture-of-experts architectures, and autonomous agent systems. Examples from energy and battery research, chemical engineering, and pharmaceutical process engineering illustrate how these methods can contribute to adaptive, scalable, and cross-domain development environments. Together, these advances point towards a transformation from isolated models and tools to integrated AI-supported ecosystems for the design, optimisation, and operation of future products and processes.