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Data-driven calibration of numerical models: bridging the gap between simulations and industrial reality

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Advances in numerical methods for the modelling of multiphase simulations have never been as meticulous and comparable to industrial systems as they are now. From fundamental research into contact mechanics and surface chemistry to improving plant-scale reactors and enabling continuous optimisation of processes and preventive maintenance of equipment with the use of digital twins, numerical modelling techniques offer academics and industries alike powerful tools to better understand and optimise the internal dynamics of a large number of systems. It is now easier and faster than ever to develop and adapt large-scale simulations, significantly reducing the human and financial costs of experimental prototyping. Simulations overcome limitations associated with experimental measurements by providing an enhanced picture of the entire system modelled.

Numerical methods include, but are not limited to, the Discrete Element Method (DEM), Computational Fluid Dynamics (CFD), Smoothed Particle Hydrodynamics (SPH), Finite Element Method (FEM), and hybrids of the aforementioned. Simulations can offer exceptional accuracy and, if correctly calibrated, provide results with quantitative precision. It is this “if”, however, that also represents their biggest drawback: without careful model development, calibration and validation, numerical methods can yield inaccurate and even unphysical results. How is the simulation precision ensured?

Ultimately, the validation of a model requires a direct comparison between simulated data and experimental measurements, whether by analysing the velocity distribution, species concentration or other model parameters. Experimental imaging and characterisation techniques provide a wealth of information about the macroscopic behaviour of the systems modelled. Incorporating such high-dimensional data into numerical simulations surpasses the capabilities of older statistical methods, requiring modern solutions – such as machine learning – to systematically determine the optimum model parameters yielding the best alignment between virtual and reality.

In this minisymposium, we will discuss the topics of i) direct comparison of novel numerically modelled systems to their industrial counterpart, i.e., digital twins, ii) recent advances in simulation methodologies and how they are used to characterise multiphase fluids and particulates as well as their current limitations, and iii) new developments in experimental data acquisition methodologies for multiphase systems. We seek to bring together future world leaders in the synergistic application of numerical models, experimental methods, and data-driven calibration to real-world problems and industrially relevant systems. By doing so, a platform will be created for exchanging ideas and developing mutually beneficial collaborations between all involved. It also gives a chance for young academics to exhibit their research findings to an audience of like-minded people at similar stages in their careers.