X International Conference on Particle-Based Methods, PARTICLES 2027
October 18-20, 2027, Barcelona, Spain

PARTICLE SIMULATIONS IN BATTERY APPLICATIONS: MANUFACTURING, USE & RECYCLING

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ABSTRACT

Battery technology is a cornerstone of Europe's transition toward sustainable energy, electrified mobility, and energy security. By fostering interdisciplinary dialogue between particle simulation experts and battery specialists, this session aims to accelerate the development of next-generation batteries that are safer, more efficient, and sustainable.

Particle-based simulations offer unique capabilities to model and understand the complex multiphysics and multiscale phenomena that dictate process and product performance relevant for the battery value chain. This invited session brings together leading researchers and practitioners, and has the prime objective to discuss (i) cutting-edge particle-based simulation methods (e.g., the Discrete Element Method), (ii) coupling strategies for co-current fluid-particle simulations (e.g., Computational Fluid Dynamics - DEM approaches), as well as (iii) strategies for sequential simulation that benefit from particle data and the use of AI/ML algorithms. Further objectives are to (I) showcase state-of-the-art particle simulation methodologies applied to battery applications, (II) identify key scientific challenges to enable next generation simulation approaches in the battery field, and (III) to bridge the gap between particle simulation experts and battery researchers as well as industry practitioners.

Topics covered include simulations of (a) electrode and battery cell manufacturing processes (e.g., powder mixing, slurry preparation, and associated rheological phenomena, as well as coating and calendaring), (b) phenomena during aging and degradation of cells (e.g., particle swelling [1], cracking, plating, as well as gas formation), (c) thermal runaway events, and (d) dismantling and recycling processes (e.g., crushing, shredding, classification and handling [2], as well as black mass treatment and the recovery of critical raw materials).

REFERENCES

[1] Yin J. et al., *Development of a P2D-based model for battery swelling prediction under mechanical constraints,* Journal of Power Sources, Vol. 677, p. 240029, 2026.

[2] Maier L. et al., *The uncertainty inherent to DEM simulations of interlocking particles,* Scientific Reports, Vol. 15, 7599, 2025.