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CONTACT FORCE MODELS BETWEEN NANOPARTICLES IN AGGLOMERATES, AGGREGATES, AND FILMS AND THEIR PARAMETERISATION

Stefan C. Endres[1], Lutz Mädler[2]

[1] Leibniz-Institute for Materials Engineering - IWT,
Faculty of Production Engineering, University of Bremen
Badgasteiner Str. 3, 28359 Bremen, Germany.
s.endres@iwt.uni-bremen.de,
URL: https://www.mimenima.uni-bremen.de/Member/eng/Endres.php
[2] Leibniz-Institute for Materials Engineering - IWT,
Faculty of Production Engineering, University of Bremen
Badgasteiner Str. 3, 28359 Bremen, Germany.
lmaedler@iwt.uni-bremen.de
URL: https://www.iwt-bremen.de/en/institute/staff/detail/prof-dr-ing-habil-lutz-maedler

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The production- and post-production properties of particle structured materials relies on fundamental models in order to gain scientific insight as well design optimal process units and controllers. Nanoparticle structured materials are often characterized by hierarchical assemblies of a distribution of primary particles in the nanoscale range (5–50 nm) which form chemically bonded aggregates (typical size range 200–300 nm) during their production. These in turn form extended particle assemblies with thicknesses in the order of 1–50 μm. Such systems characterise nanoparticle films used in gas sensors, catalysts, solar cells and battery materials. The models are also related to processes in additive manufacturing, fluidised beds, dry powder inhalers as well as fine grinding and dispersing processes. The desire to improve our understanding of these systems has driven the development of increasingly accurate and fundamental models that describe their underlying physical and chemical mechanisms of interaction [1, 2]. In this talk we review the following particle-particle contact force models:

- Particle-particle short range repulsion forces (Hertzian stress type models).
- Particle-particle attractive forces (capillary, solvation, adhesive and Coulombic forces).
- Fluid-particle interaction models CFD-DEM.
- Chemical sintering forces in particle aggregates.

Techniques for experimental validations and parameterisation of contact force models are also discussed including:

- Using AFM/TEM for measuring contact forces between primary particles in aggregate structures [3, 4].
- AFM in highly porous nanostructures [5].
- Nanoindentation [6].

- Microscopic characterisation [7].

Furthermore, an overview of available software for simulating the models as well as the use of parameter estimation and model development from molecular dynamics simulations will be given [8, 9]. Finally, we summarise the strengths and limitations of the contact models, their applicability on practical systems of nanoparticles in industry as well as propose an outlook for future developments of contact models for nanoparticle systems with a particular focus on models for nanoparticle aggregates and their interactions with multiphase fluids.

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