Microaggregation of goethite and illite: Linking mechanistic modeling and laboratory experiments

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Study microaggregate formation in silico

Why?

- study the interplay of particles in **precisely defined settings**
- in contrast to lab scenarios: easy **variation of a manifold of conditions**
- **isolation of mechanisms** / effects possible
- direct access to all parameters of resulting structures - at every time step (even not measurable ones)
- mathematical **upscaling** of structural properties possible

References

Zech, S., Dultz, S., Guggenberger, G., Prechtel, A., Ray, N. (2020):

Microaggregation of goethite and illite evaluated by laboratory experiments and mechanistic modeling, Preprint Reihe Angewandte Mathematik, ISSN 2194-5127, Erlangen.

Relates to experimental study

Dultz, S., Woche, S.K., Mikutta, R., Schrapel, M., Guggenberger, G. (2019):**Size and charge constraints in microaggregation: Model experiments with mineral particle size fractions.** *Appl. Clay Sci.* 170, 29-40. doi.org/10.1016/j.clay.2019.01.002

Extension of the work

- Rupp A., Guhra T., Meier A., Prechtel A., Ritschel T., Ray N., Totsche KU. (2019): **Application of a cellular automaton method to model the structure formation in soils under saturated conditions: A mechanistic approach.** *Front. Environ. Sci.* 7, doi.org/10.3389/fenvs.2019.00170
- Rupp A., Totsche KU., Prechtel A., Ray N. (2018): **Discrete-Continuum Multiphase Model for Structure Formation in Soils Including Electrostatic Effects**. *Front. Environ. Sci.* 6, doi.org/10.3389/fenvs.2018.00096
- Ray N., Rupp A., Prechtel A. (2017): **Discrete-continuum multiscale model for transport, biomass development and solid restructuring in porous media**. *Adv. Water Resour.* 107, 393-404, doi.org/10.1016/j.advwatres.2017.04.001

Enlarge the range of conditions and compositions of aggregate formation - use also particles used in wet lab experiments

Investigation of

- **Prototypic microaggregate forming materials (MFM)**: goethite, and illite; different in size, shape, charge loading, concentration.
- impact of **shape (aspect ratio) and size**
- impact of **edge charges** of illite/point of zero charge
- **stability** vs. particle size
- **excess particles**

Stable aggregation in terms of size and aspect ratio

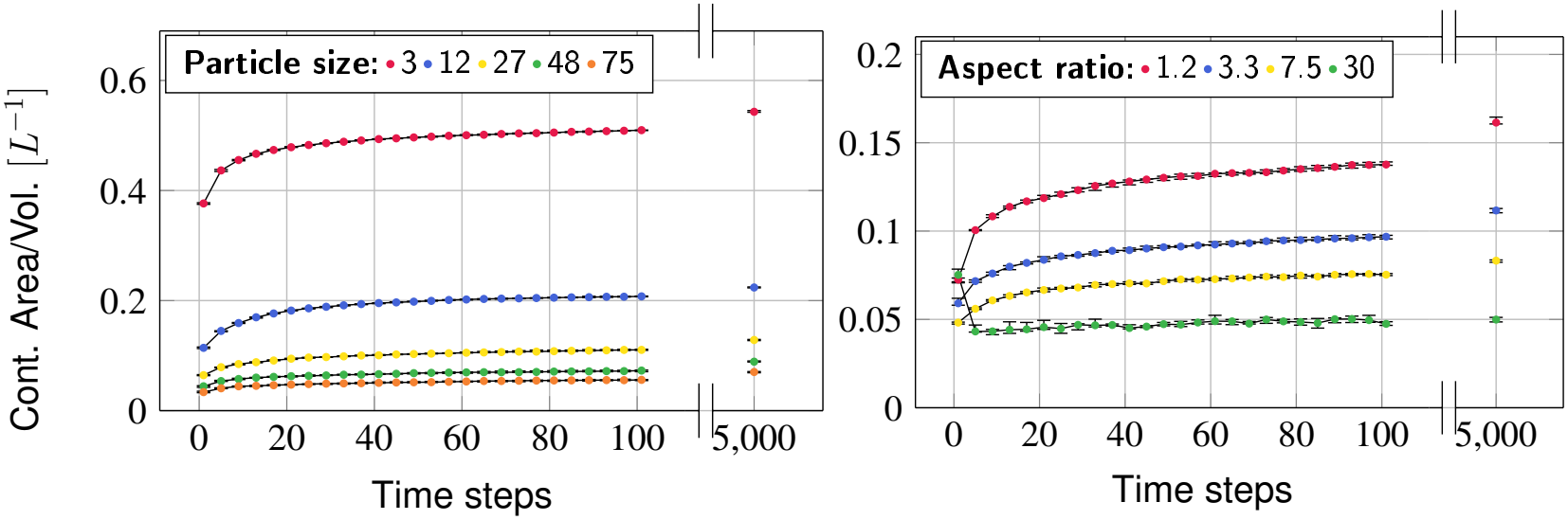

Figure: Influence of aspect ratio and size of illite building units on aggregate stability.

$\Rightarrow$ **Small in size and aspect ratio MFMs are most stable.**

Different phenotypes of structures while aggregation

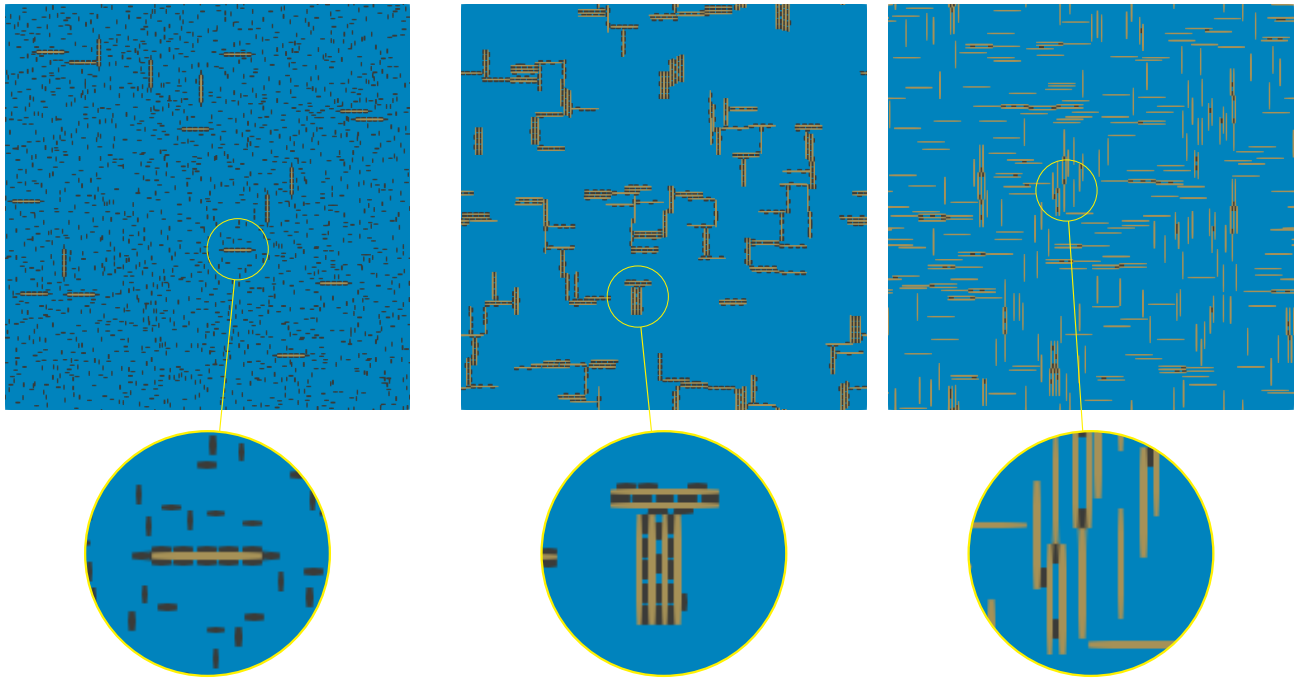

Figure: Microstructures due to heteroaggregation of fine illite with negative edge charge and coarse goethite. *Left*: 5% of goethite (**stable disperse system**), *middle*: 55% of goethite (**compact structures**), *right*: 95% of goethite (**pillar structures with hidden places**)

Optimal aggregation in terms of composition

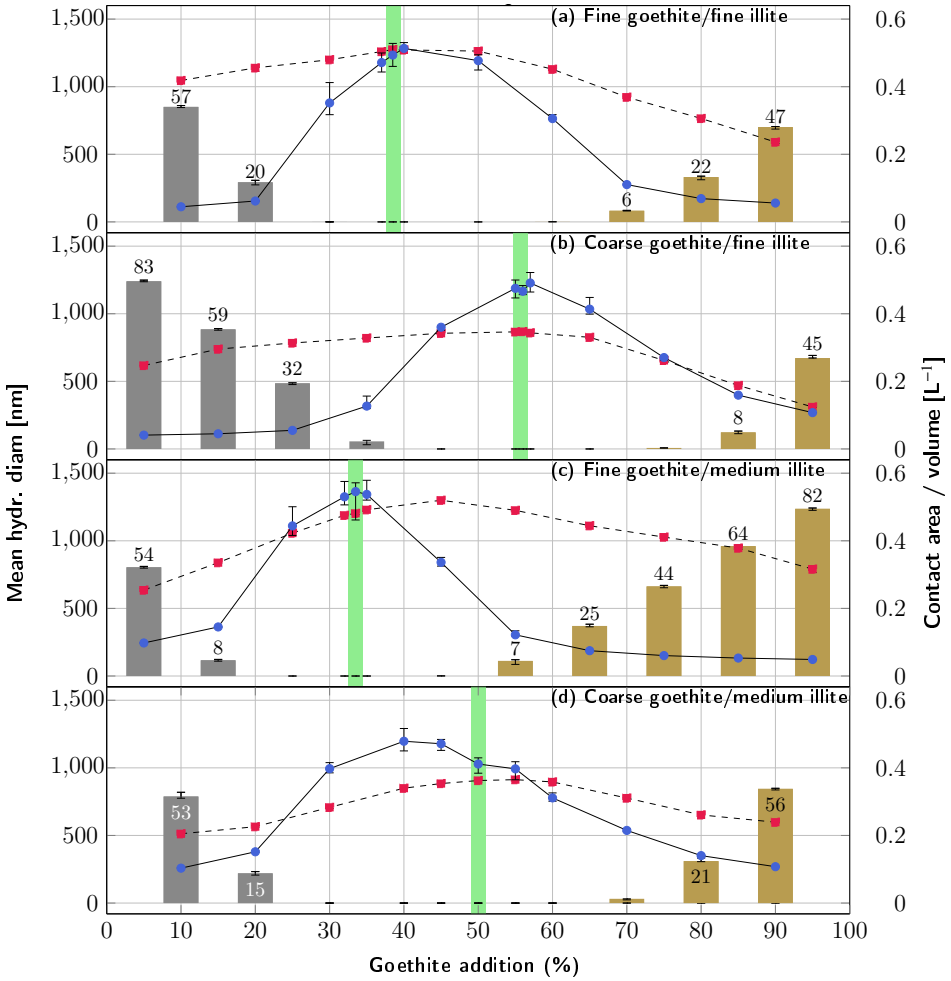

Figure: X-axis: % of portion of goethite (remaining portion is illite with negative edge charge). Left Y-axis: Mean diameter for various compositions of solid. The blue dots show the median of the mean diameter in 10 simulation runs, the black bars indicate the lower and upper quartile of the 10 simulation runs. Right Y-axis: contact area per aggregated volume (red dots). The green lines depict the point of zero charge of the system leading to strong aggregation. Bars with % of excess building units (illite in gray, goethite in brown).

Different phenotypes of structures for varying edge charge of illite

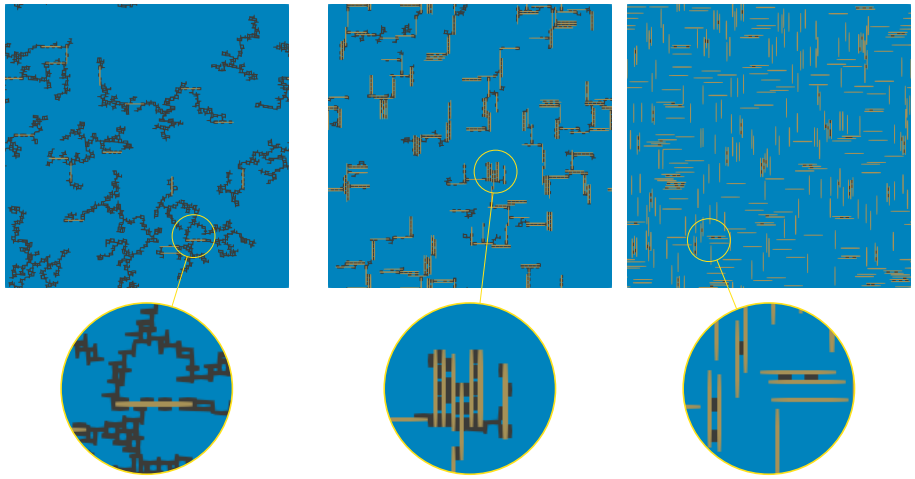

Figure: Microstructures due to heteroaggregation of fine illite with positive edge charge and coarse goethite. *Left*: 5% of goethite (**cardhouse structures**), *middle*: 55% of goethite (**compact structures**), *right*: 95% of goethite (**pillar structures with hidden places**)

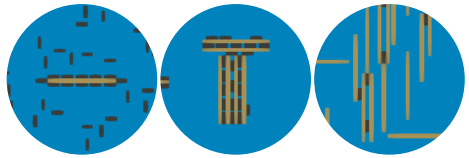

Figure: Recall situation of negative edge charge-...

Comparison with experiment

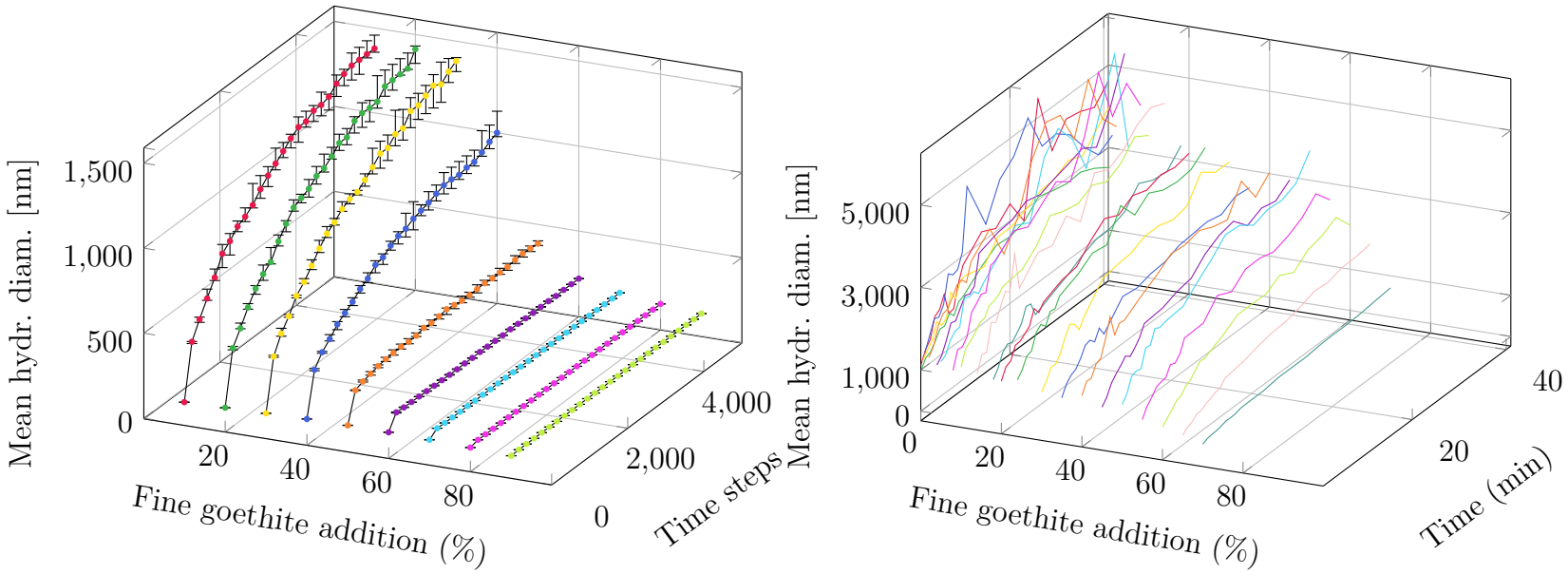

Figure: Mean (hydrodynamic) diameter (in nm) over time for different mixtures of fine goethite and fine illite with positive edge charge. Results from simulations (left) and experiments (right) show a similar qualitative behaviour.

Forward Simulation! NO FITTING OF ANY PARAMETERS!

Simulations elucidate the impact of

- **composition** of solution/ charge and ratio between MFM
  - Shielding
  - Distinct aggregate phenotypes (coiled chain like, thin long chains,..)
- relative **size** of MFM
  - surface caoting inhibiting aggregation vs. bridging supporting aggregation
- **concentration** of solution/porosity
  - higher concentration leading to larger aggregates
  - increasing complexity and size over time

on aggregation and quantification by means of characteristic values (average particle size, specific surface, compactness, ...)

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