CATALYST CARRIER SYNTHESIS: FROM PRECIPITATION TO IMPREGNATION

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A. DANDEU, M. MINIÈRE, F. SALVATORI, J-M SCHWEITZER, M. SERVEL
What is actually done

Catalyst synthesis at lab scale
- Main part of the work is done on the formulation
- No fundamental studies are done on the hydrodynamic/physical-chemistry coupling: mainly empirical approaches based on experiments

Lab’s protocol

Industrial catalyst
- Lab scale → Industrial scale: done by Axens
- Recipes are adapted to satisfy constraints imposed by each unit operation
- Experimental approach: tools at different scales
- Knowhow

Many innovative catalysts are developed and industrialized using this approach

Limits of this approach:
- Knowledge are limited to propose new formulations out of our « standard » ranges
- Promising product at lab scale which cannot be scaled-up industrially
Context

- Development of a Chemical Engineering approach

- Catalyst synthesis at lab scale
  - Reverse engineering

- Industrial catalyst
  - Scale-up rules for new catalysts

Development of multi-scale models including the main physical and chemical phenomena involved in each unit operation

- Creation of a specific team in 2015-2016
- The objective of this team is to interact with different entities involved in the catalyst manufacturing:
  - To improve existing catalyst manufacturing procedures
  - To propose new developments
RESEARCH STRATEGY

Development of Building Blocks (Collaborations, PhD, Post Doc)

- Comprehensive studies at local scale to understand which are the physical and chemical phenomena controlling catalyst textural properties
- Local measurements with specific analytical tools in controlled lab devices
- Identification of scale-up parameters (« descriptors »)
- Model development including those parameters

Make available models for industrial projects to develop innovative catalysts
1. **Boehmite gel synthesis**

   - **Raw material**
     - Aluminum sulphate
     - Sodium aluminate
     - Water

   - Precipitation
   - Washing & Filtration
   - Suspension
   - Drying atomization

   ![Boehmite powder](image)

2. **Carrier manufacturing**

   - Kneading Extrusion
   - Drying
   - Calcination

   ![Carrier extrudates](image)

3. **Catalyst manufacturing**

   - Impregnation solution
   - Impregnation
   - Drying
   - Calcination

   ![Extrudates](image)

**Product quality targets:**
- Textural properties
- Mechanical strength
- Productivity
PRECIPITATION - GELATION – PARTICLE SIZE DISTRIBUTION:

FROM DLVO THEORY TO POPULATION BALANCE
DLVO THEORY

B. Derjaguin, L. Landau, E. Verwey and T. Overbeek (1941-1948)

- DLVO modeling: Objective: modeling of the aggregation / breakage phenomena to reproduce the gelation of colloidal suspensions
  - Van de Waals potential
    \[
    W_{vdW} = -\frac{A_H}{6} \left( \frac{2 \cdot a^2}{r^2 - 4 \cdot a^2} + \frac{2 \cdot a^2}{r^2} + \ln \left( \frac{r^2 - 4 \cdot a^2}{r^2} \right) \right)
    \]
  - Electrical potential depends on
    - Activity coefficient
    - Debye length = f(Ionic strength)
  
  \[
  W_{elec} = \frac{64 \cdot \pi \cdot k_B \cdot T \cdot n_{ion} \cdot a}{K_{debye}^2} \cdot \gamma_G^2 \cdot e^{-K_{debye} \cdot h}
  \]

- Total potential
  \[
  W_{tot} = W_{vdW} + W_{elec}
  \]
Interaction forces = potential gradient

\[ \overrightarrow{F_{ij}} = -\nabla W_{tot} \]

Momentum balances

\[ m \cdot \overrightarrow{a_i} = \sum_{i \neq j} \overrightarrow{F_{ij}} - 6 \cdot \pi \cdot \eta \cdot a \cdot \overrightarrow{v} \]
Effect of the ionic strength

The energy barrier can be decreased by changing the environment (Ionic environment)

Key suspension characteristics
- Ionic strength
- Solid holdup
- Zeta potential
- Colloid radius

Repulsion controls the particle porosity and/or the mechanical strength
More repulsion leads to dense particles with a deformation risk

Aggregation and Gelation

- DLVO potential: Secondary minimum
- Use of DLVO theory for the suspension preparation steps
- Forces involved: long distance attraction (reversible)
- Aggregate geometry characterized by a fractal dimension
Aggregation and Gelation

- Use of DLVO theory for the suspension preparation steps
- 3D simulations with 1000 particles (CPU = 3 weeks)
  - Colloid radius: 50 nm
  - Ionic strength: 0.01 mol/l
  - Solid holdup: 10% vol.
  - Zeta potential: 45 mV
- Evaluation of the fractal dimension \( \Rightarrow \) fundamental parameter for aggregation modeling using population balance

Models are based on the master population balance equation (PBE)

Continuous formalism

\[
\frac{\partial f_i(x, t)}{\partial t} = \frac{1}{2} \int_0^x a(x - x', x') f_i(x - x', t) f_i(x', t) \, dx' - f_i(x, t) \times \int_0^\infty a(x, x') f_i(x', t) \, dx'.
\]

Discrete formalism

\[
\frac{dN_m}{dt} = \frac{1}{2} \sum_{i,j=1}^{i+j=m} K^A_{ij} N_i N_j - N_m \sum_{i=1}^{\infty} K^A_{im} N_i - K^B_{m} N_m + \sum_{i=m+1}^{\infty} K^B_{i} G_{im} N_i
\]


K^A: aggregation kernel
K^B: breakage kernel
Definition of discrete aggregate classes:

Based on the fractal dimension

\[ n_i = \frac{m_i}{m_p} = k_f \cdot \left( \frac{R_{g,i}}{R_p} \right)^{d_f} \]

Where \( n_i \) is the number of colloids which constitute the \( i^{th} \) aggregate

The number of colloids which constitute the \( i^{th} \) aggregate

\[ n_i = n_{i-1} + 1 + (1.08)^i \]

The gyration radius

\[ R_{g,i} = R_p \cdot \left( \frac{n_i}{k_f} \right)^{1/d_f} \]

AGGREGATION AND GELATION MODELING

- Fractal dimension: Ionic strength = 0.01 mol/l
- Calculation on the basis of 3D DLVO aggregation modeling

\[ d_f = \frac{\ln \left( \frac{n_i}{k_f} \right)}{\ln \left( \frac{R_{g,i}}{R_p} \right)} \]

<table>
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<tr>
<th>cluster number</th>
<th>R_{gyr} cluster (nm)</th>
<th>Rp (nm)</th>
<th>np_cluster</th>
<th>dim fractal</th>
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</table>
Fractal dimension: Ionic strength = 0.003 mol/l
Calculation on the basis of 3D DLVO aggregation modeling

\[ d_f = \frac{\ln \left( \frac{n_i}{k_f} \right)}{\ln \left( \frac{R_{g,i}}{R_p} \right)} \]

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<tbody>
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<td>50</td>
<td>988</td>
<td>2.48</td>
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</tbody>
</table>
Aggregation and gelation modeling

Aggregation kernel

- 2 terms for this kernel
  - Brownian agglomeration characterized by:
    - Fuchs stability ratio $W$
  - Shear induced agglomeration characterized by:
    - Collision efficiency $a$
    - Shear rate $\dot{\gamma}$

$$K_{ij} = \min \left\{ \frac{2kT}{3\eta W} \left( \frac{1}{i^{3/4} + j^{3/4}} \right) \left( i^{-1/4} + j^{-1/4} \right), \frac{4}{3\alpha \dot{\gamma} R_p} \left( \frac{1}{i^{3/4} + j^{3/4}} \right)^3 \right\}$$

Breakage kernel

- Power-law model proposed by Harshe et al.

\[ K^B_i = c_i (\eta_i)^n R_m^i. \]

According to the population balance equation we need to define the distribution \( G_{im} \) of the clusters issued from the breakage of a given aggregate

\[
\frac{dN_m}{dt} = \frac{1}{2} \sum_{i,j=1}^{i+j=m} K_{ij}^A N_i N_j - N_m \sum_{i=1}^{\infty} K_{im}^A N_i - K_m^B N_m + \sum_{i=m+1}^{\infty} K_i^B G_{im} N_i
\]

- The broken aggregates are given by a Schultz-Zimm distribution
  - \( z \) is a parameter determining the width
  - This formalism ensure that only smaller clusters are formed

\[ f_{m,k} = (a)^z + 1 (N_{fr}^s)^z \exp[-(a \cdot N_{fr}^s)] \frac{1}{\Gamma(z + 1)} \]

AGGREGATION AND GELATION MODELING

- **Solid holdup**
  \[ \varepsilon_s = \sum_i N_i \cdot \frac{4}{3} \cdot \pi \cdot R_{g,i}^3 \]

- **Viscosity**: \( \varepsilon_s \equiv \emptyset \)

- **Equation proposed by van de Ven and Takamura**

\[ \eta_s = \eta \left( \frac{1 - \phi}{\phi_c} \right)^{-\frac{5\phi}{2(2-k_0\phi_c)}} \]

- **Average gyration radius**
  \[ R_g = \frac{1}{N_0} \cdot \sum_i N_i \cdot n_i \cdot R_{g,i} \]

**Our simulation**

**Lattuada et al. (2016)**

- **Time evolution of suspension viscosity**
- **Viscosity**
- **Time evolution of average gyration radius**
FIRST COMPARISON BETWEEN EXPERIMENTAL RESULTS AND PHYSICAL MODELS

Colloidal aggregation in Brownian conditions → inspected with Dynamic Light Scattering (DLS)

No shear → \( \dot{\gamma} = 0 \)

Only aggregation kernel

\[
\beta_{ij} = \frac{2k_BT}{3\eta W} \left( \frac{1}{id_f} + \frac{1}{jd_f} \right) \left( \frac{1}{id_f} + \frac{1}{jd_f} \right)
\]

Near to IEP → the aggregation process is faster

\( W = 1 \) → \( df \) free parameter

Far IEP → the aggregation process is slower

\( W > 1 \) → \( W \) and \( df \) free parameters
IN SUMMARY

- DLVO modeling leads to an estimate of the aggregate fractal dimension
- Population balance modeling with aggregation and breakage kernels proposed by Lattuada et al. (2016) leads to the prediction of the cluster size distribution and the time evolution of suspension viscosity
- Good trends are obtained for viscosity and average gyration radius
- Population balance model is tested on an IFPEN experimental case
- This model is a tool to drive the unit operations by adapting the hydrodynamic constraints and the chemical formulation of the suspension
GEL DRYING

CONSTRUCTION OF THE BUILDING BLOCK
Objectives

Construction of a drying building block (particle drying model)
1- allow to evaluate the effects of operating conditions
2- allow to evaluate the mechanical resistance of the dry particle
3- useful to scale-up industrial dryers (belt dryer, atomizer)

Particle model

Different steps during drying
1- Particle reduction due to water evaporation
2- Crust formation
3- Elimination of water contained in the crust
4- Gas feeding
5- Crust thickening

Heterogeneity of gas velocity field

Isothermal conditions
Alumina gel drying

**Plate model**

Plate divided into 25 cells

**Drying evolution**

Gas velocity between particles ≠ Gas velocity above the plate

**Results**

- Particle shrinking
- Plate weight
- Porosity profile
- Normalized weight per cell

**Perspectives**

Particle model (Building block) used for
1- prediction of the dry particle mechanical resistance (coupled with a mechanical model)
2- Industrial belt dryer modeling
3- Atomizer modeling
Particle model for drying

Drying with $v_{gas} = 1 \text{ m/s}$
BELT DRYER

Inlet

Outlet
THE COMPLETE BOX

Solid permutation

Gas downflow

Gas upflow

Solid: Lagrangian description
Gas: Eulerian description
OBJECTS DEFINITION

- Box 1
- Box 2
- Box 3
- Box 4
- Box 5
- Box 6

Drying building block

$\cdot d_p$

$\cdot \% \text{ vol. water}$
Development of an atomizer model which includes

- The gel drying particle model developed and validated at lab scale
- A stochastic gel droplet ejection model taking into account
  - Droplet size distribution
  - Ejection angles
  - Ejection velocity
- A momentum balance for each particle taking into account friction forces and gravity
- A elastic collision model between dried particles and the wall
- **Particle-Particle collisions will be neglected** (coalescence phenomenon is not preponderant in a spray)
- The gas velocity field in an atomizer (calculated from 3D Comsol simulations)

This model is developed for a lab scale atomizer (Buchi)

This model is validated with experiments carried out on this atomizer

This model provides

- A statistical evaluation of the atomizer performances
- An 3D animation of the particle trajectories
GAS VELOCITY FIELD

3D simulations with gas only using Comsol: Velocity fields for 2, 10 and 30 m³/h
STOCHASTIC PROCEDURE

- For a given particle
  - Generate a random number $\chi_{wt}$ (between 0 and 1) for the particle size
  - Generate a random number $\chi_{\theta}$ (between 0 and 1) for initial $\theta$ angle
  - Generate a random number $\chi_{\phi}$ (between 0 and 1) for initial $\phi$ angle
  - Initial ejection velocity is set at 10 m/s
  - Start the simulation

\[
\theta = \chi_{\theta} \cdot 2\pi \\
\phi = \chi_{\phi} \cdot \tan^{-1}(R/H)
\]
EFFECT OF GAS FLOWRATE

On Yields ejection

30 µ  30 m3/h  40 µ
time/100 → 0.1 s
STATIC TRAJECTORIES FOR 40 µ

2 m³/h

30 m³/h
Evolution of the drying building block

- In some cases the particle shape is changing during drying
- Experimentally observed in a isotropic drying device (PhD Quentin Gaubert IFPEN/IUSTI)

- Single droplet levitation under drying conditions
  - Droplet levitation system using an acoustic wave
  - Optimization of the gas velocity field in order to reach isotropic conditions
Deformation model: validation

Particle model V1.0

\begin{align*}
    x &= (R + r \cos(v)) \cos(u) \\
    y &= (R + r \cos(v)) \sin(u) \\
    z &= r \sin(v)
\end{align*}

\begin{align*}
    \frac{dV_{\text{vap}}}{dt} &= (1 - \alpha)Q_{\text{vap}} \\
    R + r &= R_{\text{cr}} \\
    \frac{dV_{\text{vap}}}{dt} &= -\alpha Q_{\text{vap}} \\
    V_{\text{lin}} &= 2\pi \left( Rr^2 \left( \frac{1}{2} \sin(2\theta_0) + \frac{2}{3} r^2 \sin^2(\theta_0) \right) \right) \text{ si } R \leq r \\
    V_{\text{con}} &= 2\pi r^3 R \text{ si } R > r
\end{align*}

In progress: deformation = f(operating conditions)
CALCINATION

MOVING BED MODELING
REACTOR SCHEME

Multi-zone calcinator

Catalyst: downflow circulation in a ring
Gas: radial circulation inside the ring
REACTOR SCHEME

On each calcination zone:

- Gas operating conditions:
  - $T_g$, $Q_g$, moisture

- Optional gas recycling:
  - Outlet gas zone 1 $\rightarrow$ Inlet zone 2
Desorption of physisorbed and chemisorbed water

\[ H_2O_{(s)} \xrightarrow{k_1} H_2O_{(g)} \]

Conversion of boehmite to alumina through a reaction intermediate

\[ AlOOH \xrightarrow{k_2} \frac{1}{2} Al_2O_{3-x/2}(OH)_x + \frac{2-x}{4} H_2O_{(g)} \]

\[ Al_2O_{3-x/2}(OH)_x \xrightarrow{k_3} Al_2O_3 + \frac{x}{2} H_2O_{(g)} \]

Hypothesis: First order kinetics

\[ r_1 = k_1[H_2O_{(s)}] \]

\[ r_2 = k_2[AlOOH] \]

\[ r_3 = k_3[Al_{int}] \]

* Thèse F Karouia (2014)
REACTOR DISCRETIZATION

2D model \((r,z)\)
MASS BALANCES

**Solid molar balances**: \( C_i^s \leftrightarrow \text{[mol}_s \cdot \text{m}^{-3}\text{ particle]} \)

\[
\varepsilon_s \cdot \frac{\partial C_i^s}{\partial t} = -\frac{\partial (v_{ss} \cdot C_i^s)}{\partial z} + \sum_j \mu_{ij} \cdot r_j \cdot \varepsilon_s
\]

**Gas molar balances**: 

\[
(\varepsilon_g + \varepsilon_p \varepsilon_s) \cdot \frac{\partial C_i^g}{\partial t} = -\frac{1}{r} \cdot \frac{\partial (r \cdot v_{sg} \cdot C_i^g)}{\partial r} + \sum_j \mu_{ij} \cdot r_j \cdot \varepsilon_s
\]

**Equation of state**: 

\[
\frac{\partial}{\partial r} \left( \frac{r \cdot v_{sg}}{T_g} \right) = -(\varepsilon_g + \varepsilon_p \varepsilon_s) \cdot \frac{r}{T_g^2} \cdot \frac{\partial T_g}{\partial t} + r \cdot \frac{R}{P_{tot}} \sum_i \sum_j \mu_{ij} \cdot r_j \cdot \varepsilon_s
\]
THERMAL BALANCES

Solid thermal balance:

\[
\rho_s \cdot C_{ps} \cdot \varepsilon_s \cdot \frac{\partial T_s}{\partial t} = -v_{ss} \cdot \rho_s \cdot C_{ps} \cdot \frac{\partial T_s}{\partial z} + \sum_j r_j \cdot (-\Delta H r_j) \cdot \varepsilon_s + h_{gs} \frac{A_p}{V_p} \cdot \varepsilon_s \cdot (T_g - T_s)
\]

Gas thermal balance:

\[
\rho_g \cdot C_{pg} \cdot \varepsilon_g \cdot \frac{\partial T_g}{\partial t} = -v_{sg} \cdot \rho_g \cdot C_{pg} \cdot \frac{\partial T_g}{\partial r} - h_{gs} \frac{A_p}{V_p} \cdot \varepsilon_g \cdot (T_g - T_s)
\]
MODEL RESULTS

Sheet “color_map”:
IMPREGNATION

IMPREGNATION MODELING
OBJECTIVES

- Development of particle model for impregnation
  - Dry impregnation
  - Wet impregnation

- Comparison with experimental work based on MRI measurements

- Optimization of the impregnation step in the catalyst manufacturing procedure
CAPILLARY SUCTION MODELING

\[ \frac{d(m.\, \dot{v})}{dt} = F_{\text{capillary}} + F_{\text{friction}} \]

\[ F_{\text{capillary}} = \Delta P_{\text{Laplace}} \cdot S \]

\[ \Delta P_{\text{Laplace}} = \frac{2 \cdot \gamma \cdot \cos\theta}{R_{\text{pore}}} \]

\[ S = \pi \cdot R_{\text{pore}}^2 \]

\[ F_{\text{capillary}} = 2 \cdot \pi \cdot R_{\text{pore}} \cdot \gamma \cdot \cos\theta \]
CAPILLARY SUCTION MODELING

\[(P_1 - P_2) \cdot 2 \cdot \pi \cdot r \cdot dr + 2 \cdot \pi \cdot r \cdot z \cdot \tau - 2 \cdot \pi \cdot (r + dr) \cdot z \cdot (\tau + d\tau) = 0\]

\[d(r \cdot \tau) = \frac{\Delta P_{\text{friction}} \cdot r \cdot dr}{2 \cdot z}\]

\[\tau = -\mu \cdot \frac{dv}{dr}\]

\[\int_r^{\text{wall}} dv = \int_r^{R_{\text{pore}}} - \frac{\Delta P_{\text{friction}} \cdot r \cdot dr}{2 \cdot \mu \cdot z}\]

\[v(r) = \frac{\Delta P_{\text{friction}}}{4 \cdot \mu \cdot z} \cdot (R_{\text{pore}}^2 - r^2)\]

\[\bar{v} = \frac{\Delta P_{\text{friction}} \cdot R_{\text{pore}}^2}{8 \cdot \mu \cdot z}\]

\[F_{\text{friction}} = \Delta P_{\text{friction}} \cdot S\]

\[F_{\text{friction}} = 8 \cdot \pi \cdot \mu \cdot z \cdot \bar{v}\]
CONVECTION-DIFFUSION- ADSORPTION MODELING

- For a cylindrical particle

  - Compounds in pores during capillary suction
    \[ \varepsilon_p \cdot \frac{\partial C_i^p}{\partial t} = \frac{D_{eff}}{r} \cdot \frac{\partial}{\partial r} \left( \frac{r \cdot \partial C_i^p}{\partial r} \right) + \frac{\varepsilon_p}{r} \cdot \frac{\partial}{\partial r} \left( r \cdot \vec{v} \cdot C_i^p \right) + \sum_j \mu_{ij} \cdot r_{kin} \cdot \rho_s \]

  - Compounds in pores when the particle is completely wetted
    \[ \varepsilon_p \cdot \frac{\partial C_i^p}{\partial t} = \frac{D_{eff}}{r} \cdot \frac{\partial}{\partial r} \left( \frac{r \cdot \partial C_i^p}{\partial r} \right) + \sum_j \mu_{ij} \cdot r_{kin} \cdot \rho_s \]

  - Compounds on the solid surface
    \[ \frac{\partial C_i^*}{\partial t} = \frac{D_s}{r} \cdot \frac{\partial}{\partial r} \left( r \cdot \frac{\partial C_i^*}{\partial r} \right) + \sum_j \mu_{ij} \cdot r_{kin} \]

Washburn model

Volumetric flow rate conservation
\[ \frac{\partial}{\partial r} (r \cdot \vec{v}) = 0 \]

HYDROCARBURES RESPONSABLES
MODEL VALIDATION: DRY IMPREGNATION

Case of 0,2M $[\text{Ni}^{2+}]$

Adsorbed Nickel

Nickel in pores
MODEL VALIDATION: WET IMPREGNATION

Case of 0,2M [Ni^{2+}]

Adsorbed Nickel

Nickel in pores
Identifcation and study of relevant solid descriptors during boehmite synthesis

Thesis starting in 2018
Giullia Ferri
OBJECTIVES

- Construction of an unique solid structure model where the empirical parameters are adjusted for each unit operation step

- Variations of these parameters through the different steps should:
  - allow to evaluate their sensitivities
  - allow to evaluate their impact on the final textural properties

- The final objective is to estimate the values of those parameters for different unit operation in order to reach a given set of textural properties.
1. Improvement of the solid construction model (dry and wet media)

- Solid structural model: Stochastic assembly of elementary particles. The stochastic methodology is based on specific distribution functions such as:
  - Fractal dimension
  - Agglomerates size
  - Aggregates size
  - Preferential sticking faces of the elementary particles
  - ...

- Distribution functions
  - Continuous or discretes
  - Different types (log-normal, gaussian,...)
  - Characterized by a limited number of parameters (mean, standard deviation,...)

- Calculation of the global properties of the reconstructed solid
  - Size pore distribution
  - Porous volume
  - SBET
  - Crystal size distribution
  - ...

Thèse Haisheng Wang (Mines de Paris / IFPEN 2016)

2 scales model
Model parameters
  - Elementary particle size
  - Size of aggregates
  - Number of elementary particles in aggregates
  - ...
Validation on SBET, Vp, TEM images, Nitrogen desorption, ...
2. Solid analytical characterization at each step
   - What are the analytical techniques available?
     - SAXS
     - Mercury porosity
     - MEB
     - ...
   - Reliability in wet conditions
   - Development or modification of specific analytical methods in order to define new descriptors
   - Are all these methods enough to sensitize the global set of textural properties?

3. Optimization of distribution function parameters in order to reproduce the analytical results obtained at each steps.
   - Follow their evolution after each steps
   - Sensitivity analysis to identify which steps are critical for the final textural properties

4. Modeling of the distribution parameters based on physical-chemical descriptors (interaction with the DLVO model)
   - pH, zeta potential, Re, shear stress, Drying severity...
EXPERIMENTAL STUDY AND MODELLING OF A COLLOIDAL GEL RHEOLOGY UNDER PHYSICO-CHEMICAL AND HYDRODYNAMIC CONSTRAINTS

Thesis starting in 2019
Iana Sudreau
From lab to ind. scale

- CFD development with complex fluid
- population balance implementation
- CFD + fluid model validation

Complementary PhD proposal (2020)

Population balance modeling of gelation process
- macroscopic scale, observation $\mu(t), \dot{\gamma}(t)$
- laminar
- turbulent

Compartmental model coupled with population balance

Structuration and breakage modeling of colloids aggregates
- scale: nm
- observation: colloidal structure

| pH, $C_s$, $r_c$, $\zeta$ | $D_f$, $\dot{\gamma}(t)$ | $S: |\mu(t)|_{\dot{\gamma}=\text{cte}}$, $\dot{\gamma}(x, y, z)$ | $S: \mu(t, \dot{\gamma})$ |
|--------------------------|--------------------------|-------------------------------------------------|--------------------------|

$C_s$: salt concentration, $r_c$: colloid radius, $\zeta$: zeta potential, $D_f$: fractal dimension, $\mu$: viscosity, $\dot{\gamma}$: shear rate
STRATEGY – COMPARTMENTAL MODELING

- shear rate field obtained from CFD simulation (COMSOL / FLUENT)
- shear rate data transposed to a structured grid (FORTRAN code)
- compartmentalization according to the shear rate field
- calculation of mean entrance and outlet compartmental flow rate
- population balance modeling inside each compartment

velocity field from CFD simulation – \([\text{m.s}^{-1}]\)

structured mesh

shear rate compartmentalization
determination of mean entrance and outlet compartment flow rate

population balance modelling run inside each compartment
Innovating for energy

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