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Strategies for Controlled Latex Particle Coagulation incorporating CFD analysis

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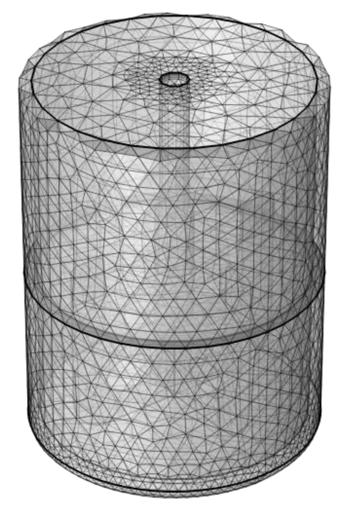
Introduction

Coagulate PMMA polymer system:

- Minimise fouling in the reactor
- Narrow Particle Size Distribution (PSD)
- Homogenous morphologies (HM)

Optimum reactor/impeller geometry → Homogeneous shear

Verify by Computational Fluid Dynamics (**CFD**) using **COMSOL Multiphysics**



Physical Model → **Turbulent flow-kε** (↑ Re)

Momentum balance → **Navier-Stokes**
Mass conservation → **Continuity equation**

Methodology

Coagulation

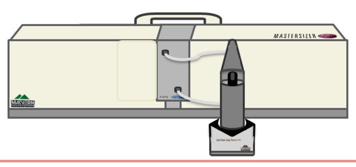
100 mL reactor
NaCl addition 1 h + 3h mixing
T= 25, 50, 75 or 90 °C
Speed= 200, 400 or 700 rpm
NaCl: 0.3 or 1 M

$$G = \sqrt{\frac{\epsilon}{\nu}}$$
Average shear rate

$$Pe = \frac{3\pi\mu G r_i r_j (r_i + r_j)}{2k_B T}$$
Peclet number

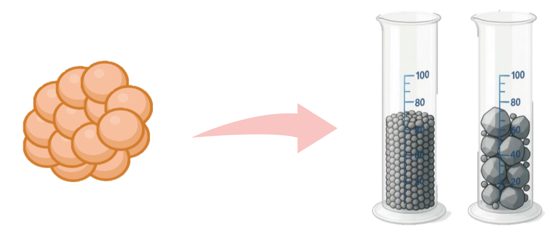
$$W' \approx \frac{1}{2\kappa a} e^{\left(\frac{V_{Tmax}}{k_B T}\right)}$$
Fuch stability ratio

Laser diffraction



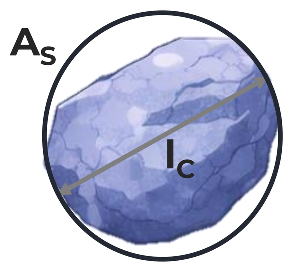
SEM

Bulk density calculation



$$\rho_B = \frac{Weight\ of\ powder\ (g)}{Bulk\ volume\ of\ powder\ (cm^3)}$$

2D-fractal dimensión



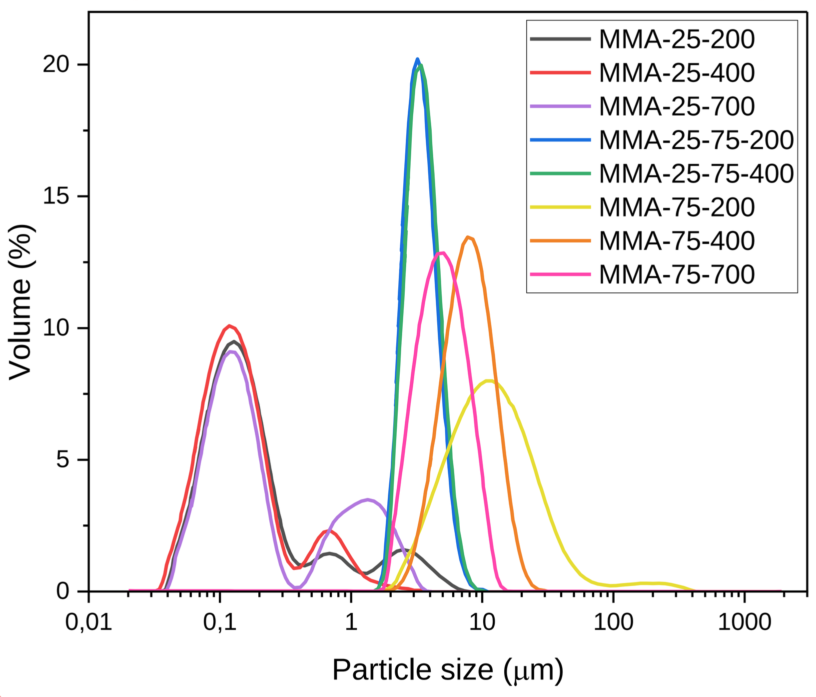
$$A_S \propto l_c^{D_2}$$

From1-2
(↑ homogeneous)

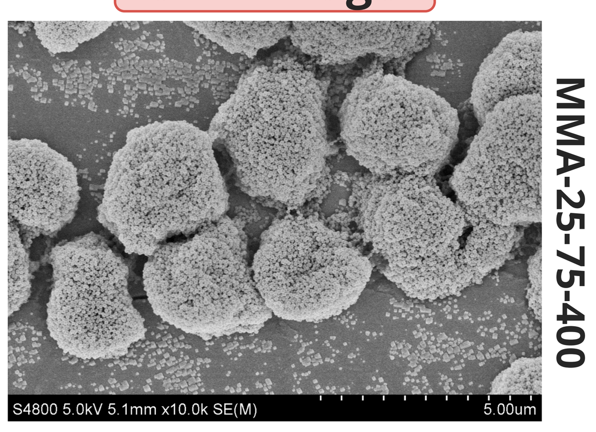
Results

Experimental results

Volume Particle size distribution (PSD)

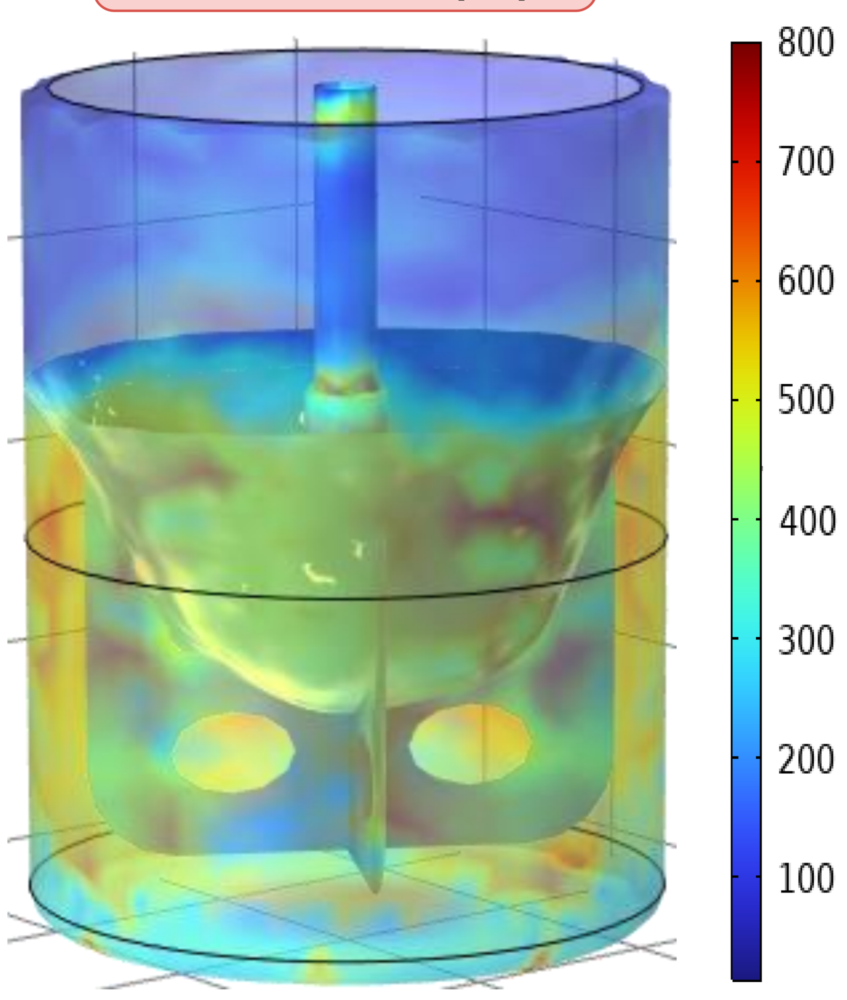


SEM image

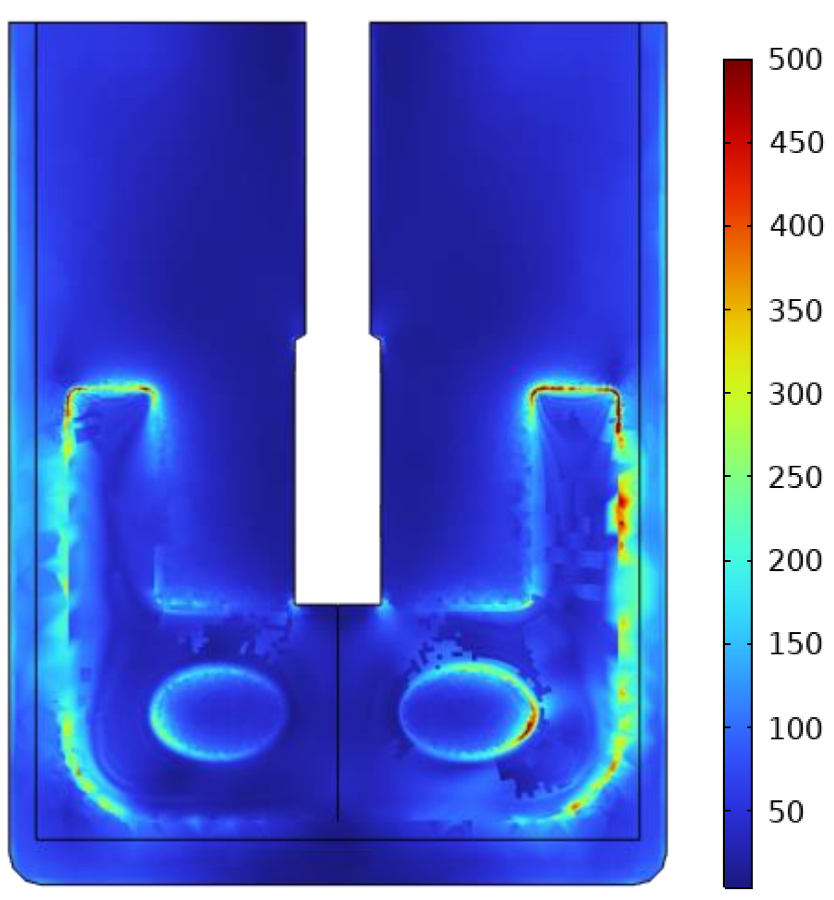


Experiment T	Narrow PSD	HM
25 °C	✗	✗
75 °C	✓	–
25-75 °C	✓	✓

CFD: Shear rate in reactor wall (s^{-1})

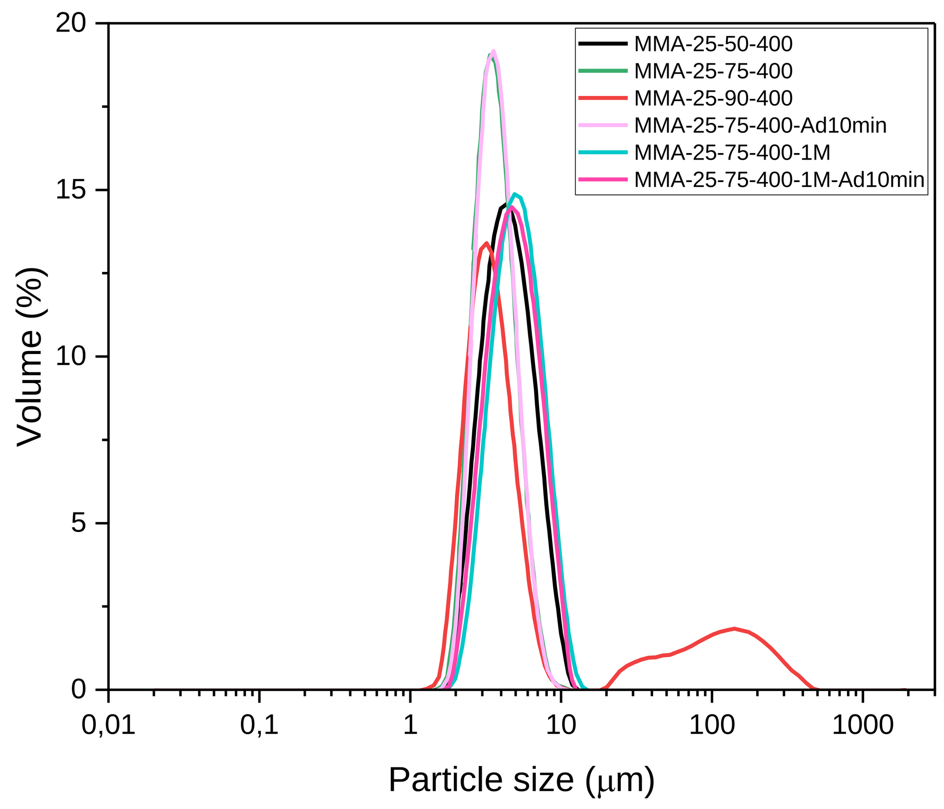


CFD: Shear rate cut plane (s^{-1})

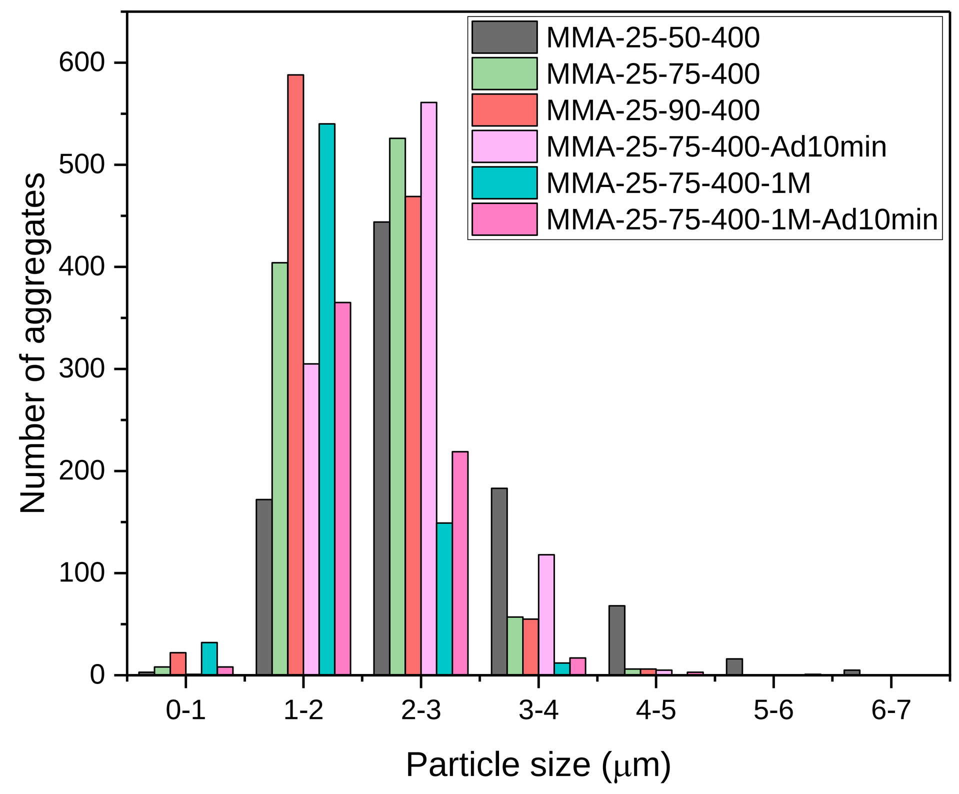


Average shear rate				
	Wall (s^{-1})	Bottom (s^{-1})	Reactor (s^{-1})	Experimental (s^{-1})
400 rpm	371	287	356	286

Volume Particle size distribution (PSD)



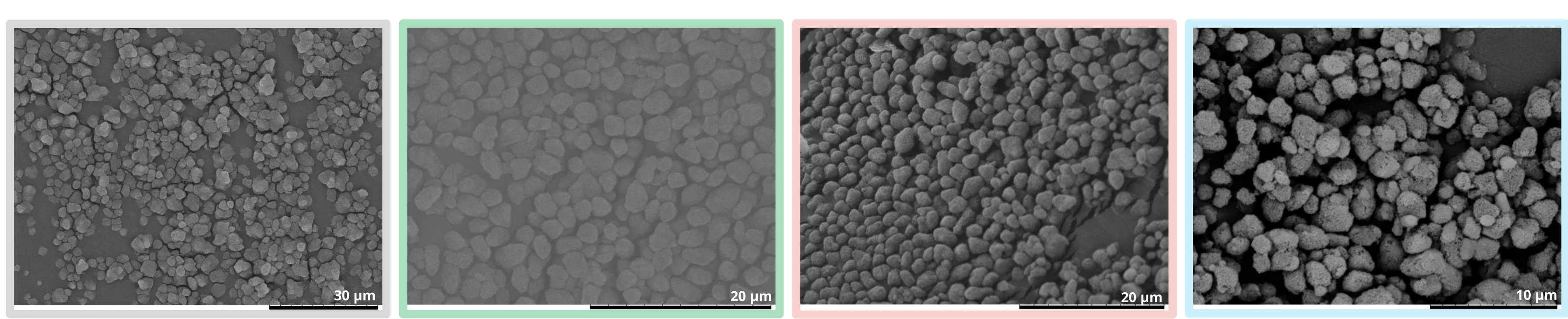
Number Particle size distribution (PSD)



Experiment	Pe	W'	$dp_{volMaster}$ (µm)	dp_{volSEM} (µm)	D_2	Bulk density (g/cm^3)
MMA-25-50-400	1.61	$6.46 \cdot 10^9$	4.8	3.8	1.82	0.36
MMA-25-75-400	1.50	$6.46 \cdot 10^9$	3.5	2.6	1.87	0.35
MMA-25-90-400	1.43	$6.46 \cdot 10^9$	3.8	2.6	1.73	0.26
MMA-25-75-400-Ad10min	1.50	$6.46 \cdot 10^9$	3.6	2.8	1.78	0.32
MMA-25-75-400-1M	1.50	0.15	5.5	2.2	1.67	0.30
MMA-25-75-400-1M-Ad10min	1.50	0.15	5.1	2.6	1.67	0.30

Morphology (SEM)

MMA-25-50-400 | MMA-25-75-400 | MMA-25-90-400 | MMA-25-75-400-1M



Conclusion

Temperature control

50 °C → Not enough E for better arrangement (D_2)

75 °C → Perfect T to maintain enough E and particle-cluster aggregations (Higher D_2 and Bulk density)

90 °C → Close to Tg. Penetration between aggregates

NaCl concentration

0.3 M → Minimum coagulant ensures controlled coagulation and better particle arrangement in the aggregates.

1 M → Excess of coagulant **does not improve** homogeneity (D_2) and powder packing. Less compact aggregates and lower stability (W')

CFD

- Able to recreate experimental reactor.
- **Average shear rate** → same range as experimental value
- **Local shear rate** → impeller blades and reactor wall

Key outcome

Control of operating conditions lead to narrow Volume and Number PSD, homogeneous morphologies (↑ D_2) and ↑ bulk density

MMA-25-75-400

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