

Determining an Empirical Coefficient for Particle-Surface Interactions in Discrete Element Method Simulations

Ryan Duong, Chemical Engineering
Mentor: Heather Emady, Associate Professor
School for Engineering of Matter, Transport and Energy



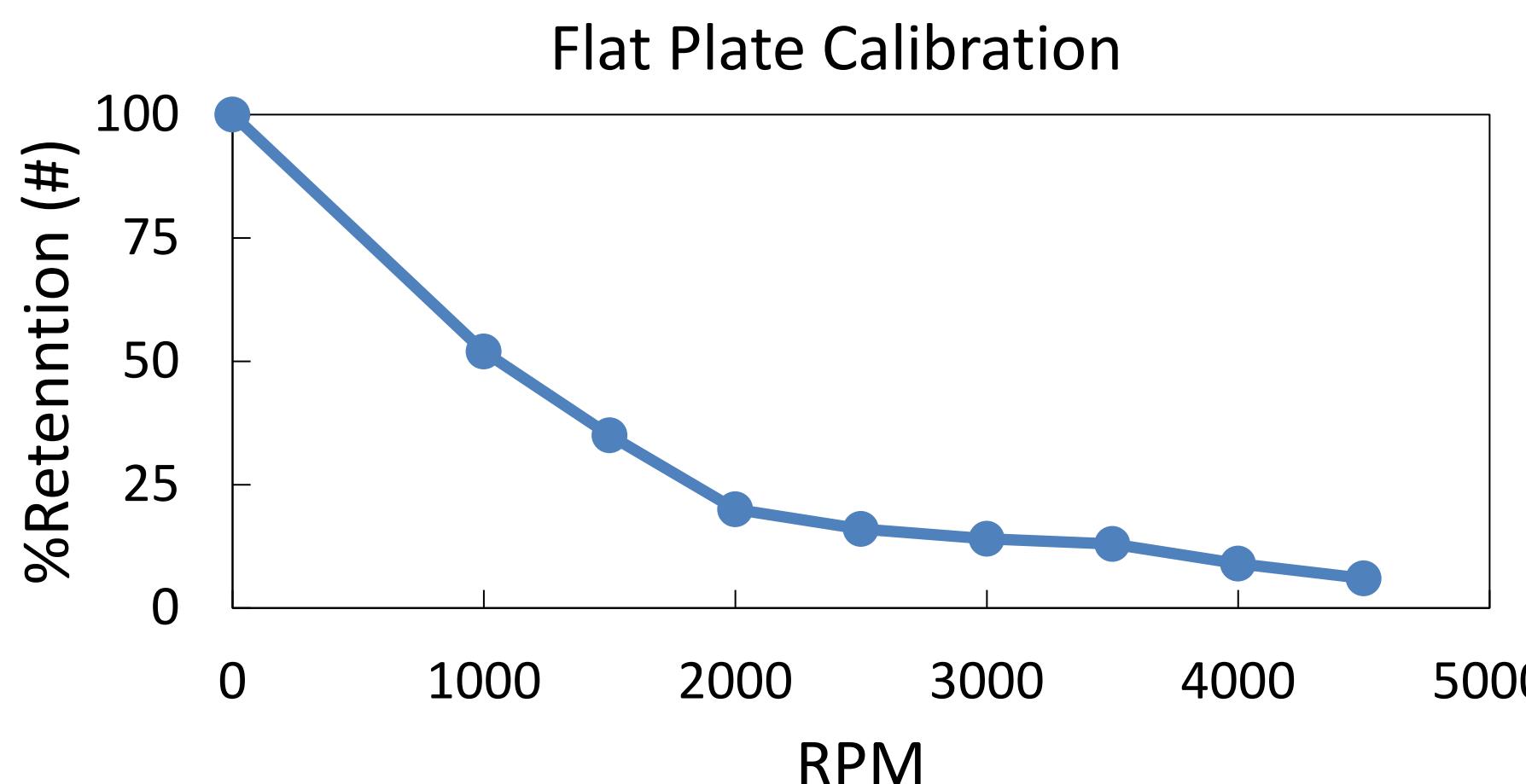
Creating material specific particle-surface adhesion coefficients enables more accurate and realistic computer simulation predictions for real-world situations

Background

- Discrete Element Method (DEM) simulations model particle behavior [1]
- Used to replicate existing processes

Methods

- 32-38 μm polyethylene microspheres
- 3D printed high-speed resin flat plate
- Centrifuge at 1000-4500 RPM & image
- Reproduce in EDEM simulation



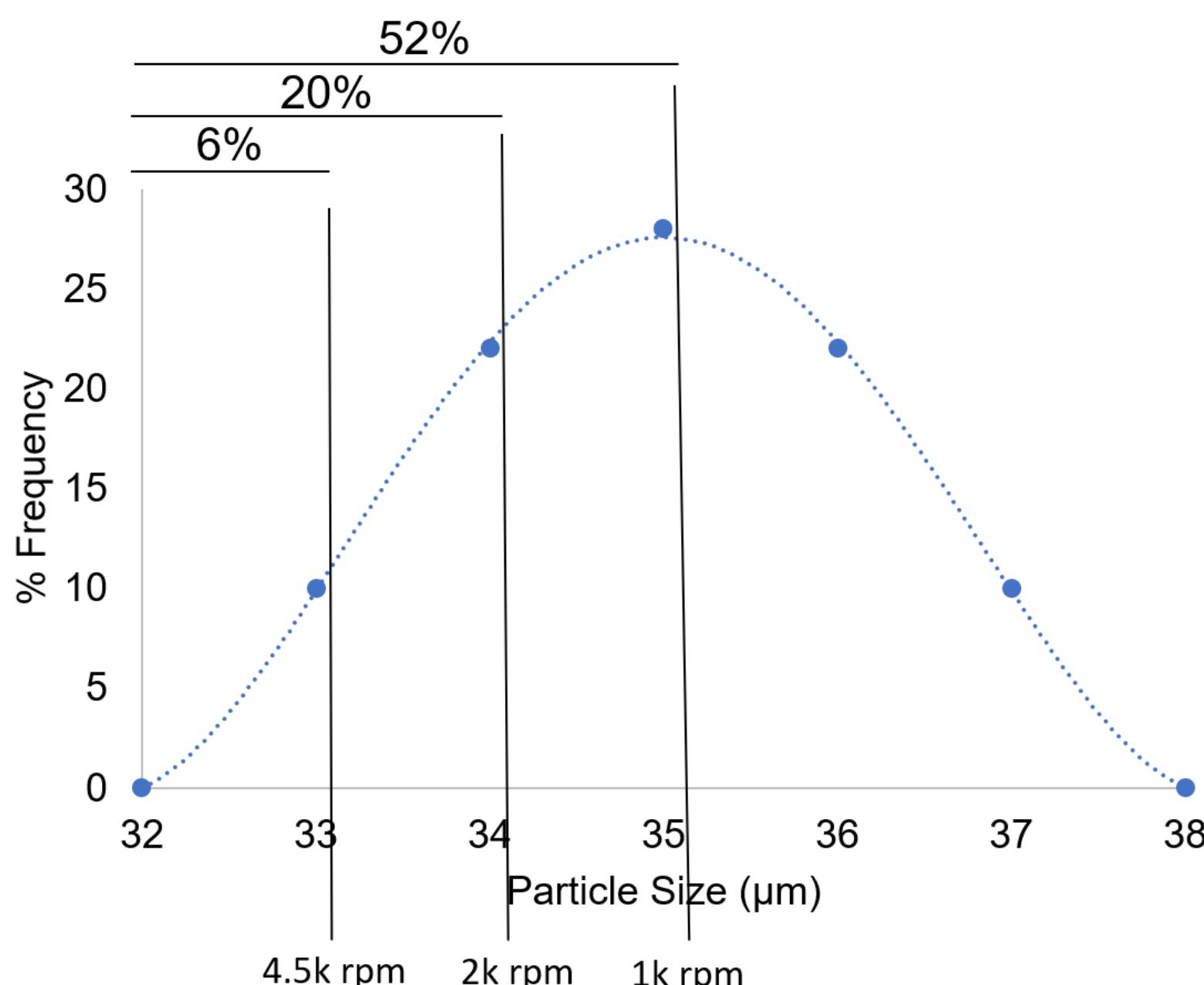
Contact Model of Interest: [2]

- Johnson-Kendall-Roberts (JKR) v2:

$$F_n = \frac{4E^*a^3}{3R^*} - (8\pi\Gamma E^*a^3)^{\frac{1}{2}}$$



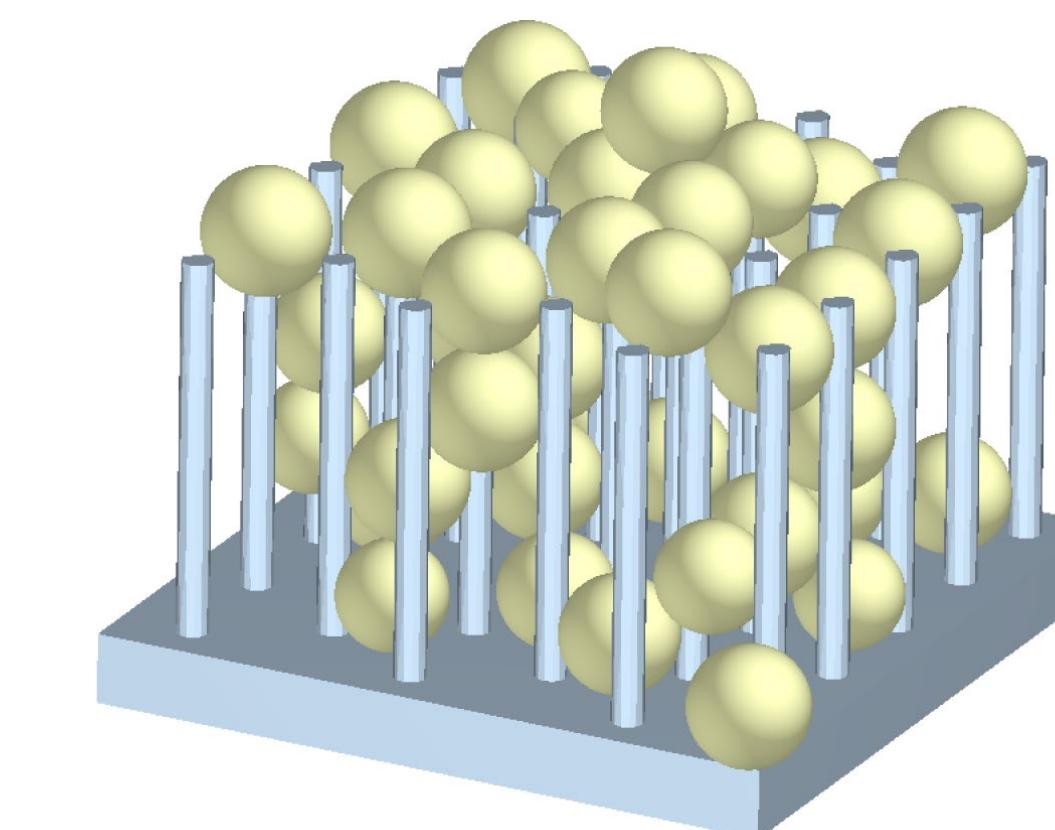
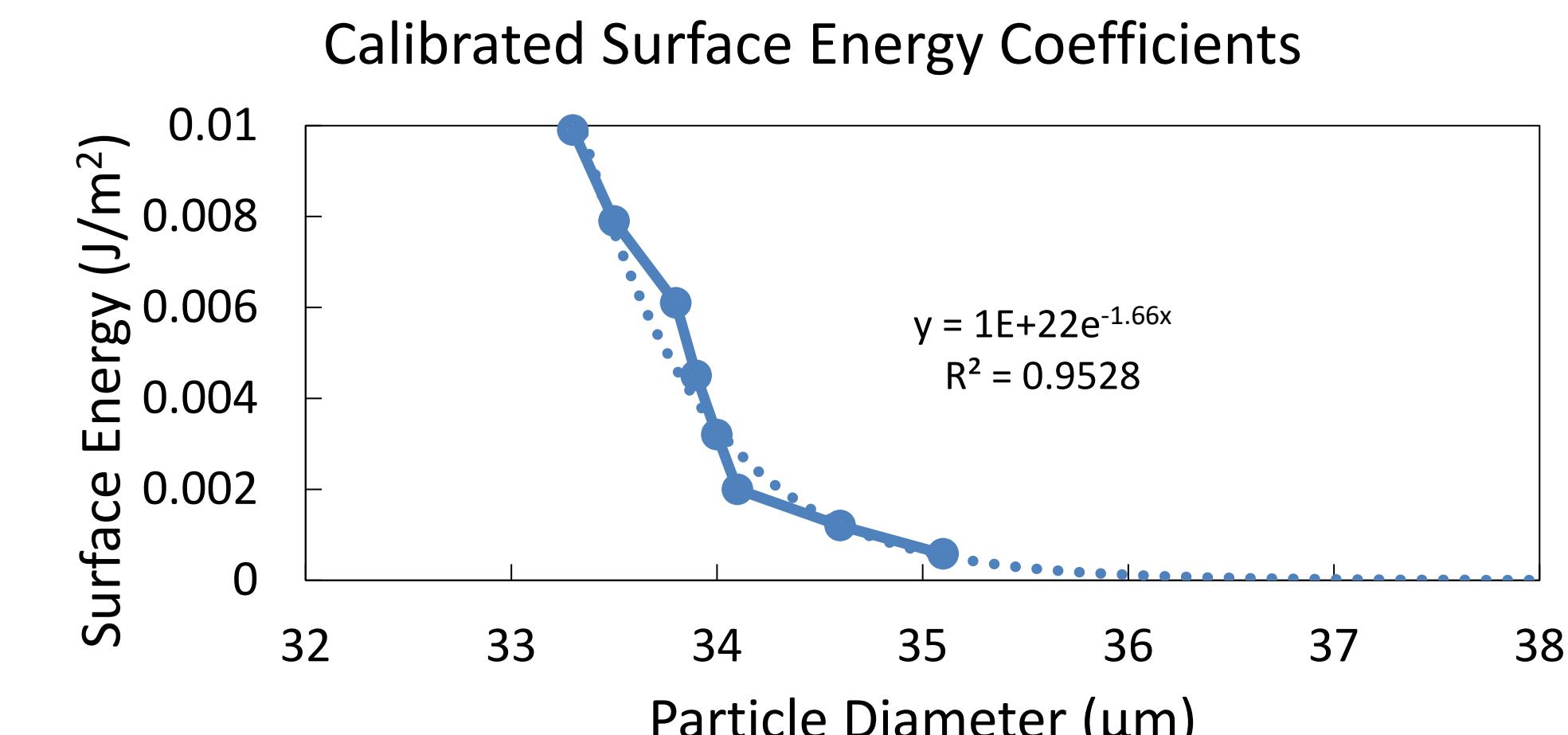
- E^* = Relative Elasticity
- R^* = Relative Radius
- Γ = Interfacial Surface Energy
- a = Contact Radius



- Manipulate gravity as constant pull off force (RPM equivalents)
 - Manually adjust surface energy until particles below a certain size stick
- Experimentally calibrate Γ to match desired %-retention curve per particle size
 - Account for capillary forces, electrostatics & more

RPM	% Particles Remaining	% Particles in Bin	Max Particle Size Remaining (μm)	Surface Energy (J/m^2)
0	100	48	38.0	4.00E-06
1000	52	17	35.1	5.80E-04
1500	35	15	34.6	1.20E-03
2000	20	4	34.1	2.00E-03
2500	16	2	34.0	3.20E-03
3000	14	1	33.9	4.50E-03
3500	13	4	33.8	6.10E-03
4000	9	3	33.5	7.90E-03
4500	6	6	33.3	9.90E-03

Results



Particle Size (μm)	Predicted Γ (J/m^2)
38	4.00E-06
37	2.12E-05
36	1.11E-04
35	5.86E-04
34	3.08E-03
33	1.62E-02
32	8.52E-02

Impacts

- Enable future hair-like material research with polyethylene-resin simulations as prospective design
- Enhance understanding of sensitivity of model parameters

References

[1] Zhu, H. P., Zhou, Z. Y., Yang, R. Y., & Yu, A. B. (2007). Discrete particle simulation of particulate systems: Theoretical developments. *Chemical Engineering Science*, 62(13), 3378–3396. <https://doi.org/10.1016/j.ces.2006.12.089>

[2] Altair EDEM. (2025). Base Contact Models: EDEM Contact Models. https://help.altair.com/edem/topics/creator_tree_physics/the_edinburgh_elasto_plastic_adhesion_model_eepa_r.htm