

Particle-scale DEM model for investigating calendering effects in dry electrode manufacturing



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BACKGROUND AND AIM

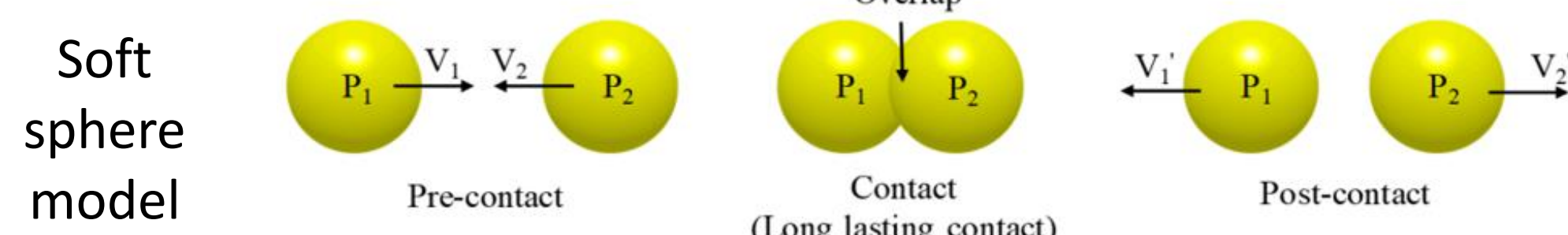
- Lithium-ion batteries** are the cornerstone of modern energy storage, delivering high energy density and reliability across applications from portable electronics to electric vehicles [1]. Their performance is tightly linked to electrode design and manufacturing processes.
- Calendering** plays a vital role in enhancing the performance of lithium-ion battery electrodes by altering their structural, mechanical, and transport properties. However, understanding the underlying mechanics, particularly the interplay between pressure, deformation, and interfacial behaviour, remains a challenge. Advanced simulation tools like DEM provide new opportunities to capture these effects with high fidelity.
- In this study**, we use Discrete Element Method (DEM) simulations to compare uniaxial (flat-plate) and roller-based calendering approaches for evaluating their effects on porosity, stress distribution, tortuosity, conductivity, and adhesion strength, and assessing which approach better represents real industrial calendering.

METHODOLOGY

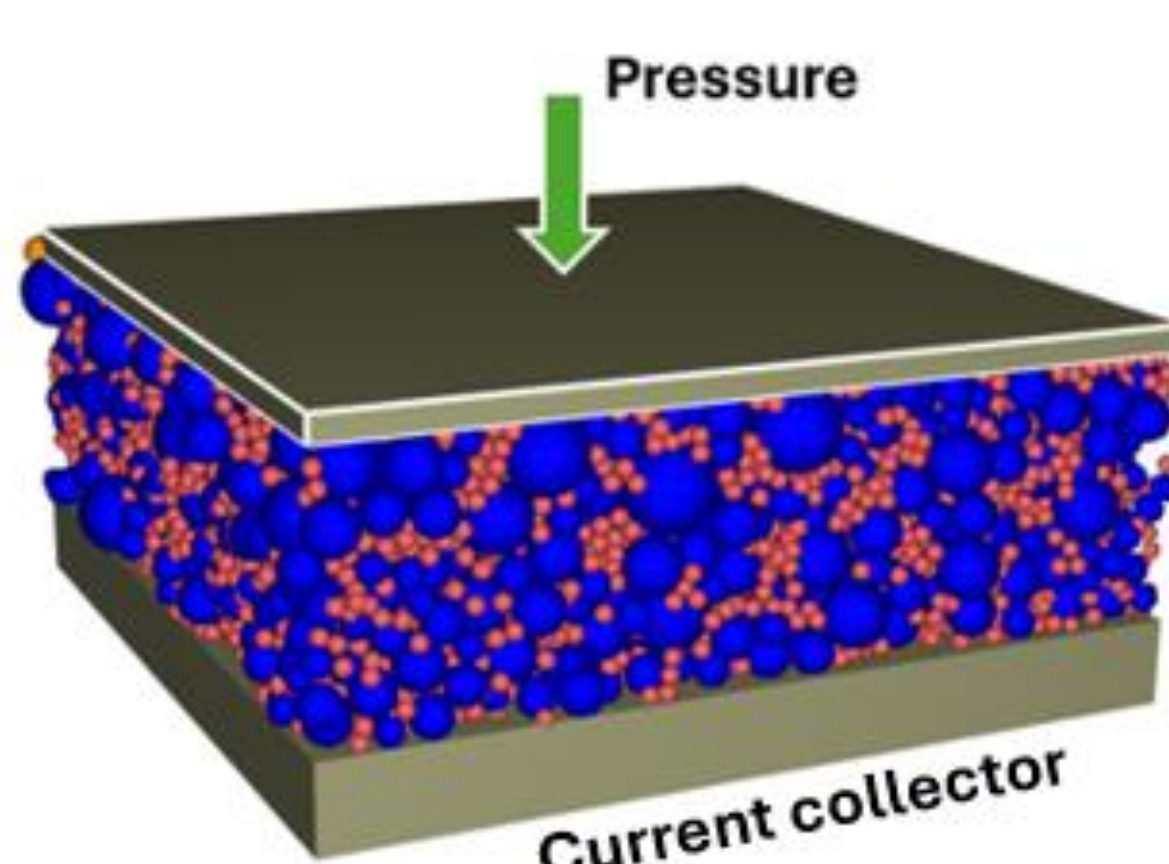
Discrete Element Method (DEM) is a numerical approach used to simulate the behavior of particulate materials by resolving the motion and interaction of individual particles. Each particle acts as a separate element whose contacts, collisions, and force transmissions are tracked over time according to Newton's laws of motion.

$$m_i \frac{dv_i}{dt} = \sum (F_{ij}^n + F_{ij}^t) + m_i g \dots \dots \dots (1)$$

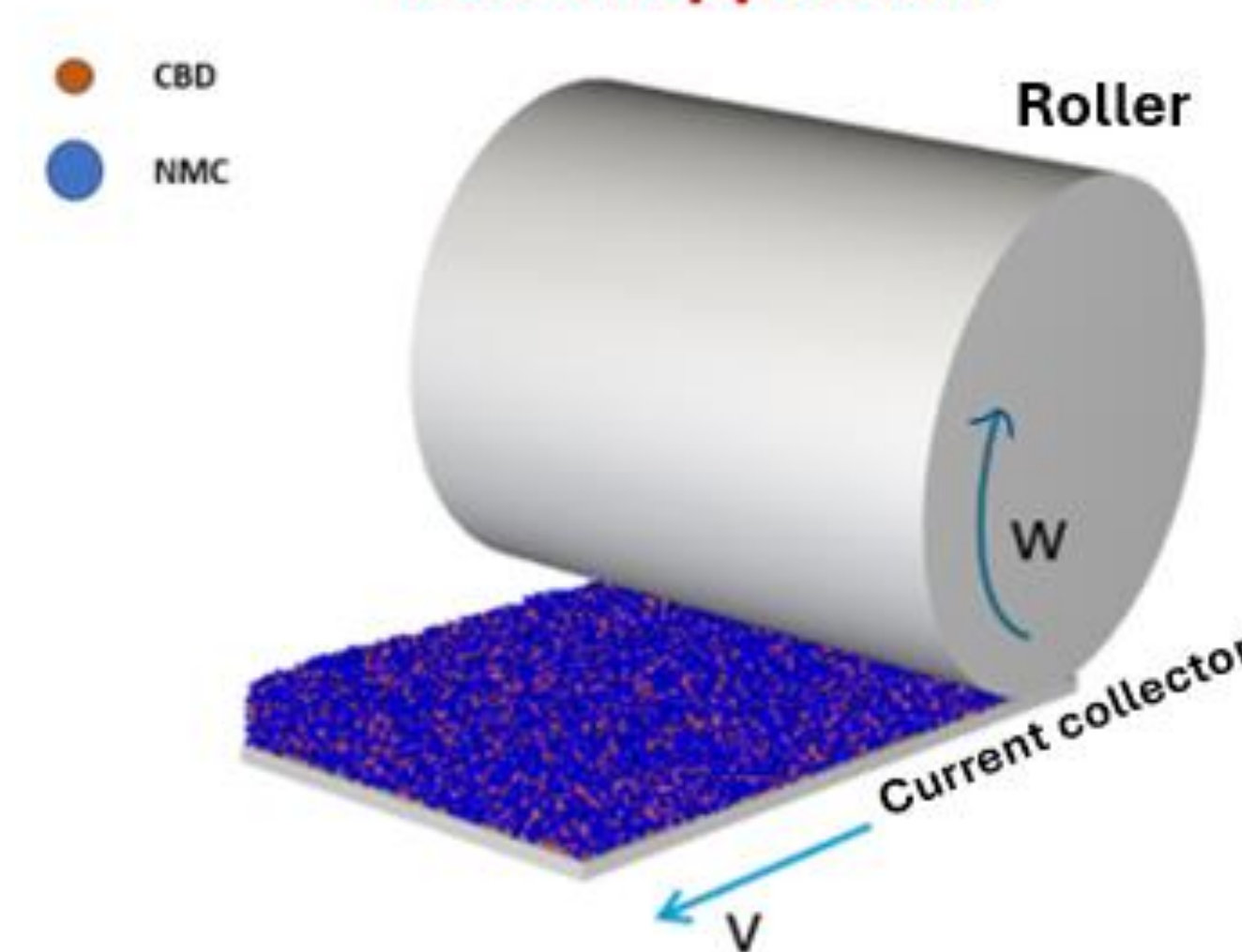
$$I_i \frac{d\omega_i}{dt} = \sum (R_i \times F_{ij}^t - \tau_{ij}^r) \dots \dots \dots (2)$$



Uniaxial (Flat Plate) Approach



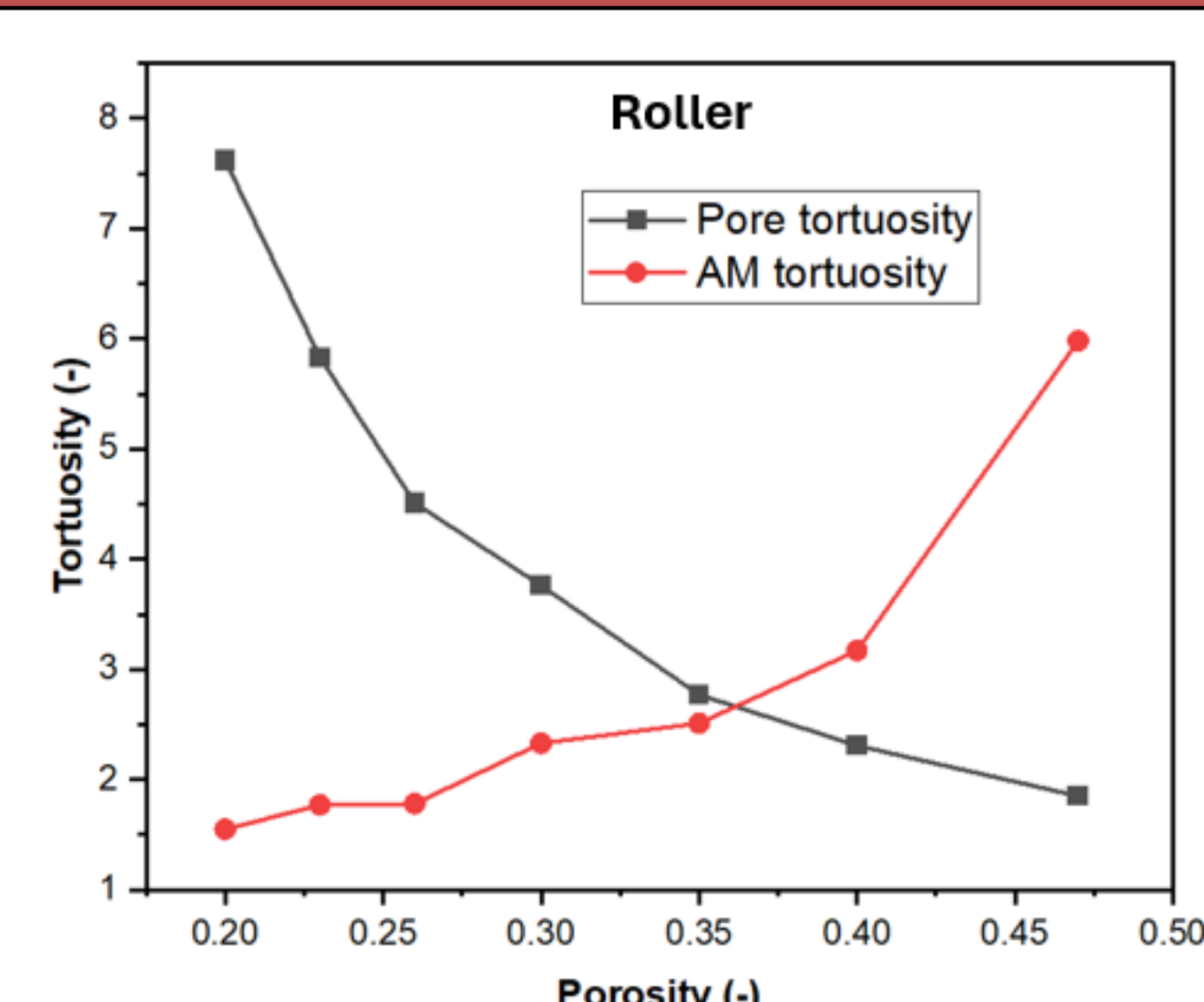
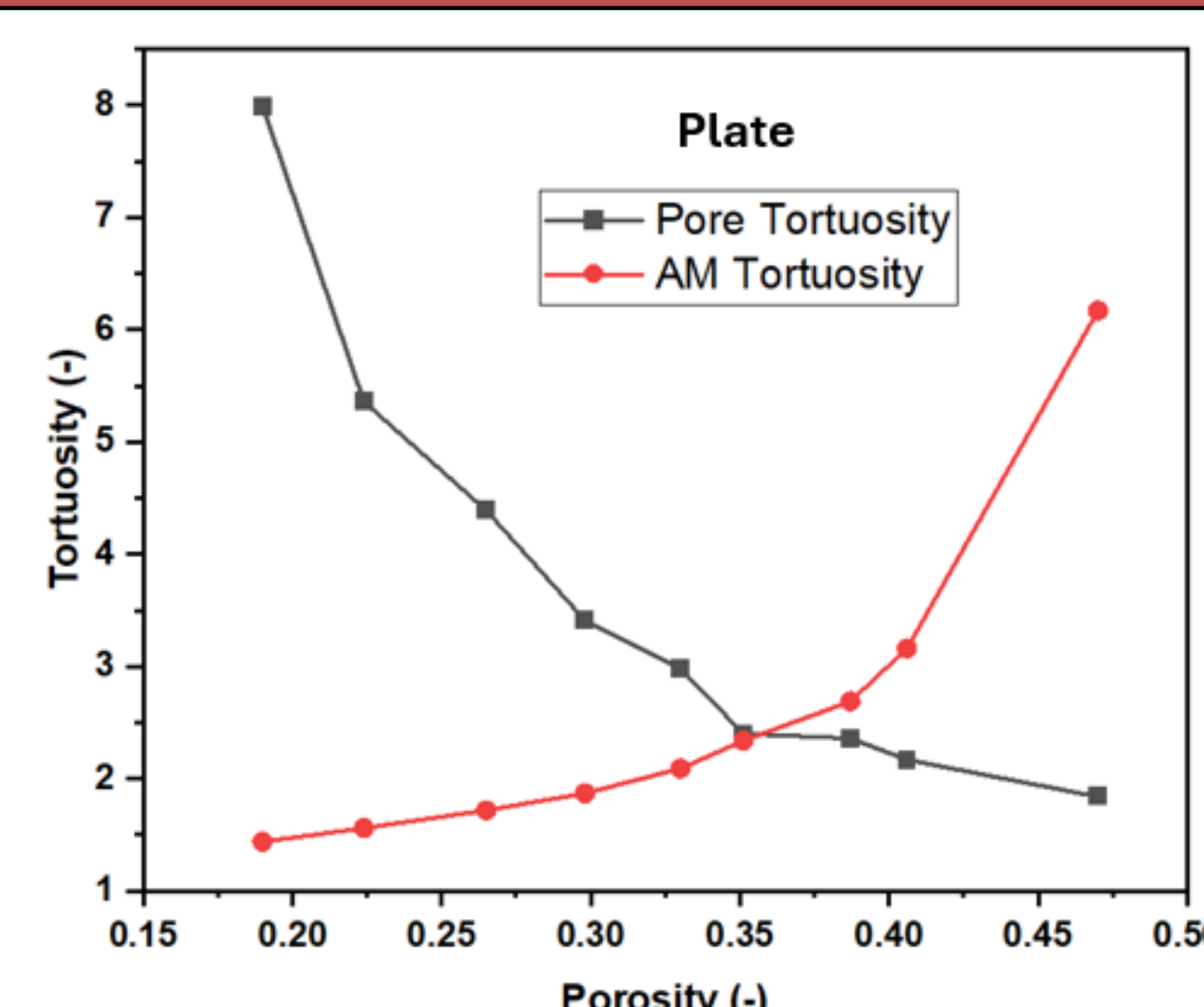
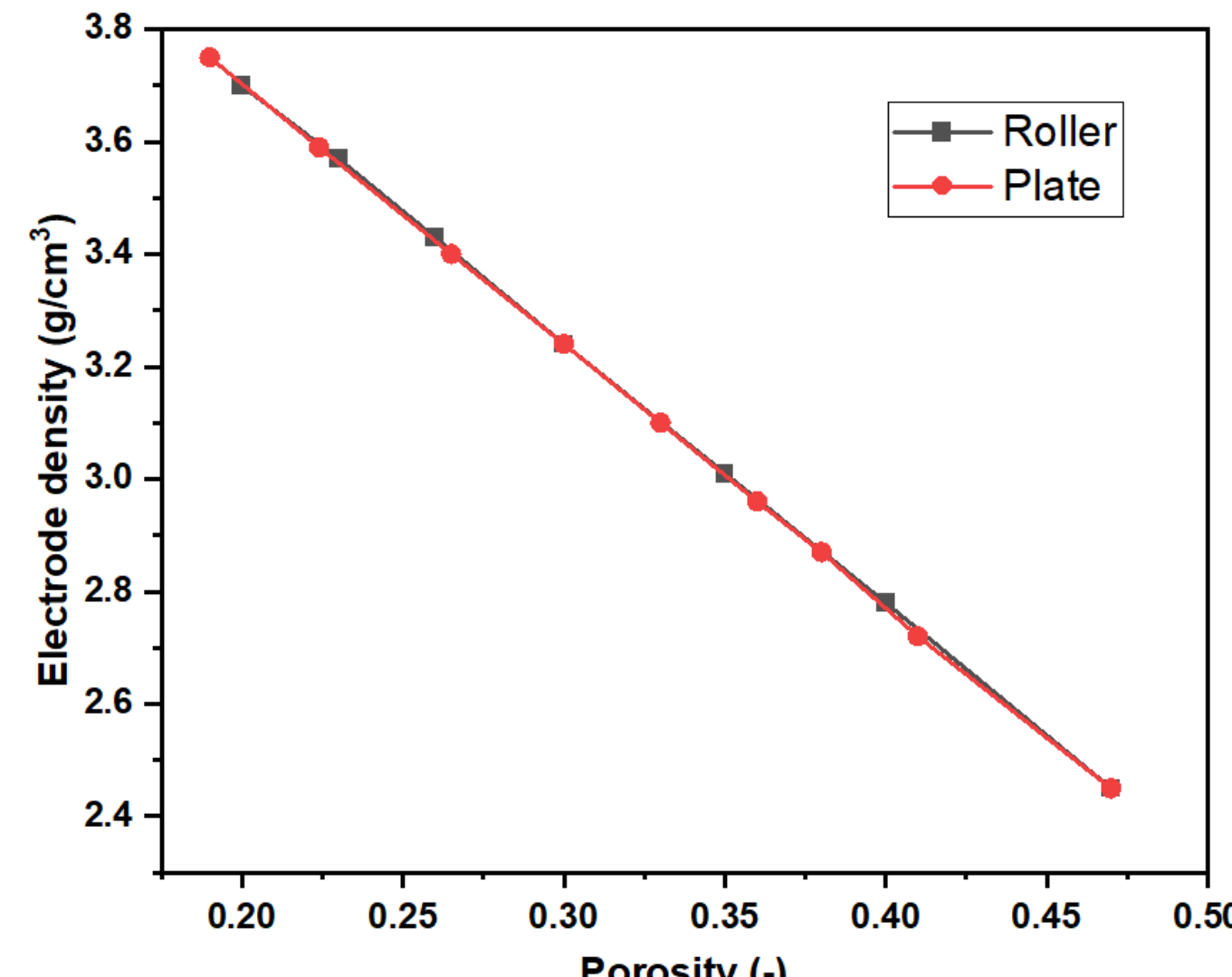
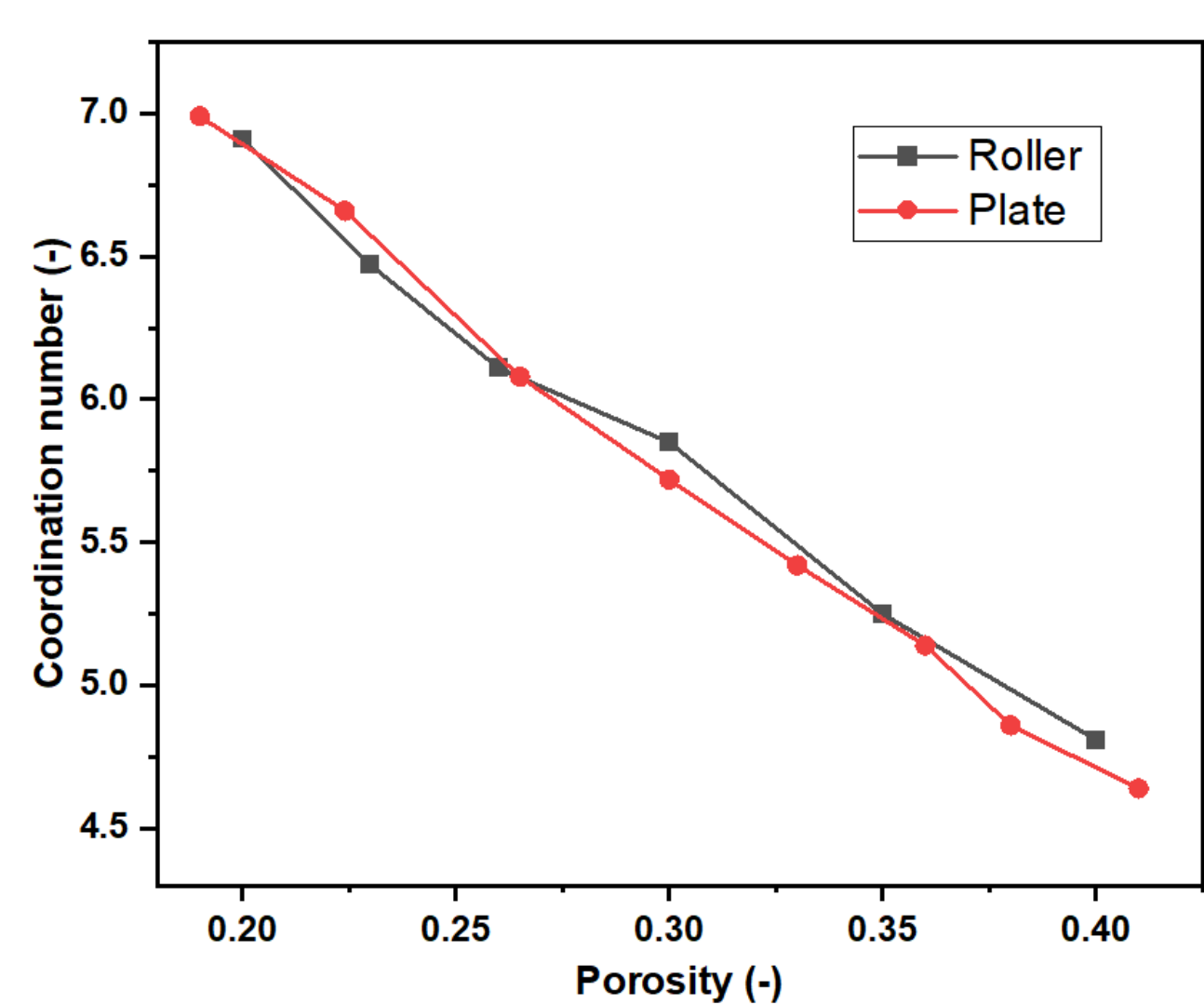
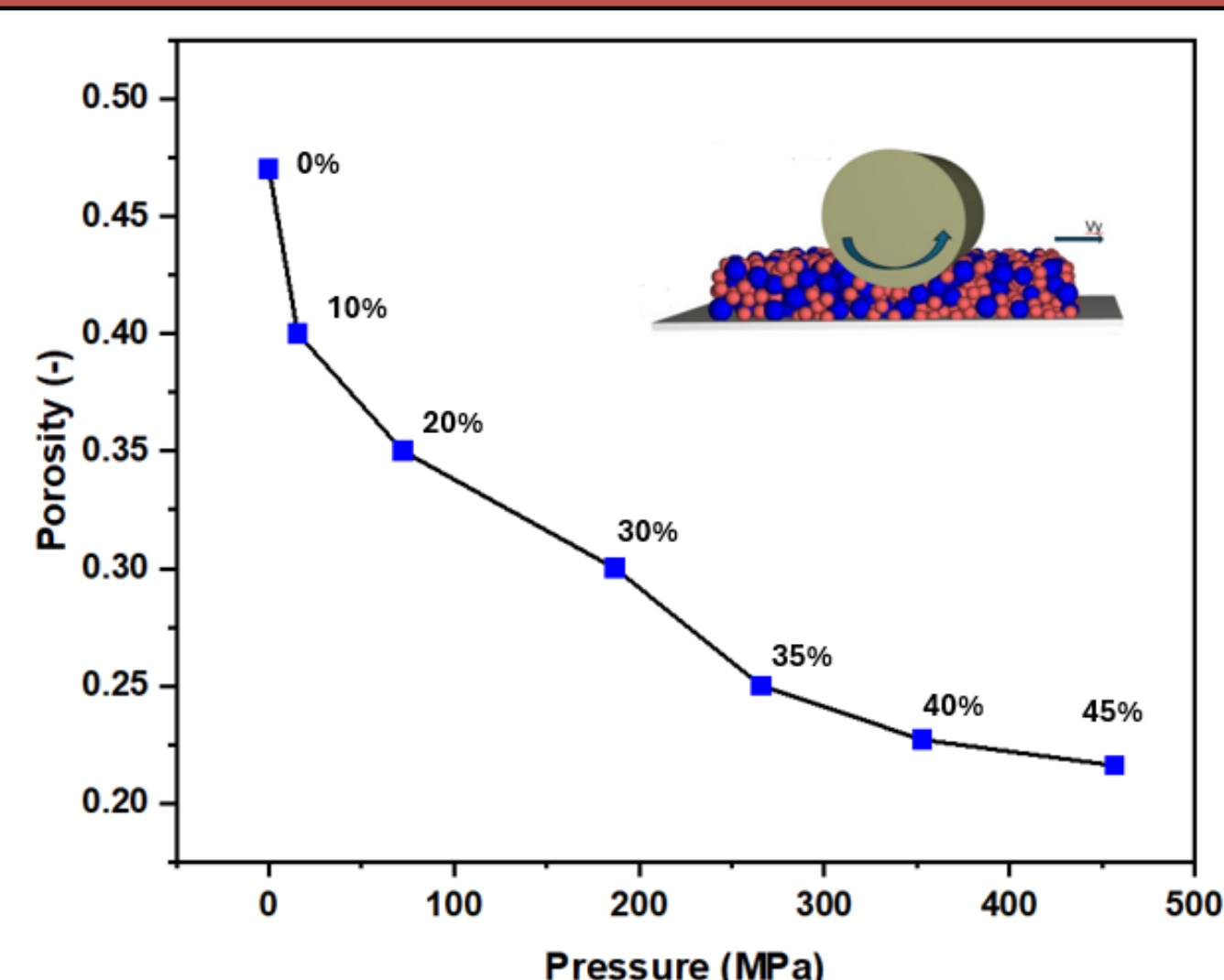
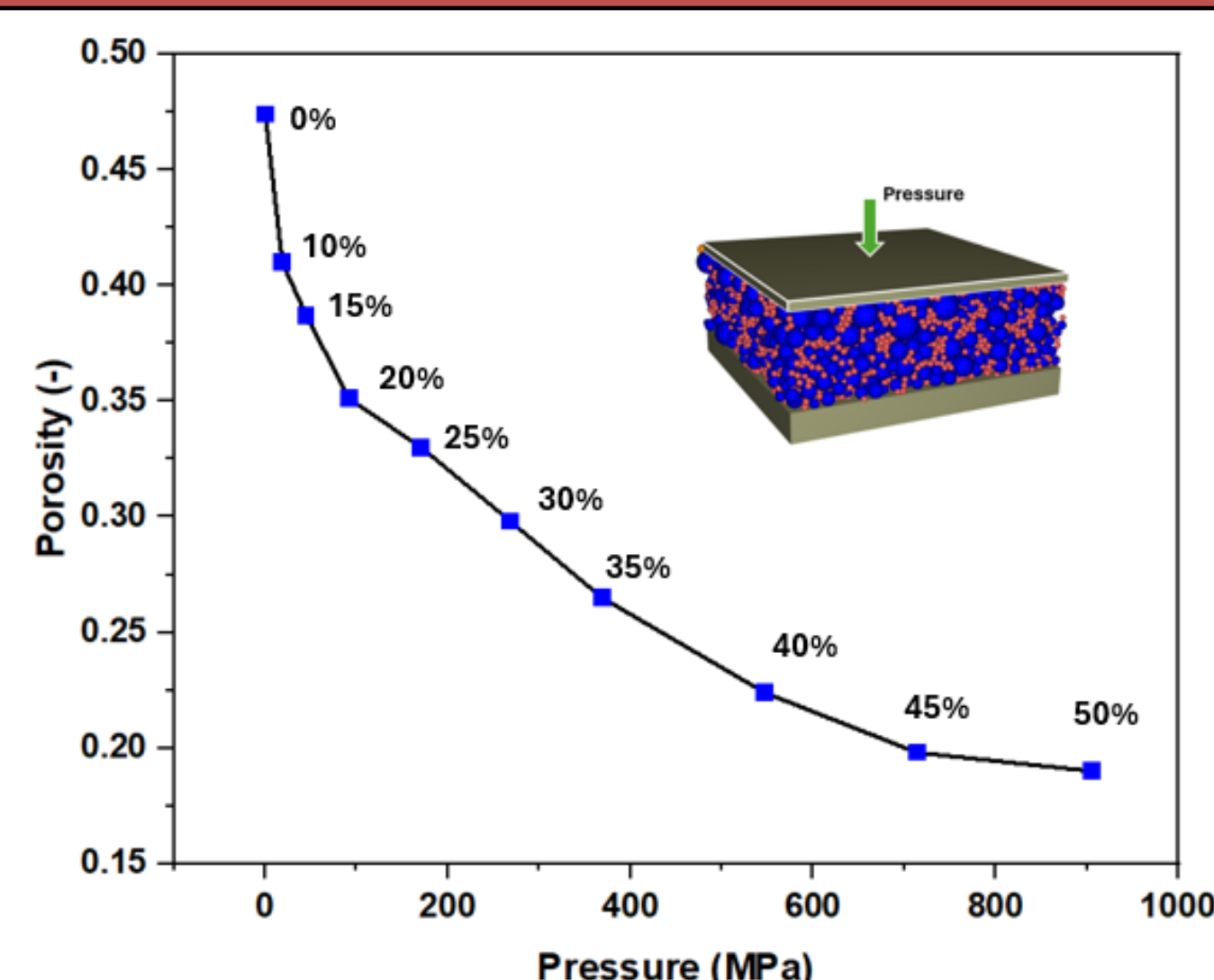
Roller Approach



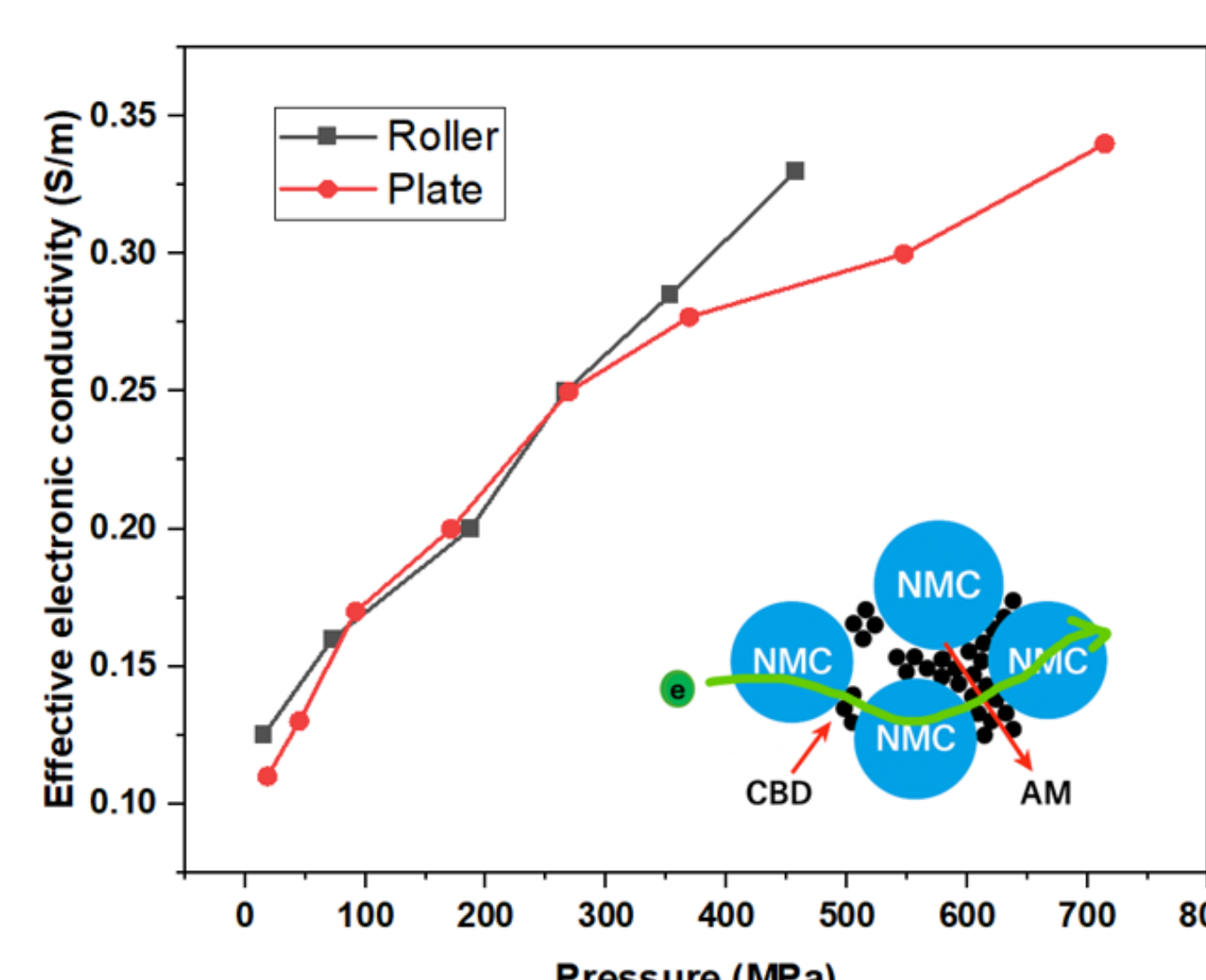
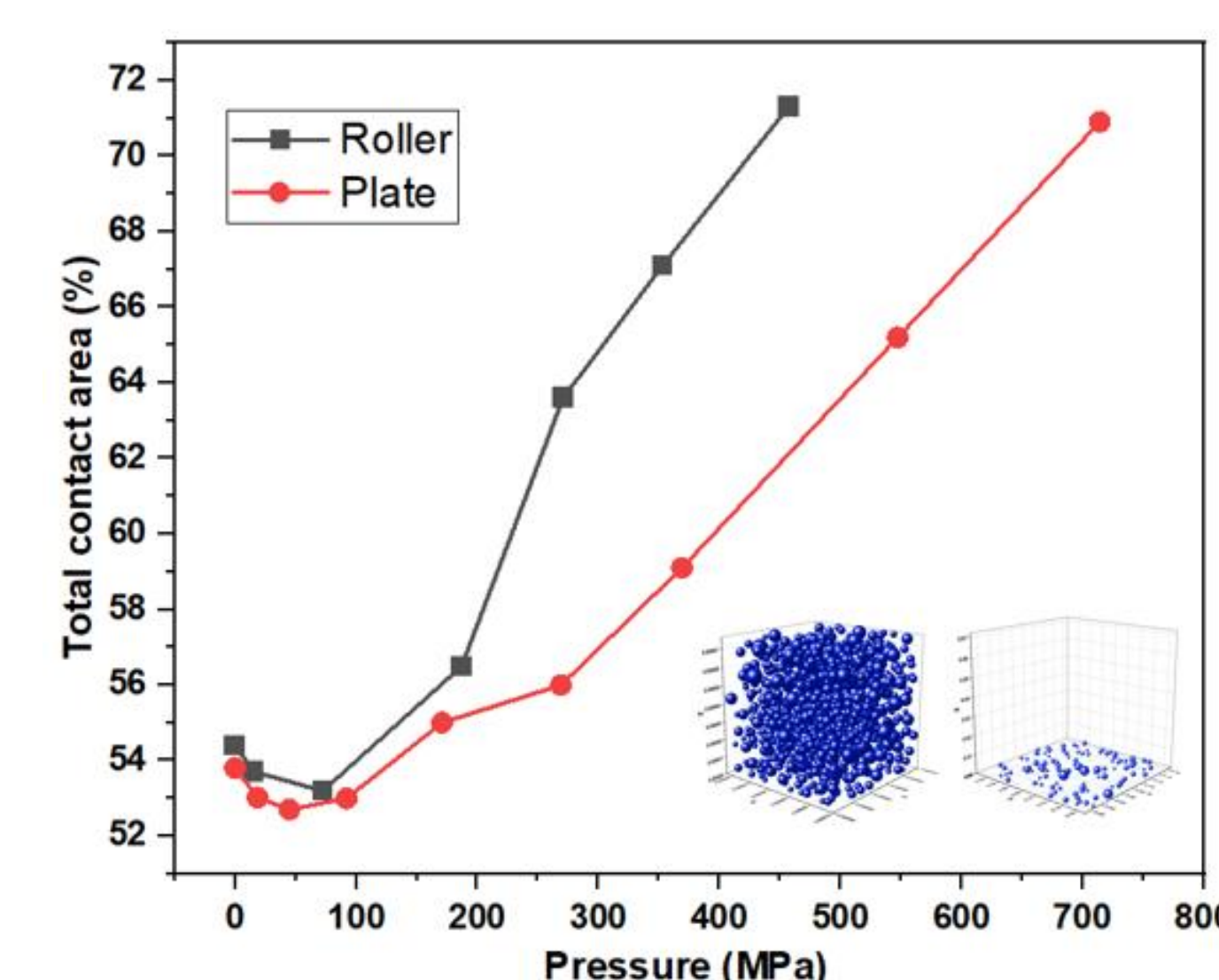
DEM model used	Hysteretic linear spring model
Model Domain	100 μm/100μm/75μm (Plate) 500 μm/100μm/75μm (Roller)
Boundary	Periodic (X & Y) - plate approach Periodic (X) - roller approach
Upper plate (roller) - movable	Steel
Bottom plate (current collector) - fixed	Aluminium
Materials	NMC + CBD (CB+PTFE)

Materials	Poisson's ratio	Density (g/cm ³)	Young's Modulus (GPa)
NMC-622	0.25	4.74	75
CBD	0.3	2.0	1.9
Aluminium	0.3	2.7	68.9
Steel	0.3	7.9	208

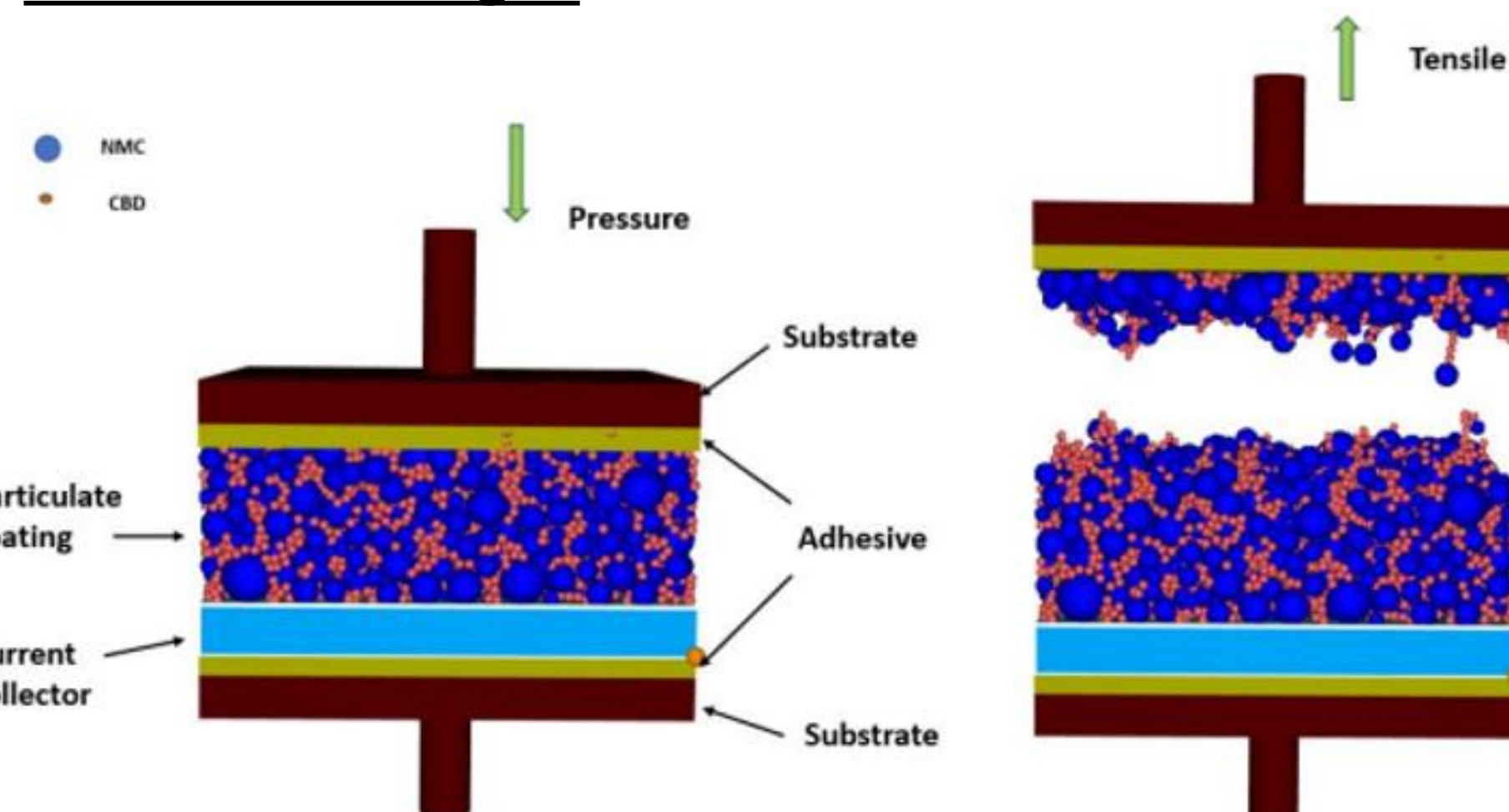
RESULTS AND DISCUSSION



Tortuosity factors were determined using **TauFactor** (MATLAB) [2], while effective electronic conductivity was computed using an **in-house Lattice Boltzmann Method (LBM)** solver developed by Prof. Cai's research group [3].

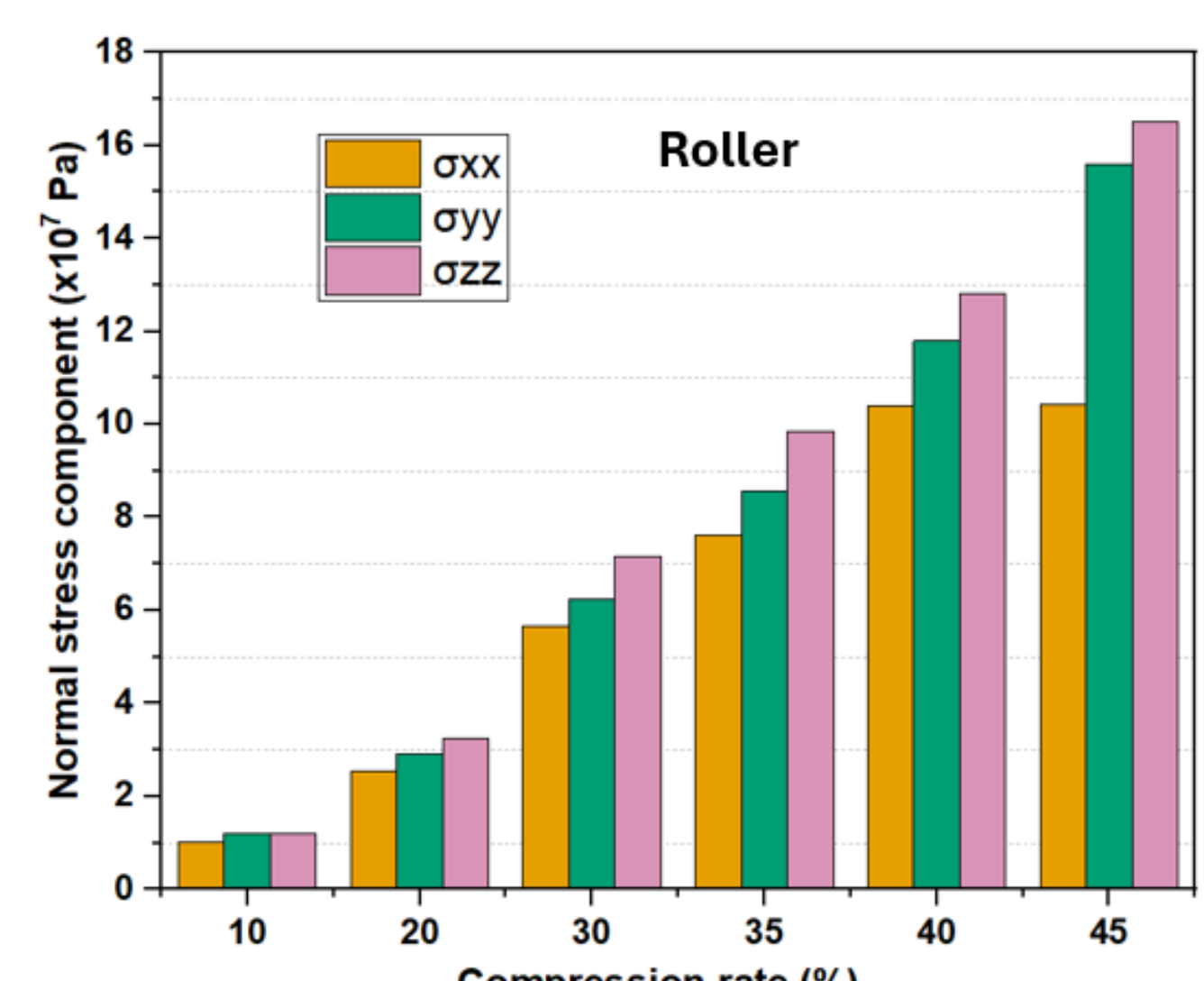
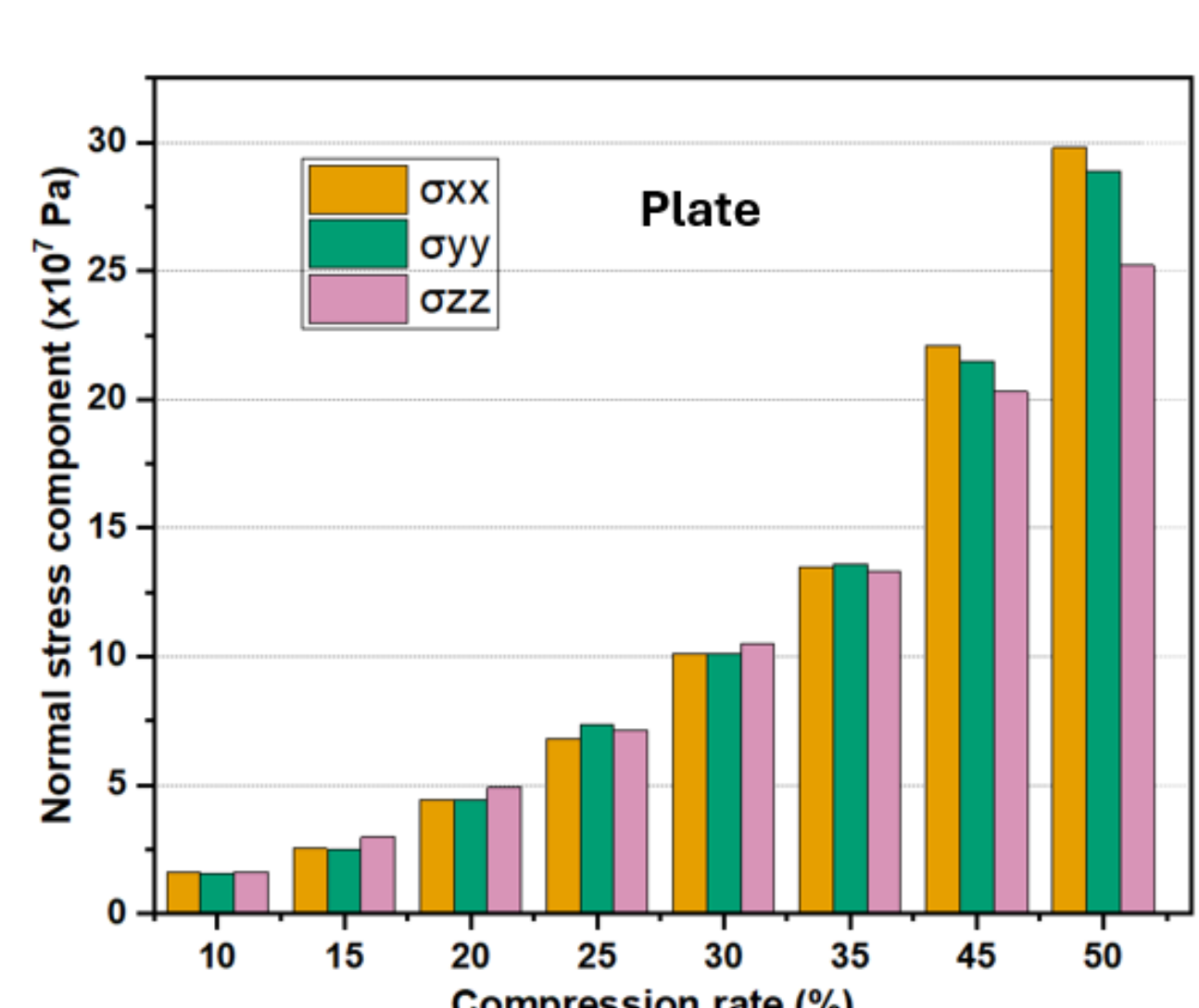


Adhesion strength



Discussion: Adhesion strength of 82 kPa was achieved, with failure occurring within the coating layer (cohesion failure)

Discussion: Increasing calendering pressure reduces porosity and enhances particle packing, reflected by higher coordination number and density. Normal stresses (σ_{xx} , σ_{yy} , σ_{zz}) rise uniformly with compression, confirming effective load transfer. The roller method achieves similar densification at lower stress, indicating smoother and more efficient compaction.



CONCLUSION:

- Both plate and roller DEM models captured key densification trends: reduced porosity, higher coordination number, and improved conductivity.
- The roller approach achieved comparable compaction at lower pressures, showing smoother stress distribution and more realistic particle rearrangement.
- While the flat-plate model is useful for fundamental studies, the roller-based DEM framework provides a more realistic and physically representative approach for industrial calendering and process optimization.

[1] Kwade, A., Haselrieder, W., Leithoff, R., Modlinger, A., Dietrich, F. & Droeder, K. *Nat. Energy* 3, 290–300 (2018).

[2] Cooper, S.J., Bertel, A., Shearing, P.R., Kilner, J.A. & Brandon, N.P. *SoftwareX* 5, 203–210 (2016)

[3] Huang, J., Hu, J., Zhang, D., Du, Y., Wu, C.-Y. & Cai, Q. *J. Energy Storage* 114, 115692 (2025)