G005

Discrete Element Modeling of Particle-Scale Resistive Heating

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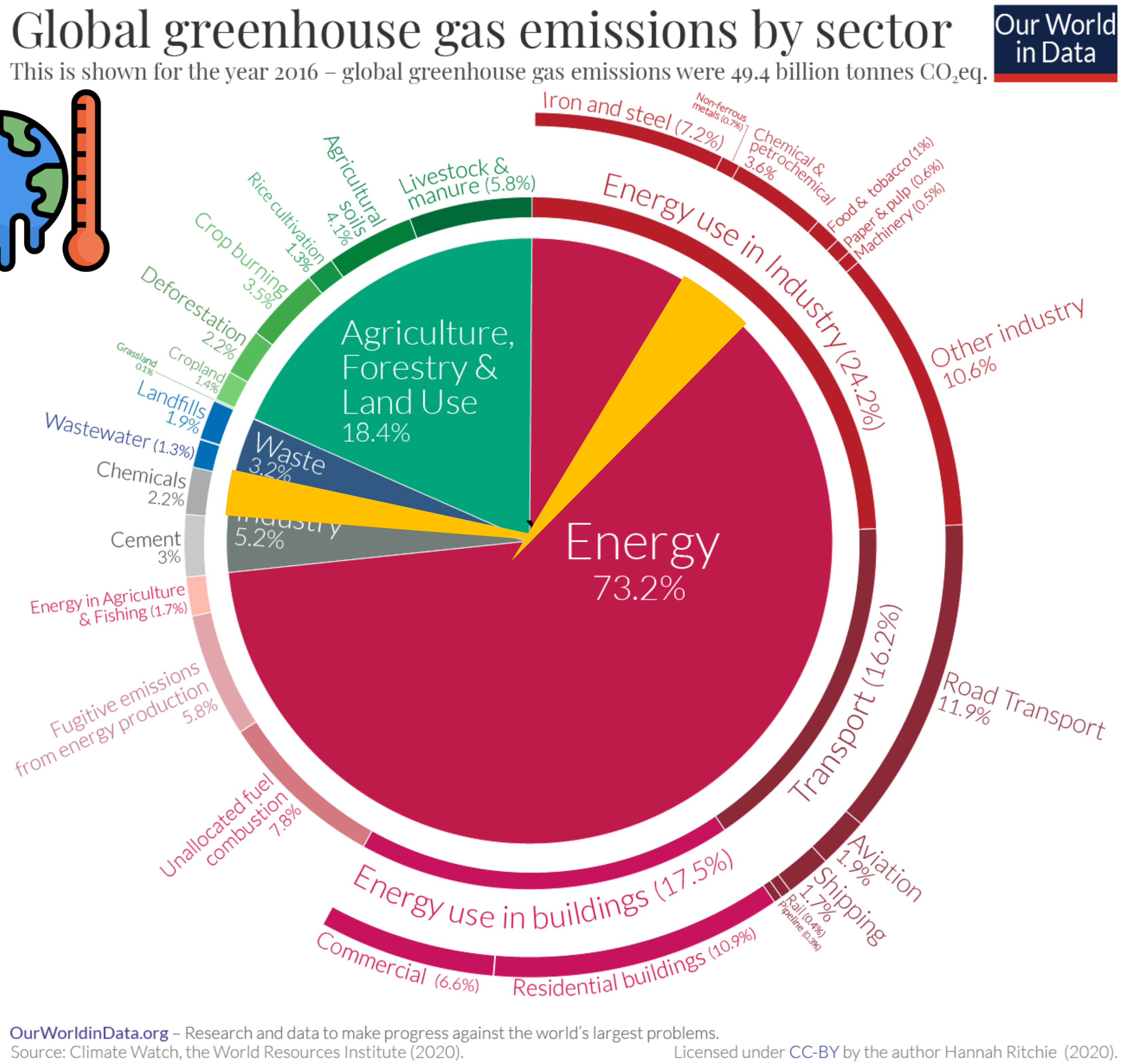
MaCKiE

CO_2 emission by chemical industry

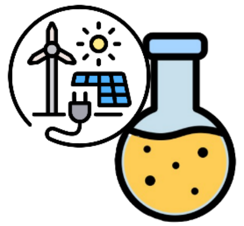


Chemical Industry

~6% of the total worldwide CO_2 emissions

~30% of the total industry CO_2 emission

→ **62% Energy emissions**



Electrified chemical Industry

~ potential of reducing 50% reducing the CO_2 of the industry

→ **1.43 billion tones $CO_{2,eq}$**

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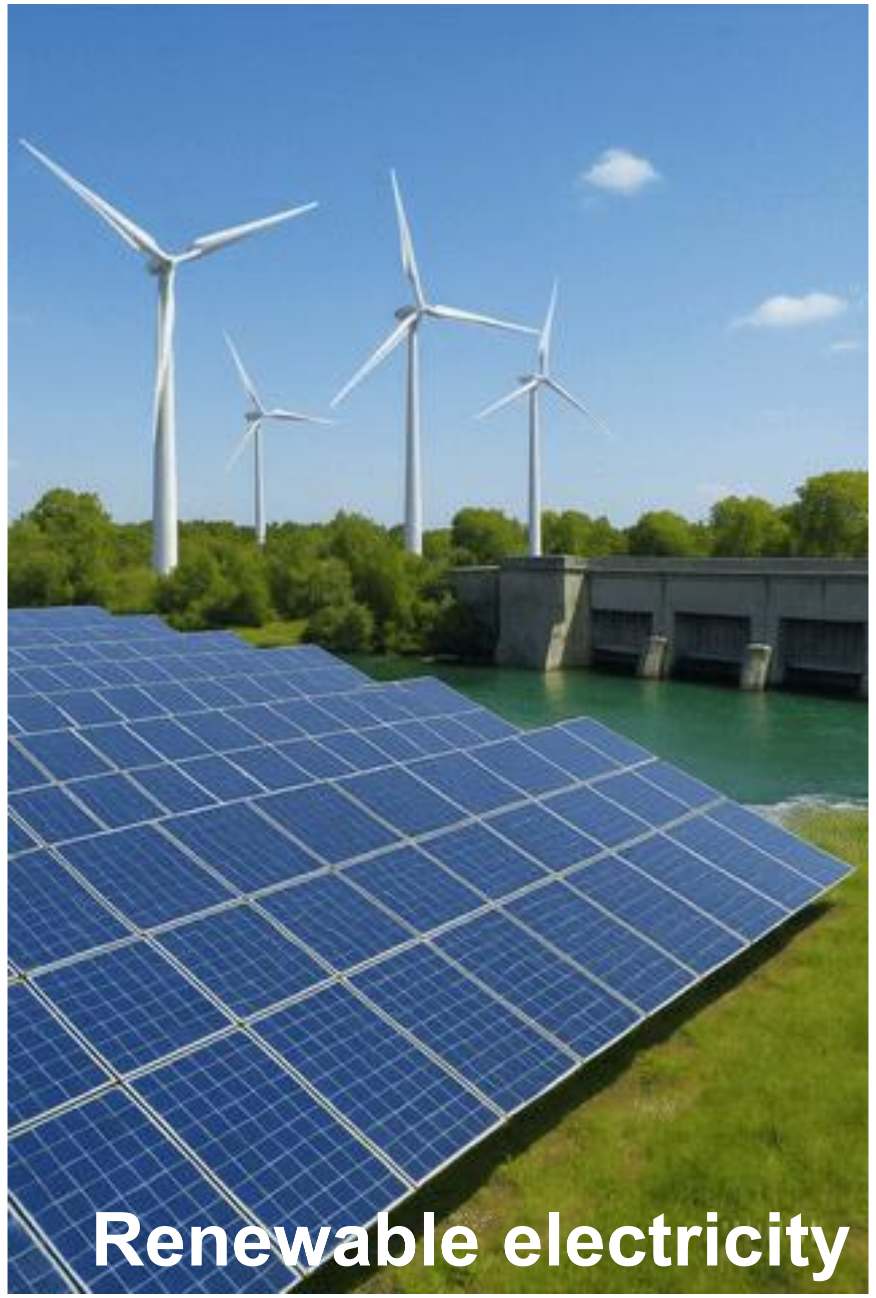
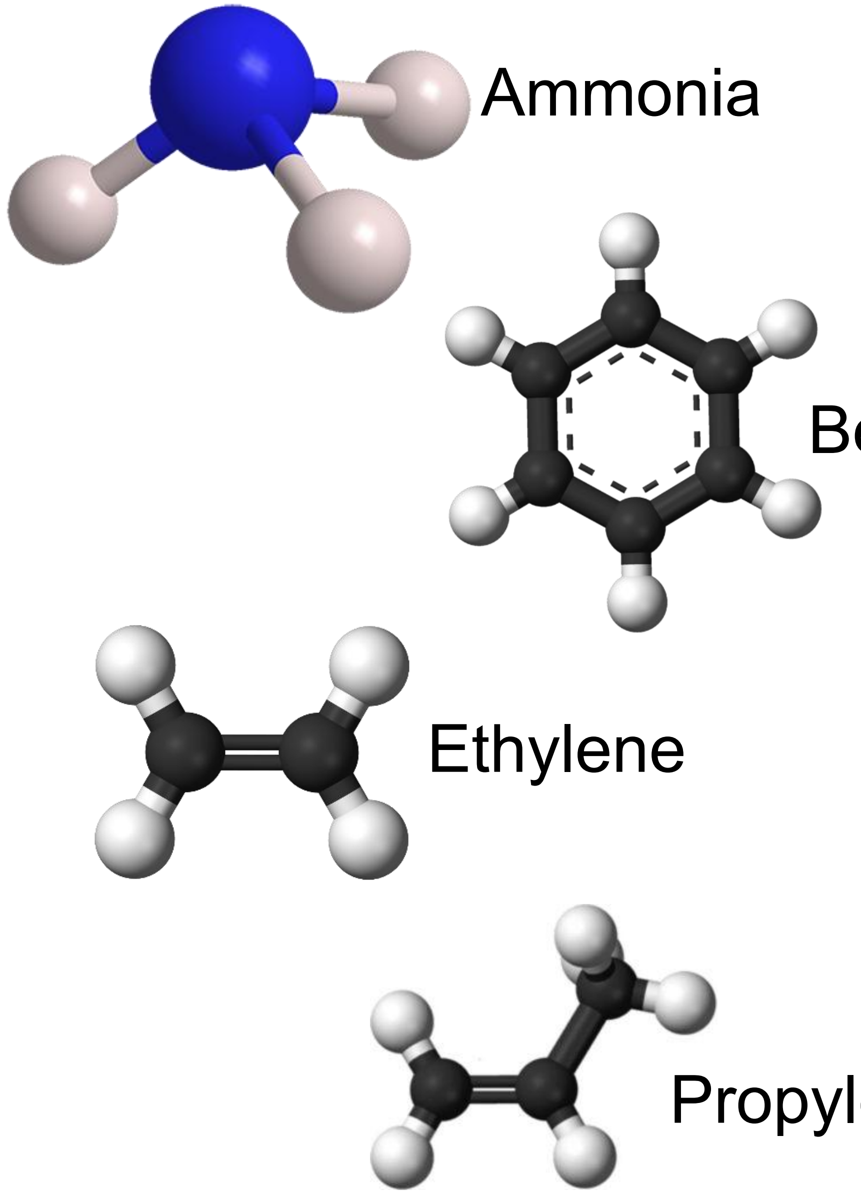
Roelofsen, et al., Plugging in: What electrification can do for industry, (2020).

Electrification

Power-to-heat (conversion of electrical energy from renewable sources to thermal energy)



Chemical plant



Chemical building blocks

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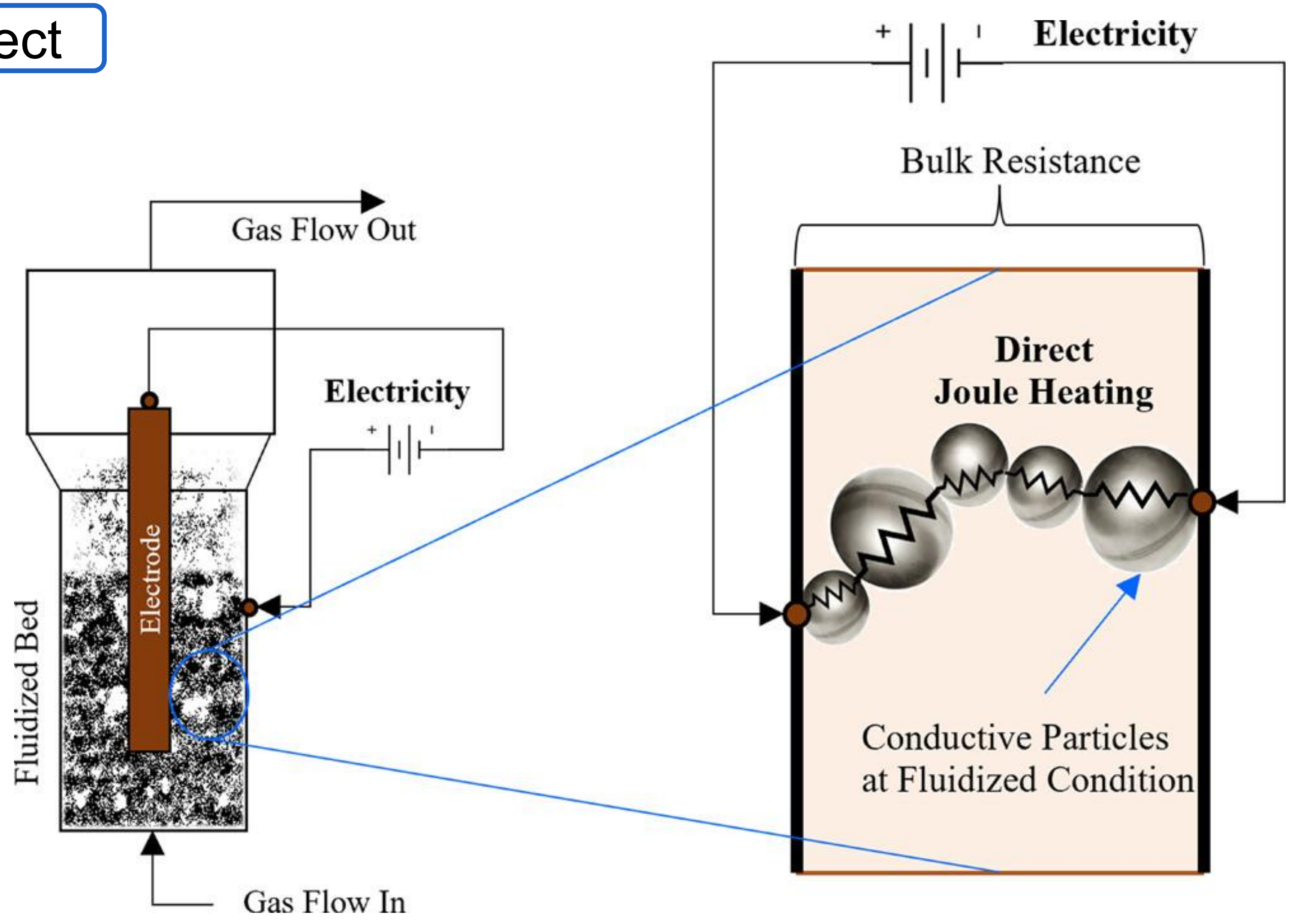
Electrified gas-solid fluidized bed reactors (e-Beds)

Electrically heated fluidized bed

- **Resistive heating**
  - **Direct** — ***Conversion of electrical to thermal energy directly on material in the reactor***
  - In-direct
- Induction heating
- Electromagnetic Irradiation heating
- Sonication
- Plasma heating
- Gas preheating



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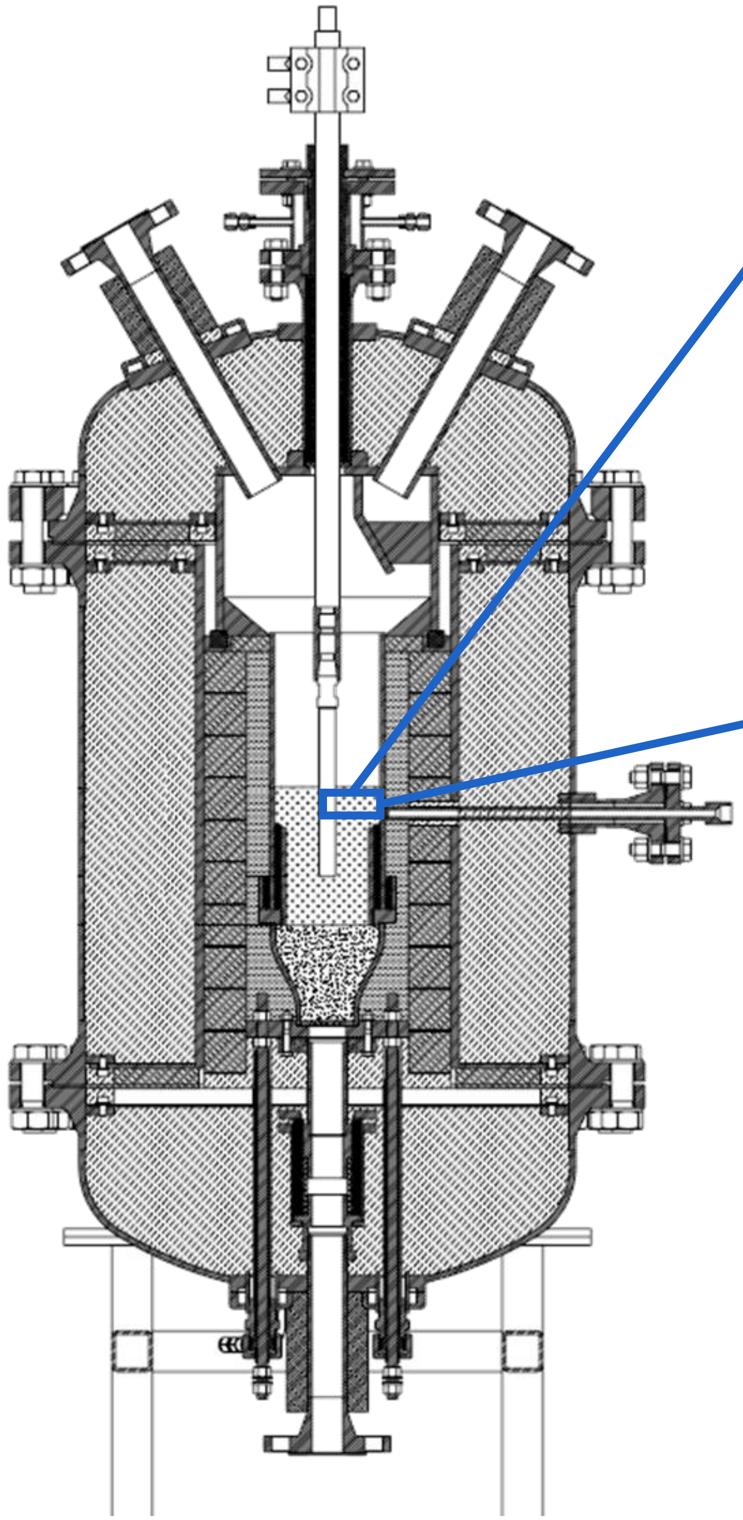
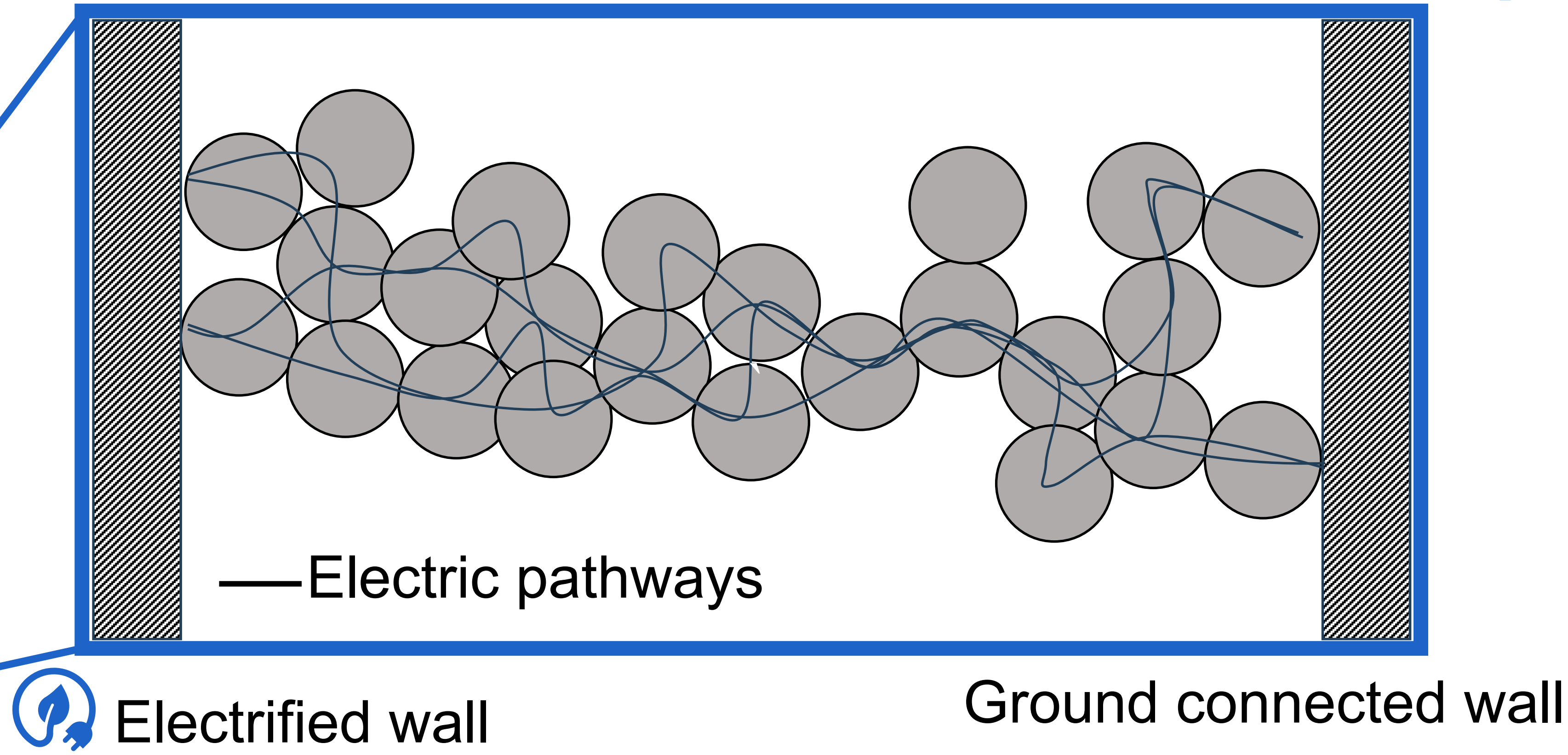
Ahmed I., et al., Ind. & Eng. Chem. Res., (2024). https://doi.org/10.1021/acs.iecr.3c04232

Electrified gas-solid fluidized bed reactors (e-Beds)





Electrified environment:

On ***Hydrodynamics***

- Change of interparticle interaction force

On ***Heat Transfer***

- Conduction particle-particle/particle-wall
- Convection particle-gas
- Joule heating at particle scale
- Radiation of particles at high temperature

Physics at the **particle scale**

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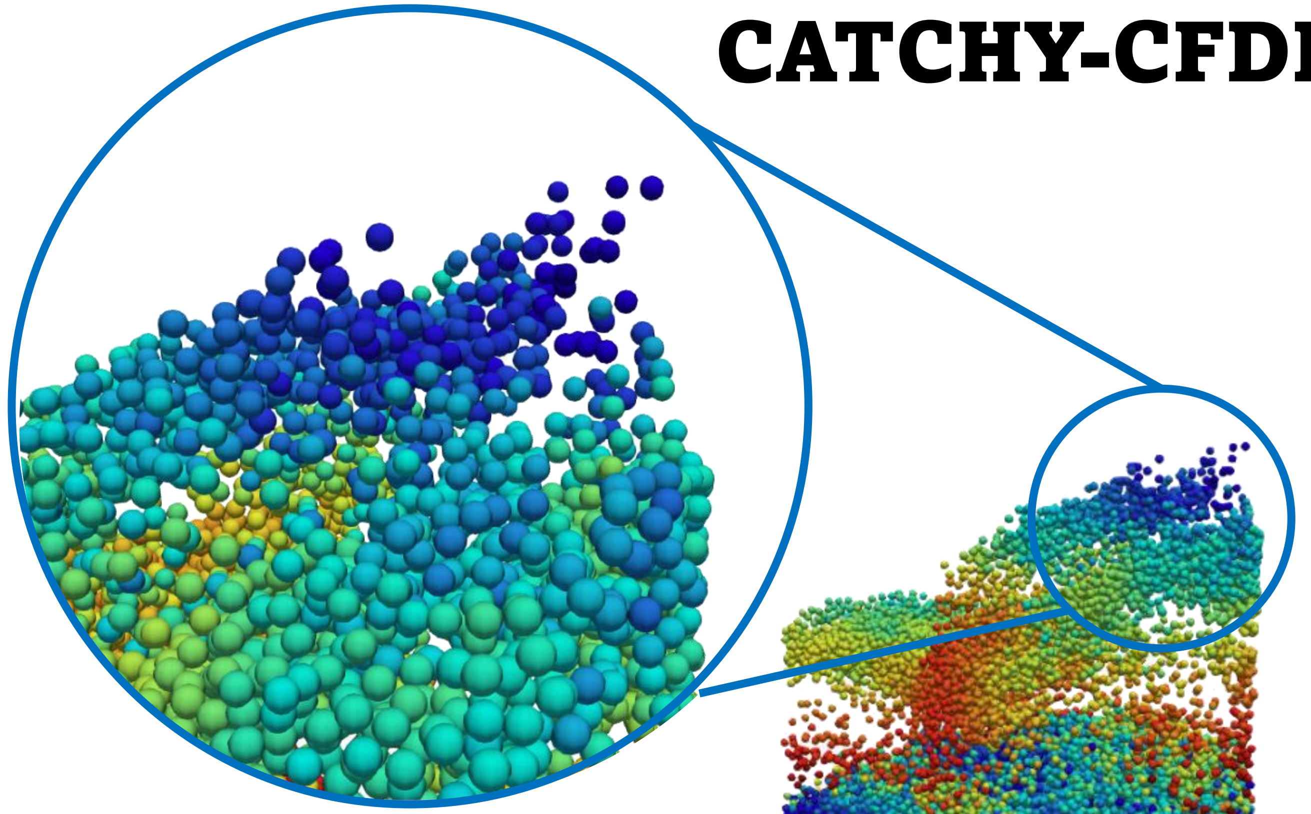
Methodology

CATCHY-CFDEM



<u>Gas-Solid Systems</u>

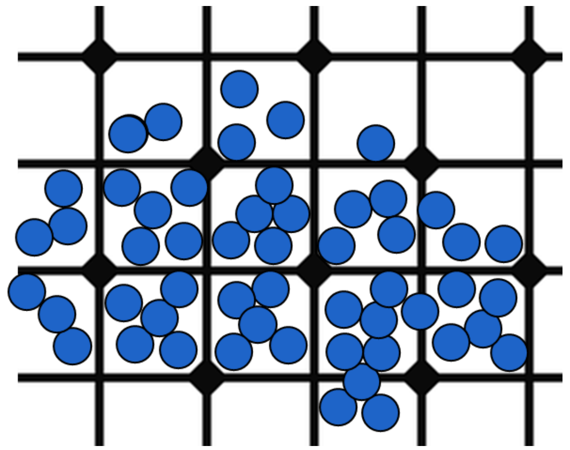
- Euler-Euler
- **Euler-Lagrange *(CATCHY-CFDEM)***
  - **Goal:** First framework to model dynamic electric conduction and joule heat in e-Beds

Fluid Dynamics (CFD-OpenFOAM):

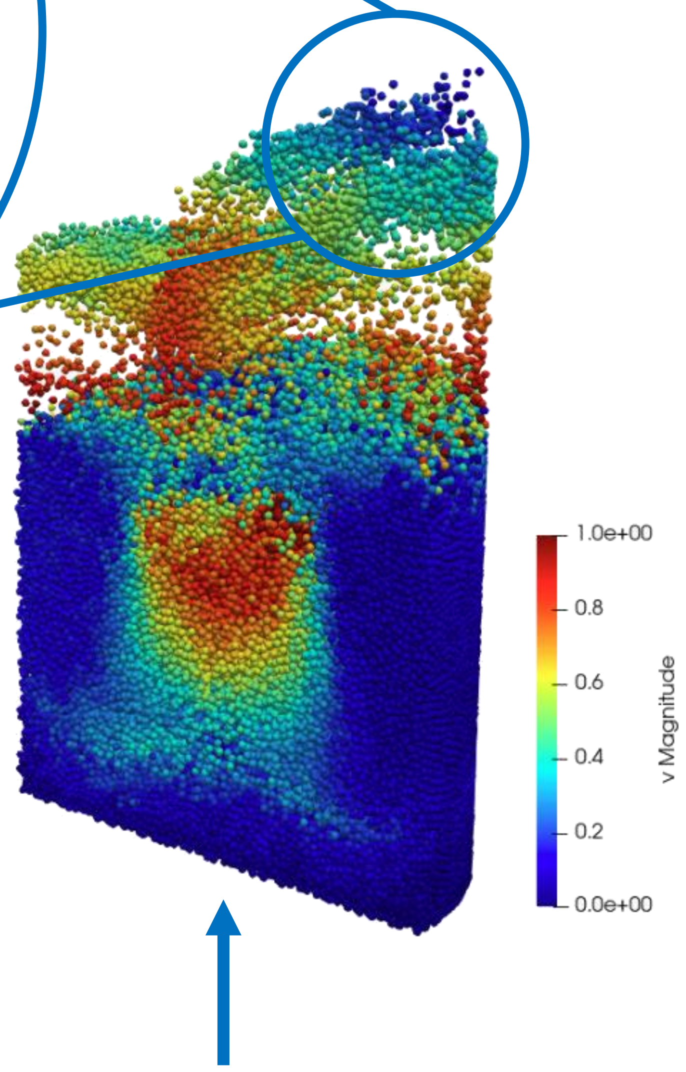
- Hydrodynamic
- Heat transfer

Particle modeling (DEM-LIGGGHTS):

- Force balance (2nd law of Newton)
- Energy balance



Unresolved CFD-DEM

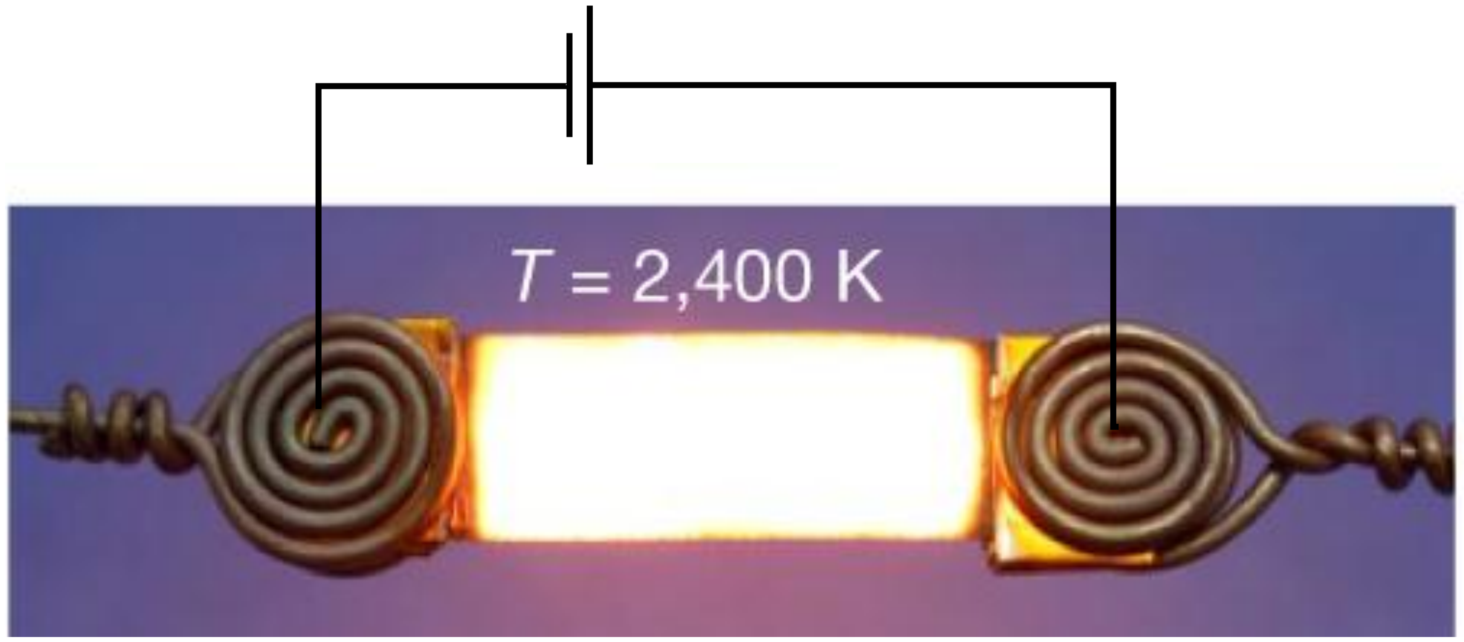


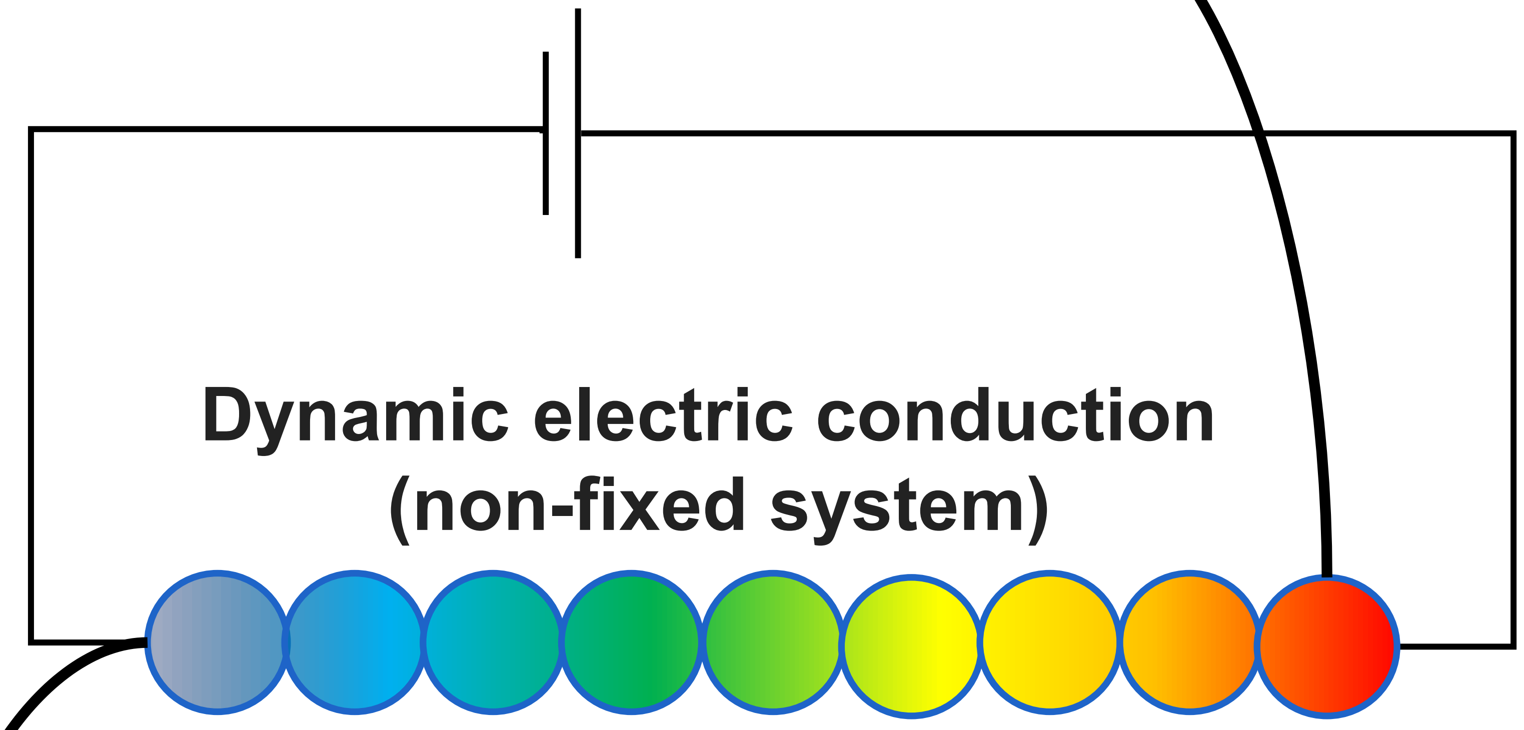
Inlet gas

Wéry, et al. *Chem. Eng. J.*, (2024). https://doi.org/10.1016/j.cej.2024.155247

Challenges in dynamic electric conduction

Identifying conductive electric pathways within the system





One static solid object

Multiple dynamic solid objects (!)

Joule heat at particle scale

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Dong, Qi, et al., Nature, (2022) https://doi.org/10.1038/s41586-022-04568-6

Dynamic electric conduction

Identifying electrical pathways within the system

Contact matrix based on neighbor list of particles at each time-step

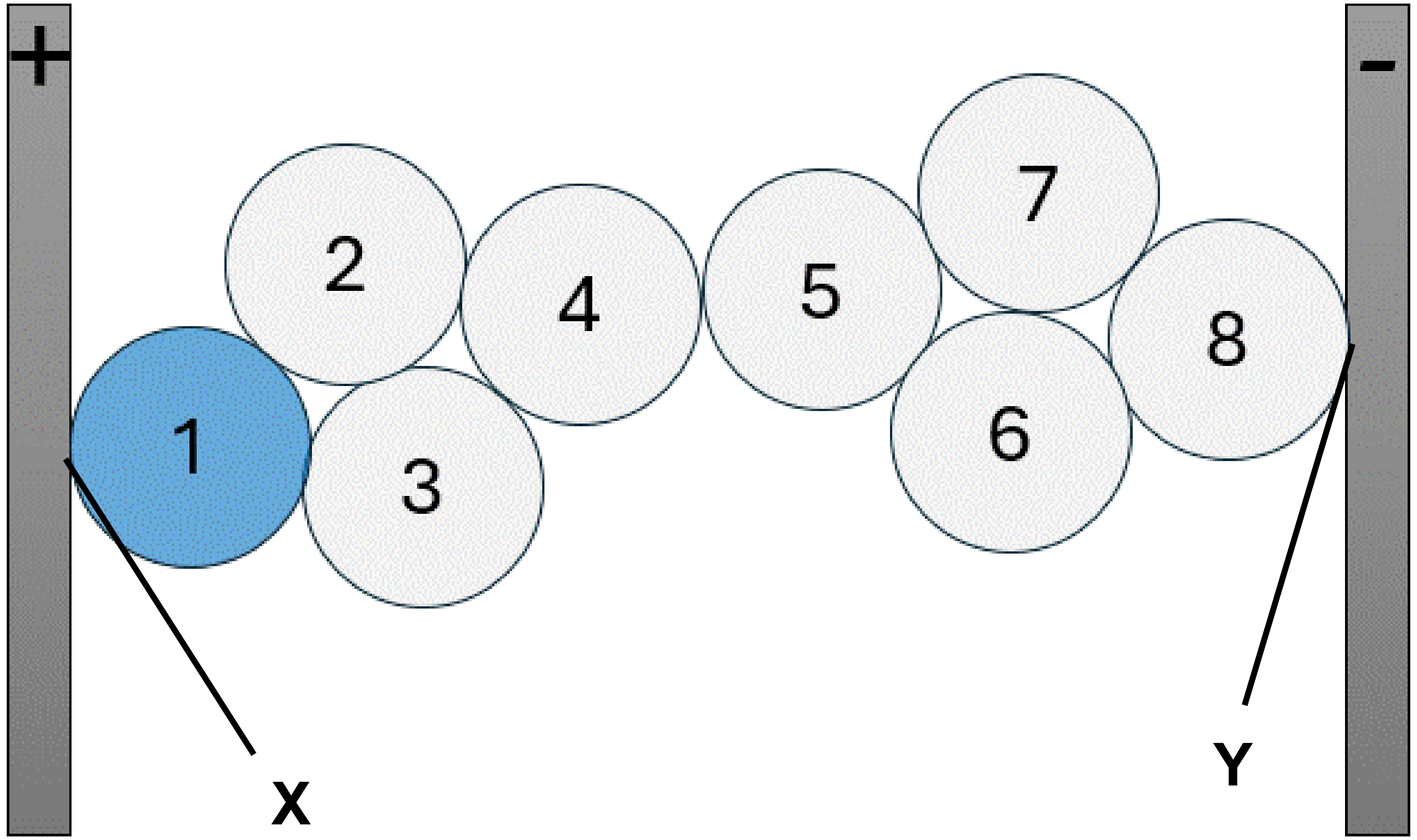
	M								C
	1	2	3	4	5	6	7	8	-
1	n	a	a	0	0	0	0	0	X
2	a	n	a	a	0	0	0	0	0
3	a	a	n	a	0	0	0	0	0
4	0	a	a	n	a	0	0	0	0
5	0	0	0	a	n	a	a	0	0
6	0	0	0	0	a	n	a	a	0
7	0	0	0	0	a	a	n	a	0
8	0	0	0	0	0	a	a	n	Y

a: p-p contact ,

X: p-w contact with source,

Y:p-w contact with sink

Resistor Network Model



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Dynamic electric conduction

Applying the conservation law of electric current density on each cluster of particles

- **Conservation law**
- Contact electrical resistance
- Numerical solve
- Electric current
- Joule heat

$$\nabla \cdot j = 0 \Rightarrow \sum_{j=1}^{N_{nb}} j_{ij} = 0 \Rightarrow \sum_{j=1}^{N_{nb}} \sigma_i \frac{V_i - V_j}{d_{ij}} = 0$$

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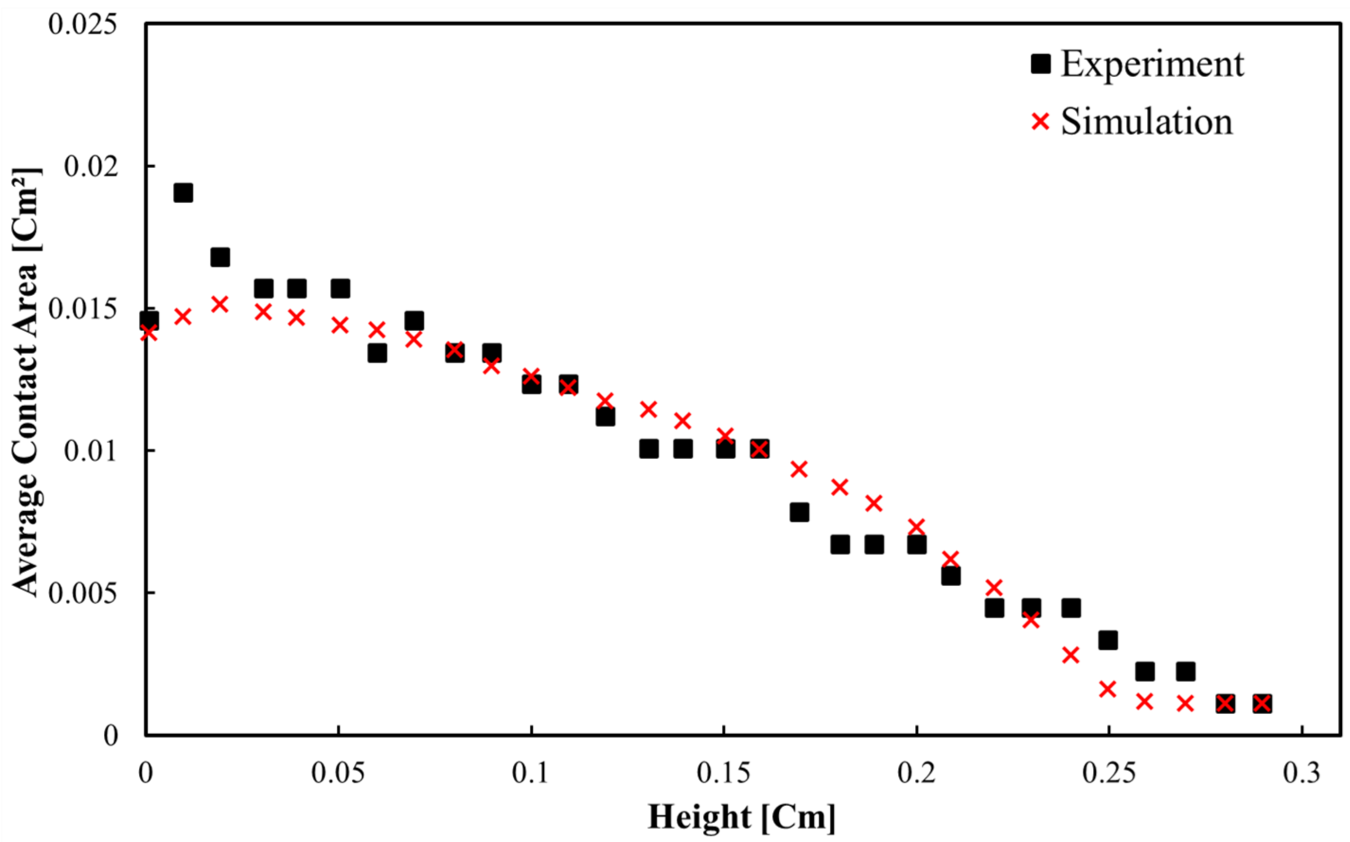
Dynamic electric conduction

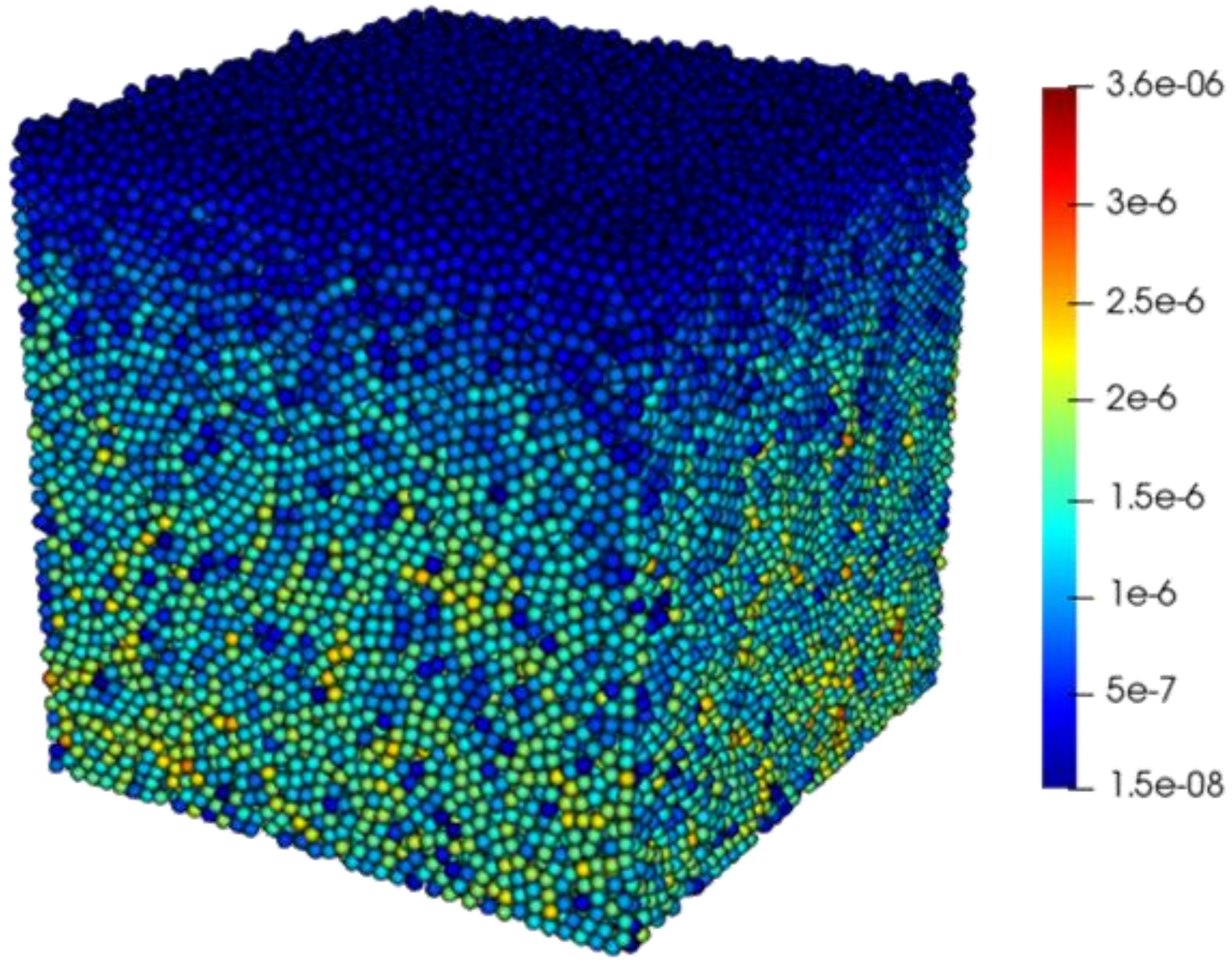
Defining the electrical resistance (analogy with conduction heat transfer)

- Conservation law
- **Contact electrical resistance**
- Numerical solve
- Electric current
- Joule heat

$$\sum_{j=1}^{N_{nb}} \frac{V_i - V_j}{R_{\sigma,ij}} = 0\,, \qquad \frac{1}{R_{\sigma},ij} = \frac{4r_c}{\frac{1}{\sigma_{p,i}} + \frac{1}{\sigma_{p,i}}}$$

dependency of electrical resistance to contact area (radius)





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Govender N., et al., Chem. Eng. Sci. (2020). https://doi.org/10.1016/j.ces.2020.115584

Dynamic electric conduction

System of linear equations for particles in an identified electric pathway

- Conservation law
- Contact electrical resistance
- **Numerical solve**
- Electric current
- Joule heat

Direct-solvers:

- Gauss elimination

Iterative Solvers:

- Jacobi method
- Conjugate gradient
- Bi-Stablized method Conjugate gradient (BiCGStab)

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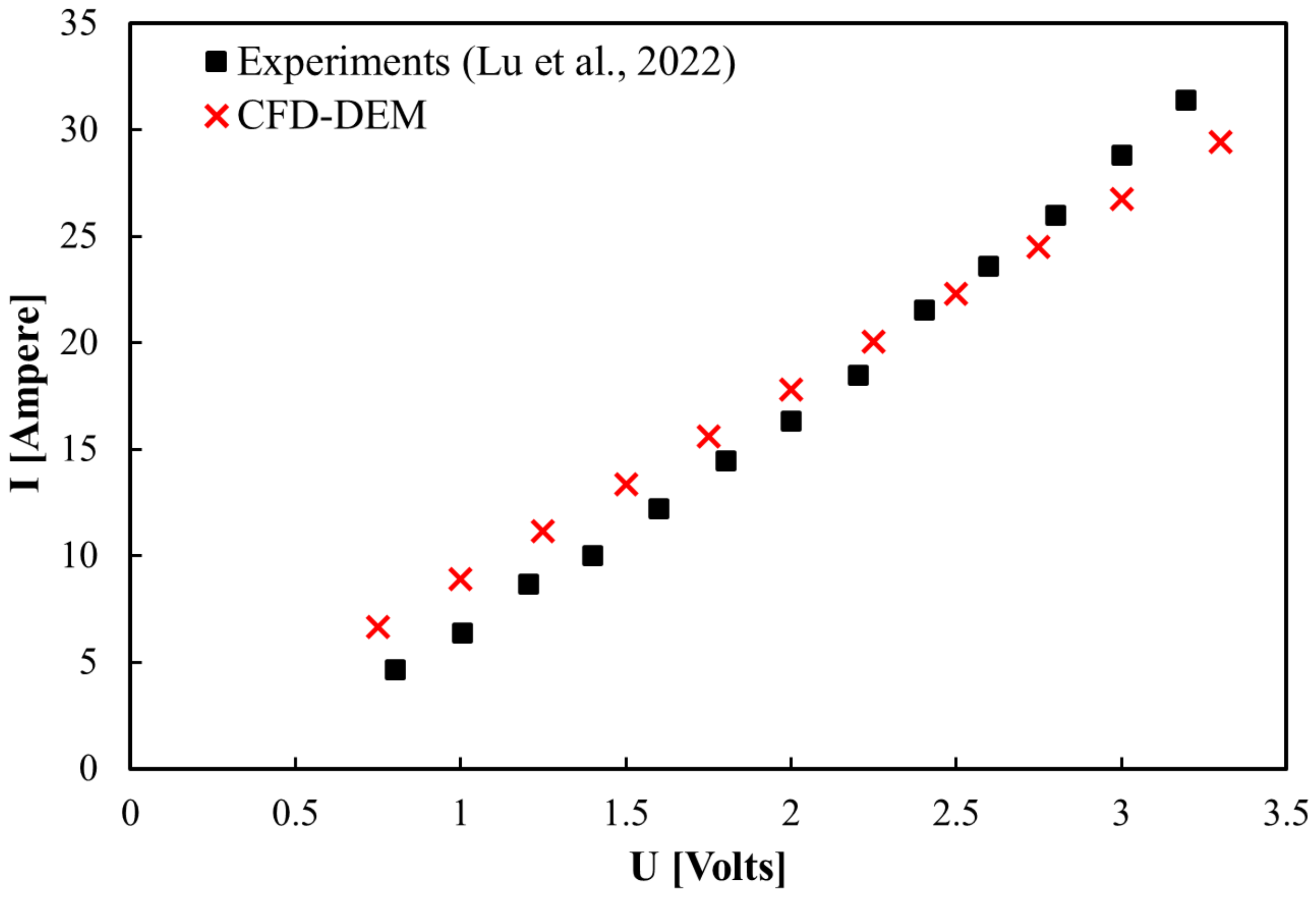
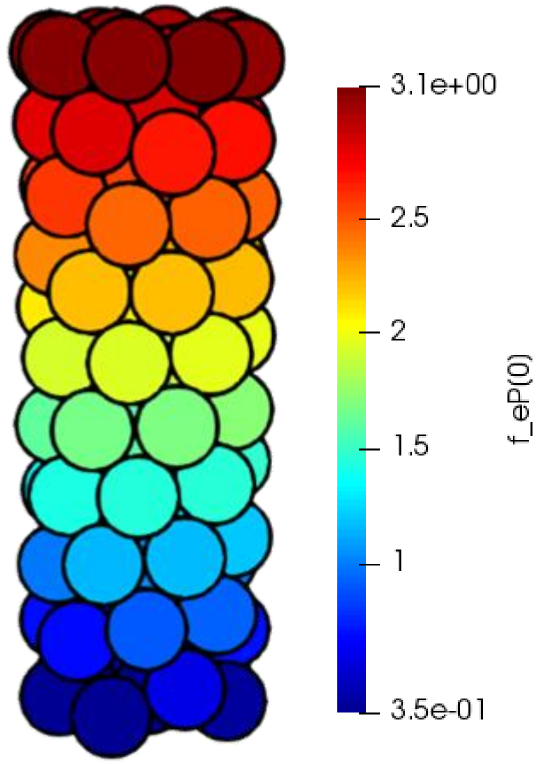
Dynamic electric conduction

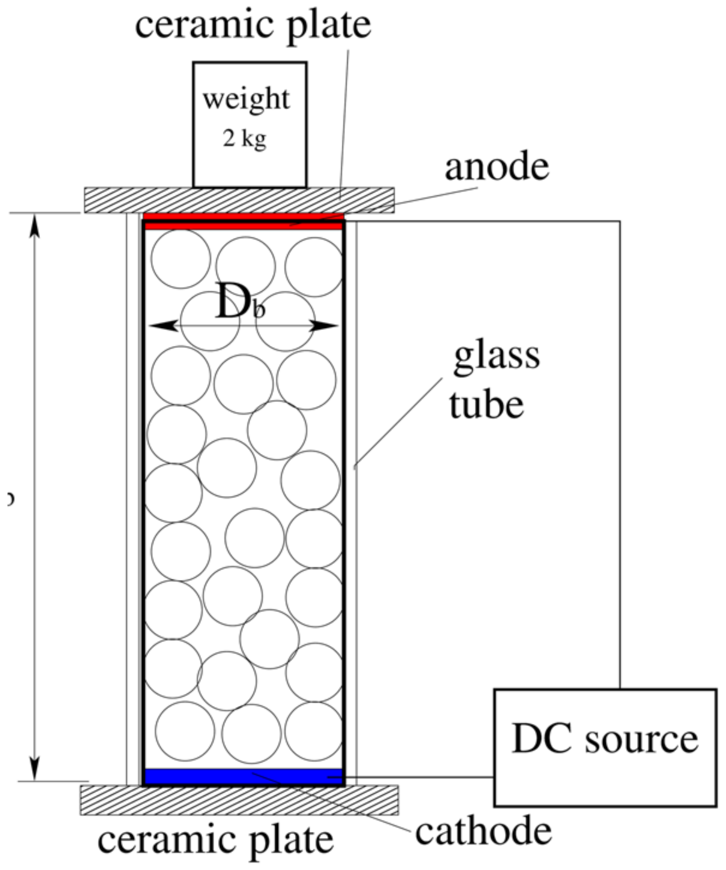
Calculating electric current

$$I_{ij} = \frac{V_i - V_j}{R_{\sigma,ij}},$$ pair-particle in contact (i,j)

- Conservation law
- Contact electrical resistance
- Numerical solve
- **Electric current**
- Joule heat



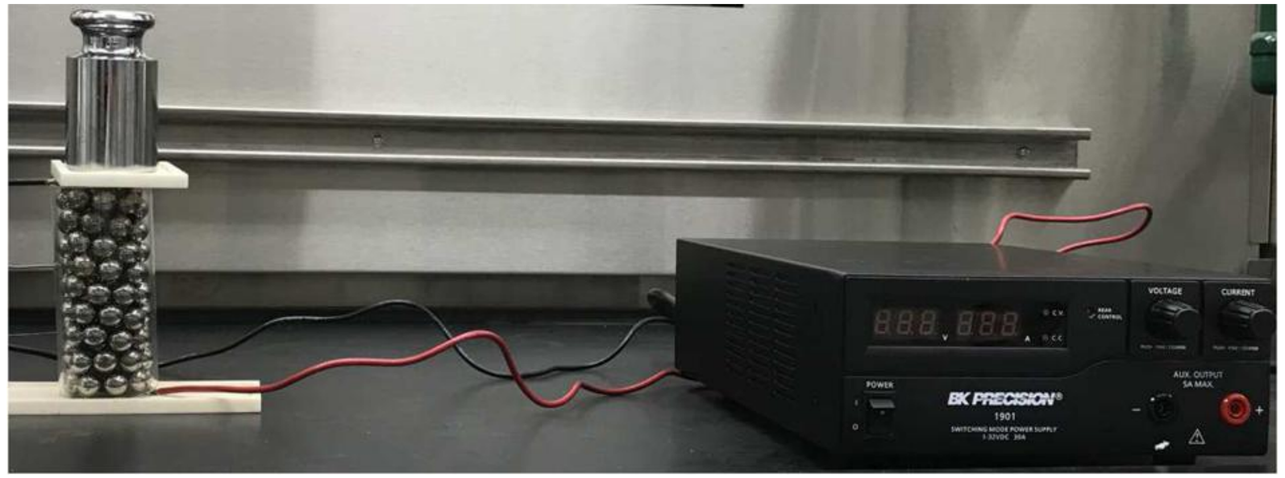




d_p=0.0127 m

P=7800 kg/m^3

N_p= 86 (Carbon steel particles)



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Lu, et al. ASME. J. Energy Resour. Technol. (2022). https://doi.org/10.1115/1.4053303

Dynamic electric conduction

Joule heating calculation at each time step

- Conservation law
- Contact electrical resistance
- Numerical solve
- Electric current
- **Joule heat**

$$Q_e = P = I_{ij}^2 \cdot R_{\sigma,ij} = \frac{1}{2}\sum_{j=1}^{N_{nb}} \frac{\left(V_i - V_j\right)^2}{R_{\sigma,ij}}$$

½ for each particle i and j

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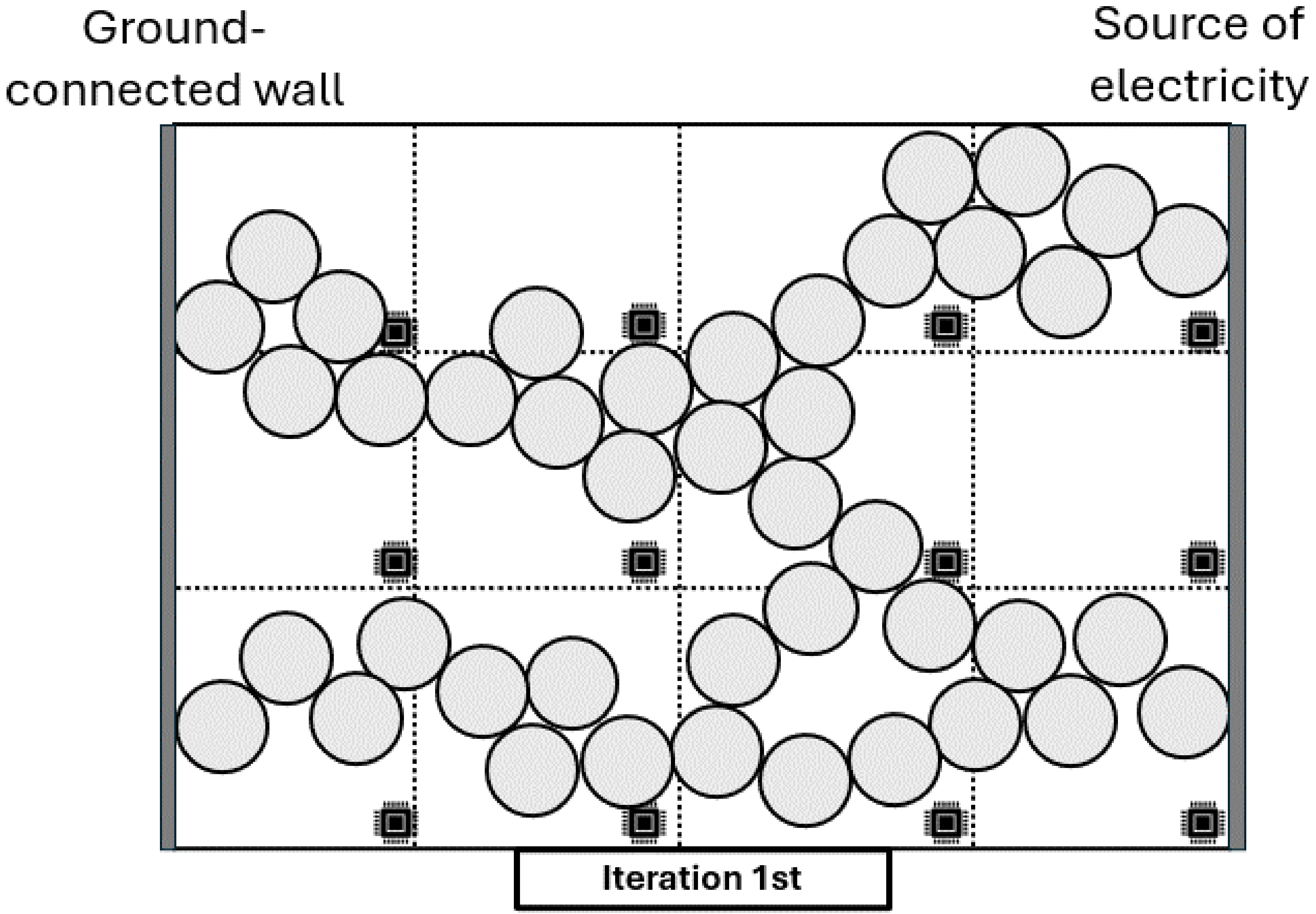
Up-scaling

Iterative chain detection using label-propagation algorithm

Algorithm

1. *Start from the p-w contacts with source of electricity*
2. *Transfer the unique flag of p-w contact by p-p contacts*
3. *Repeat step 2 for all found particles in an iterative approach*
4. *Complete chain, if p-w contact with ground connected wall*



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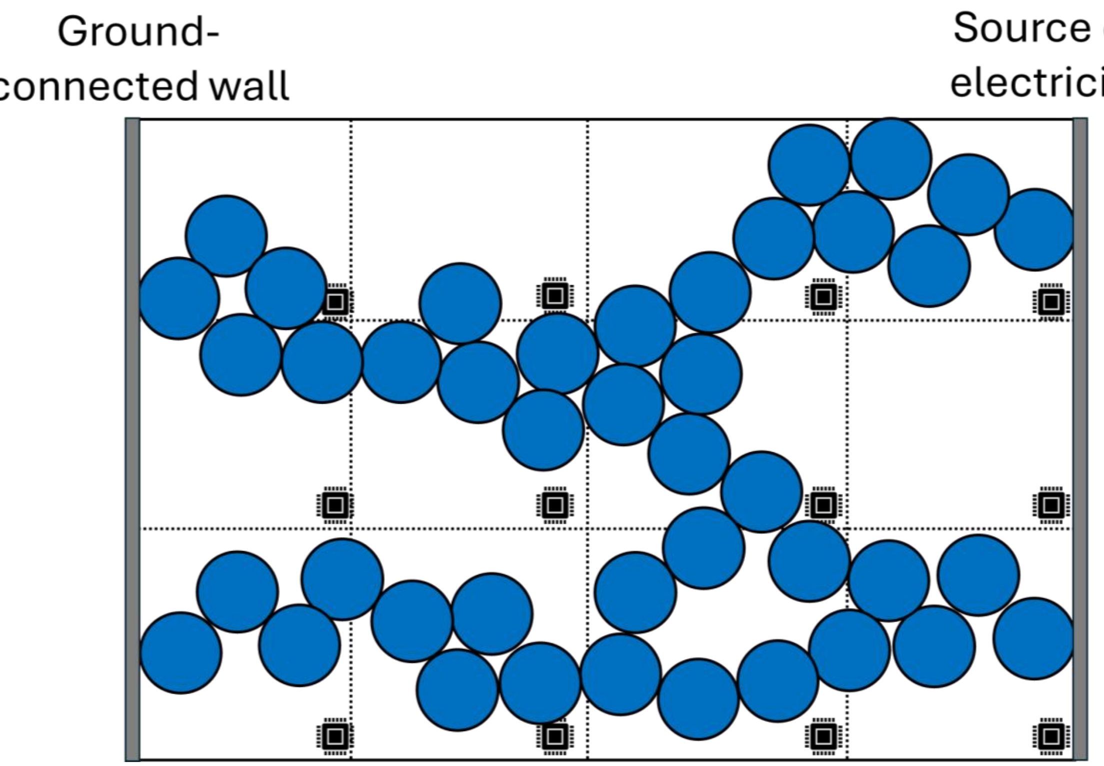
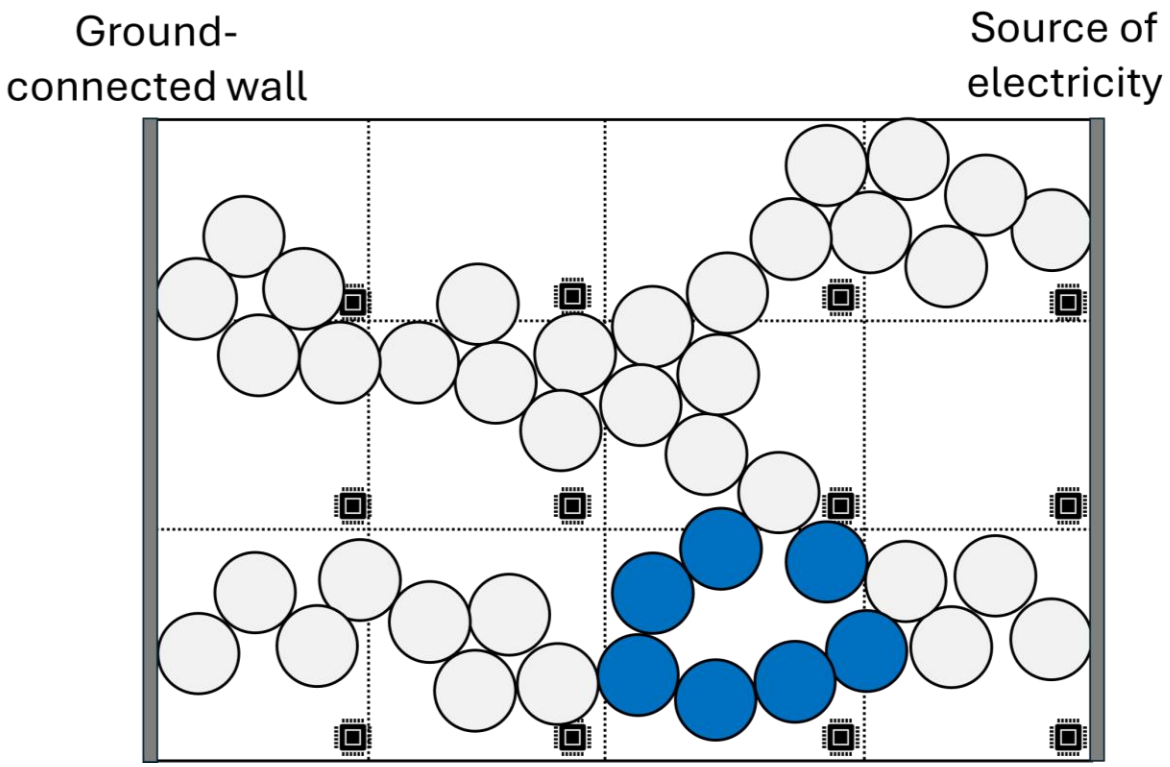
Up-scaling

From chains to particles

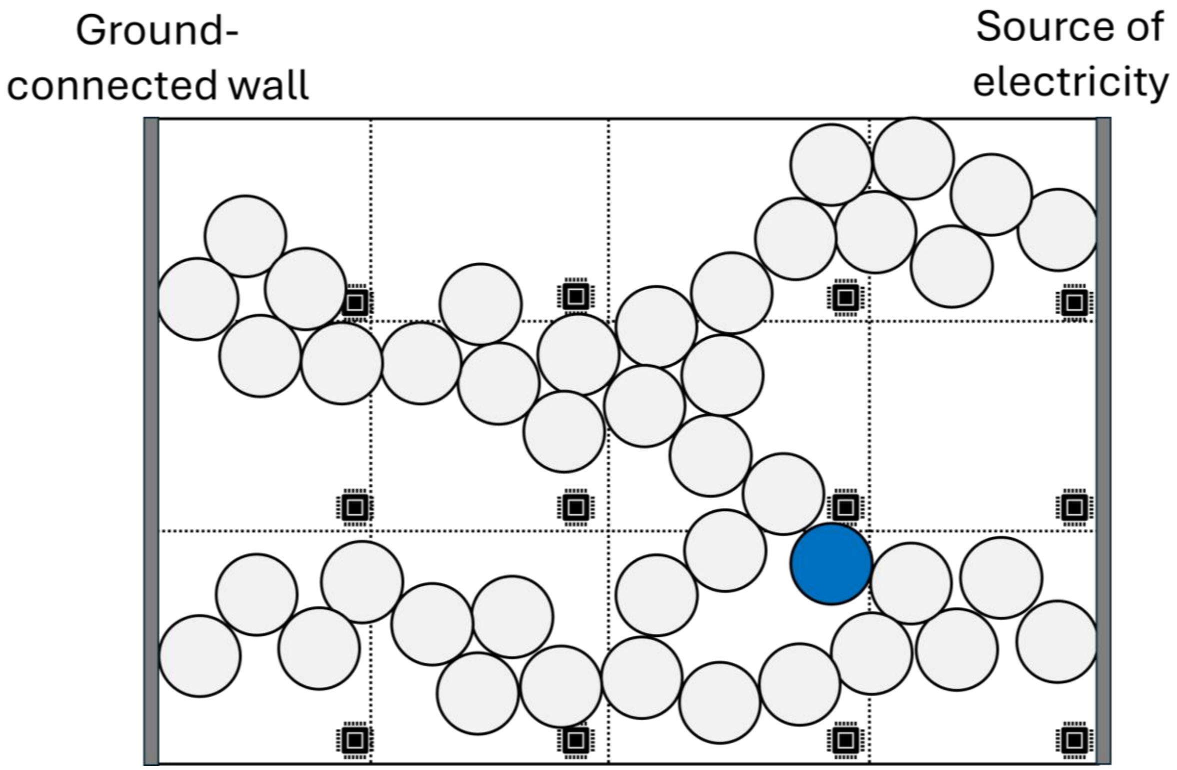


Connected conductive electric pathway



Segments of a connected conductive electric pathway

Block-BiCGStab solvers



Particles of a connected conductive electric pathway

Use charge conservation as a convergence criteria

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Up-scaling

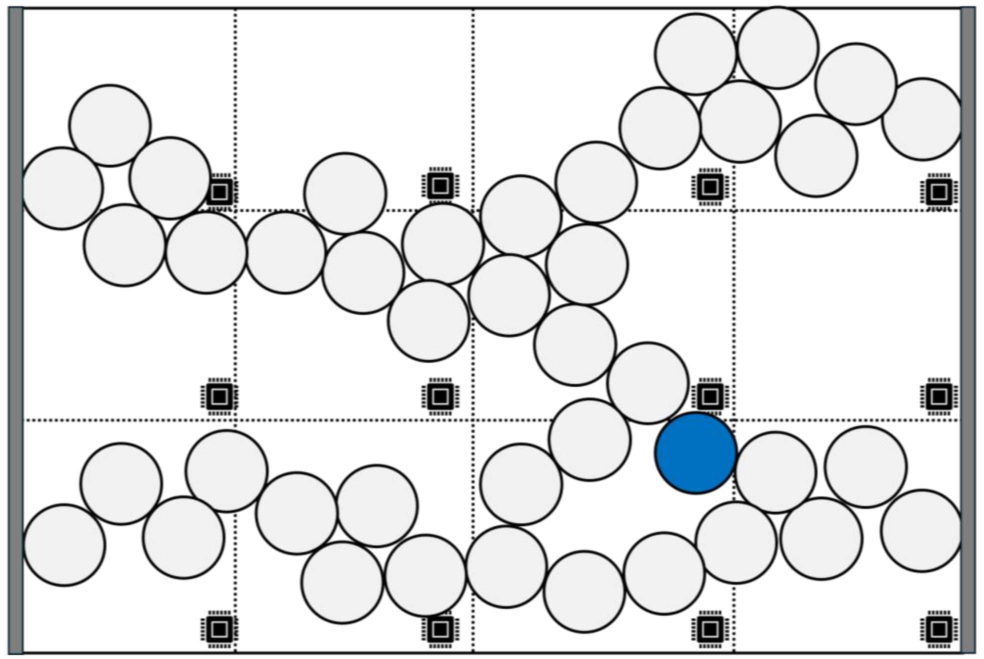
From chains to particles

$$\nabla \cdot j = 0 \Rightarrow \sum_{j=1}^{N_{nb}} j_{ij} = 0 \Rightarrow \sum_{j=1}^{N_{nb}} \sigma_i \frac{V_i - V_j}{d_{ij}} = 0$$

Electric potential balance
$$\left(\sum_{j \epsilon N(i)} \frac{1}{R_{ij}} + \frac{1}{R_{wall,i}} \right) V_i - \sum_{j \epsilon N(i)} \frac{V_j}{R_{ij}} = \frac{V_{wall,i}}{R_{wall,i}}$$

Jacobi update per particle
$$\begin{cases} V_i^{k+1} = (1-\omega) V_i^{(k)} + \omega \dfrac{\sum_{j \epsilon N(i)} \frac{V_j}{R_{ij}} + \frac{V_{wall,i}}{R_{wall,i}}}{\sum_{j \epsilon N(i)} \frac{1}{R_{ij}} + \frac{1}{R_{wall,i}}} \\ I.C.: \quad V_i^{(0)} = 0 \qquad \omega: relaxation\ factor \end{cases}$$

Convergence criteria: Conservation of charge ($I_{in} = I_{out}$)



Particles of a connected conductive electric pathway

Use charge conservation as a convergence criteria

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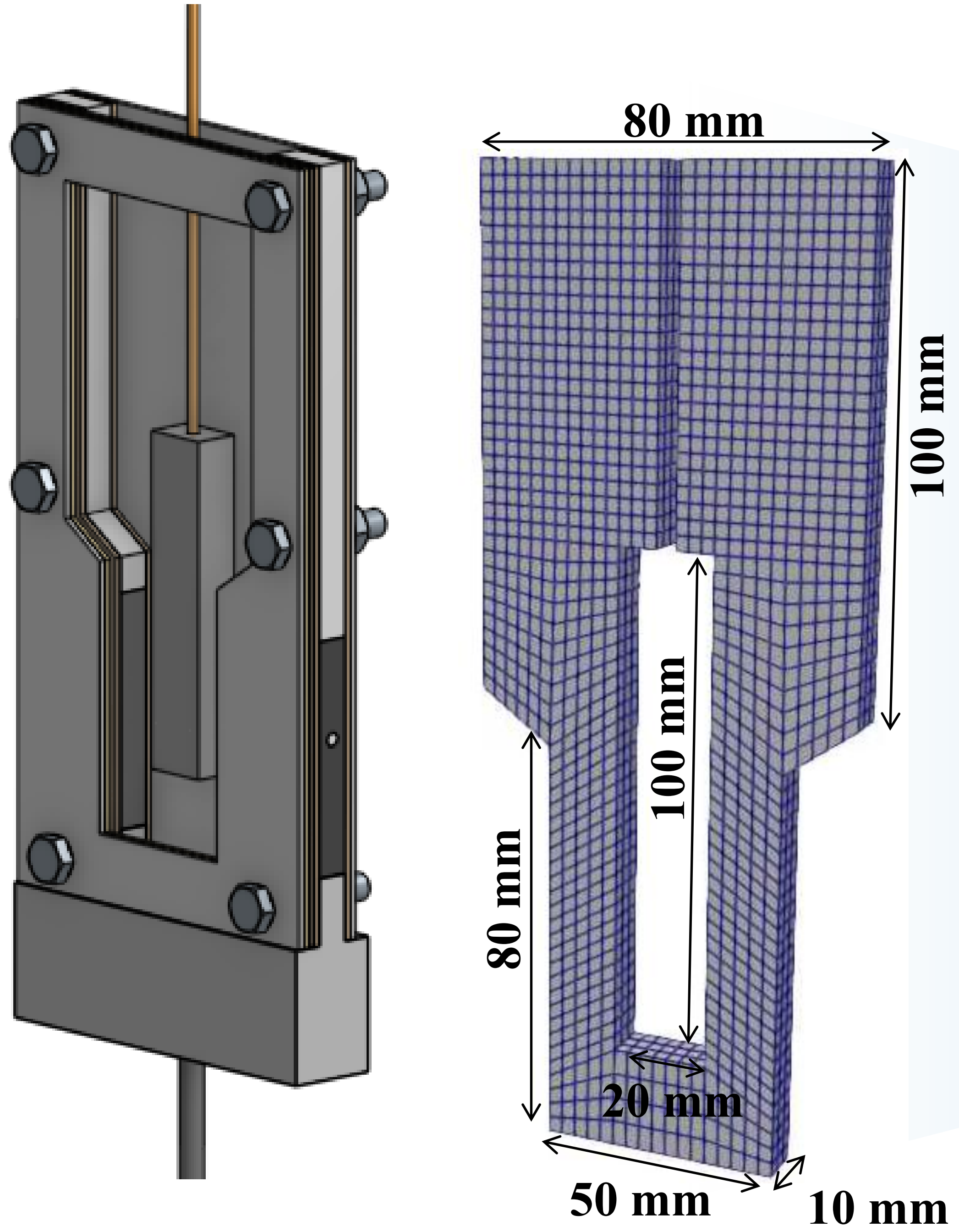
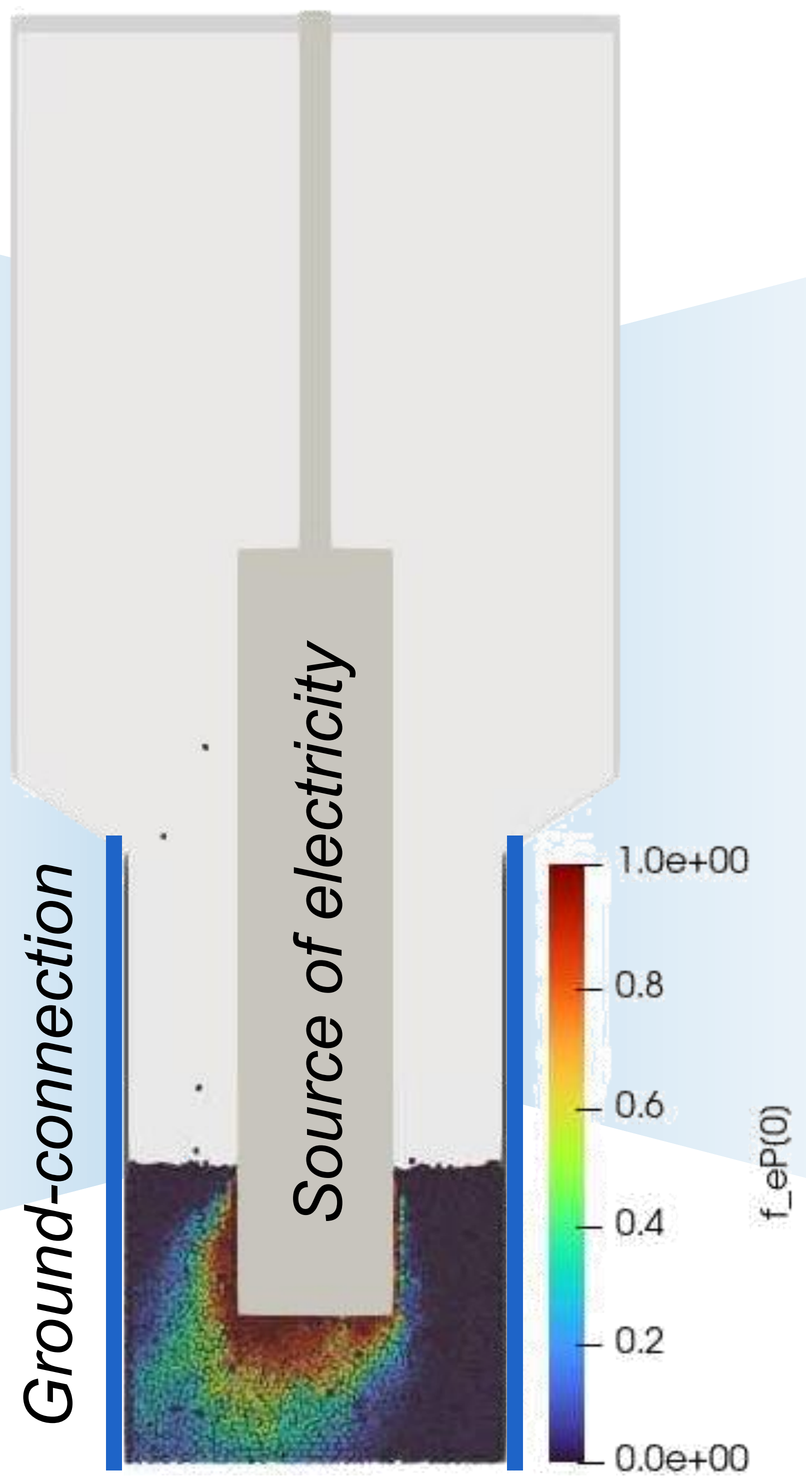
Fixed-condition

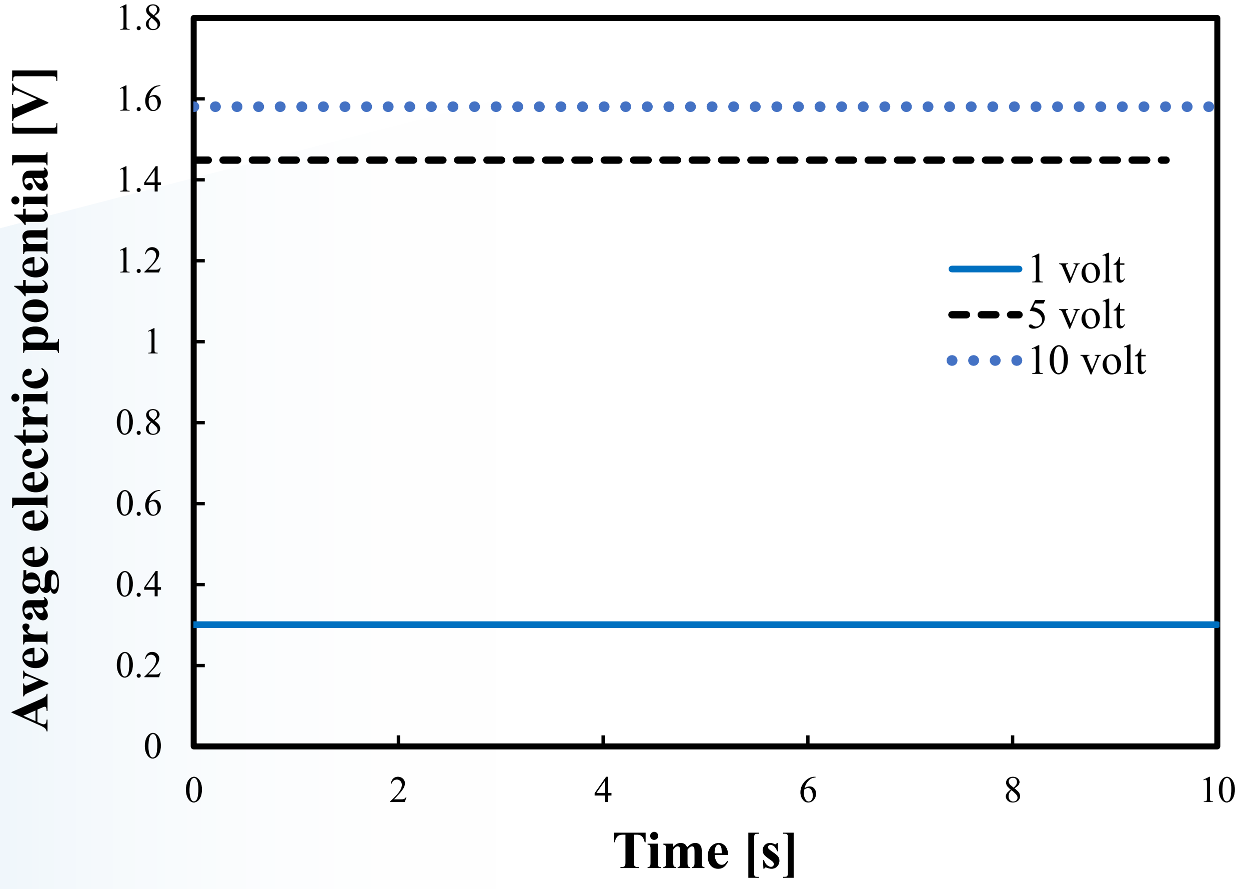


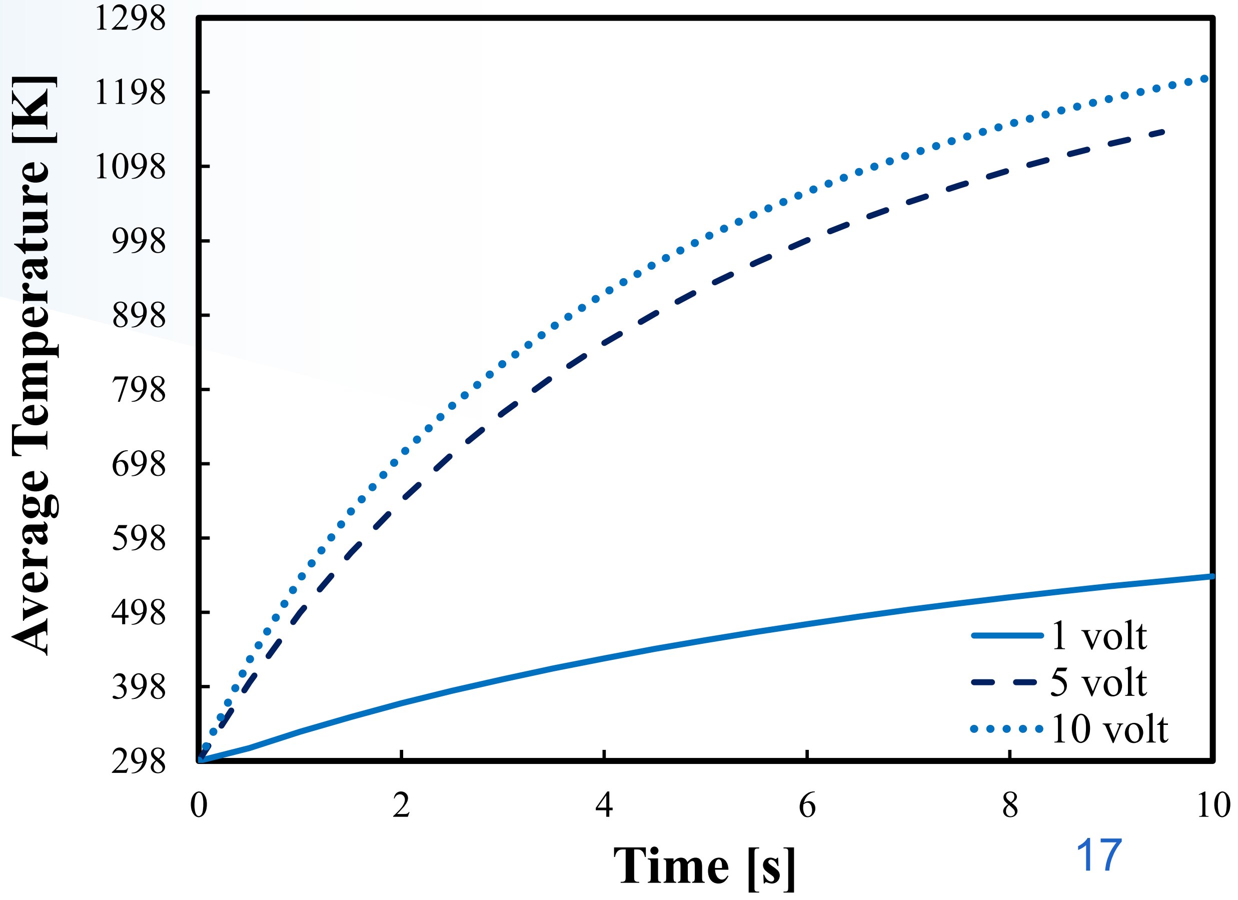
Proto-type 2D e-Bed



Electric potential distribution

Static bed → constant bulk electric resistivity





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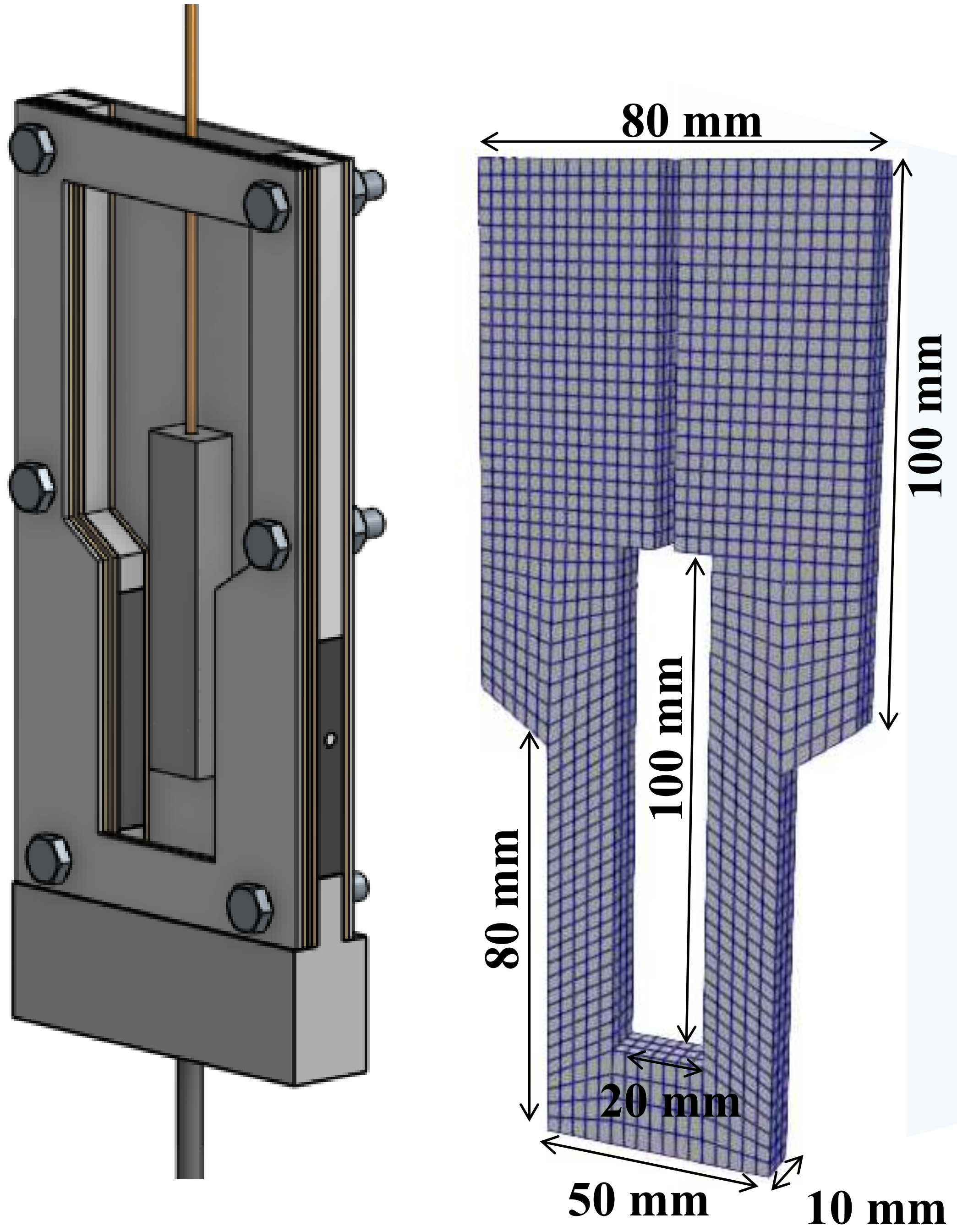
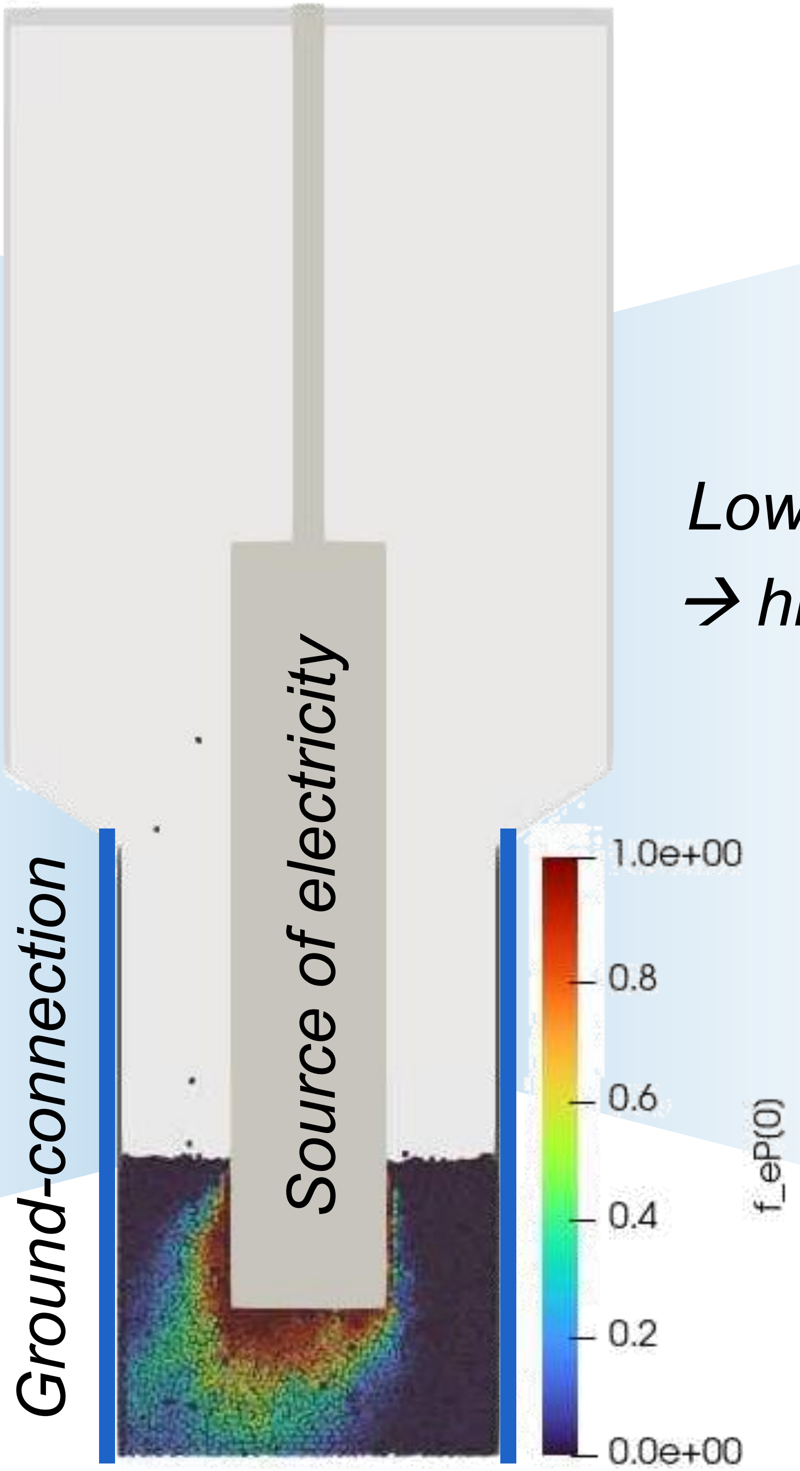
d_p=1mm
P=2500 kg/m^3
N_p= 20k

Fixed-condition

Static bed → constant bulk electric resistivity



Proto-type 2D e-Bed

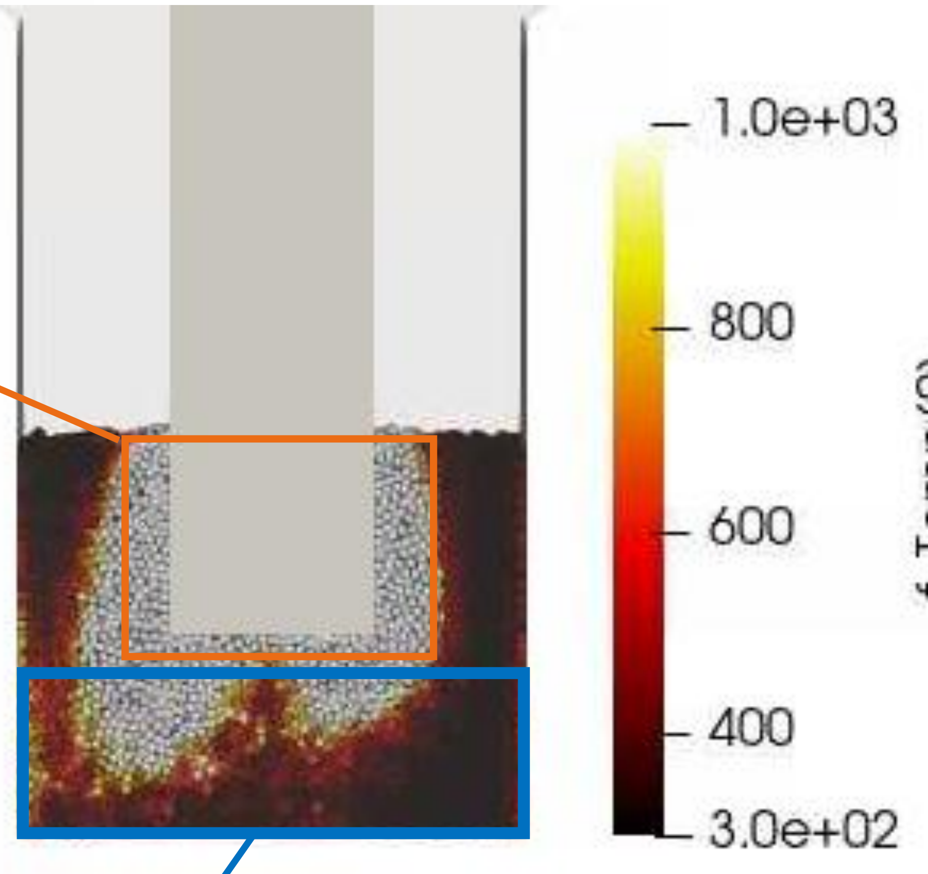


Electric potential distribution

Particle temperature distribution

Hot area

Lower p-p contacts → higher resistance



Dense bed (higher p-p contacts → lower electrical resistivity)

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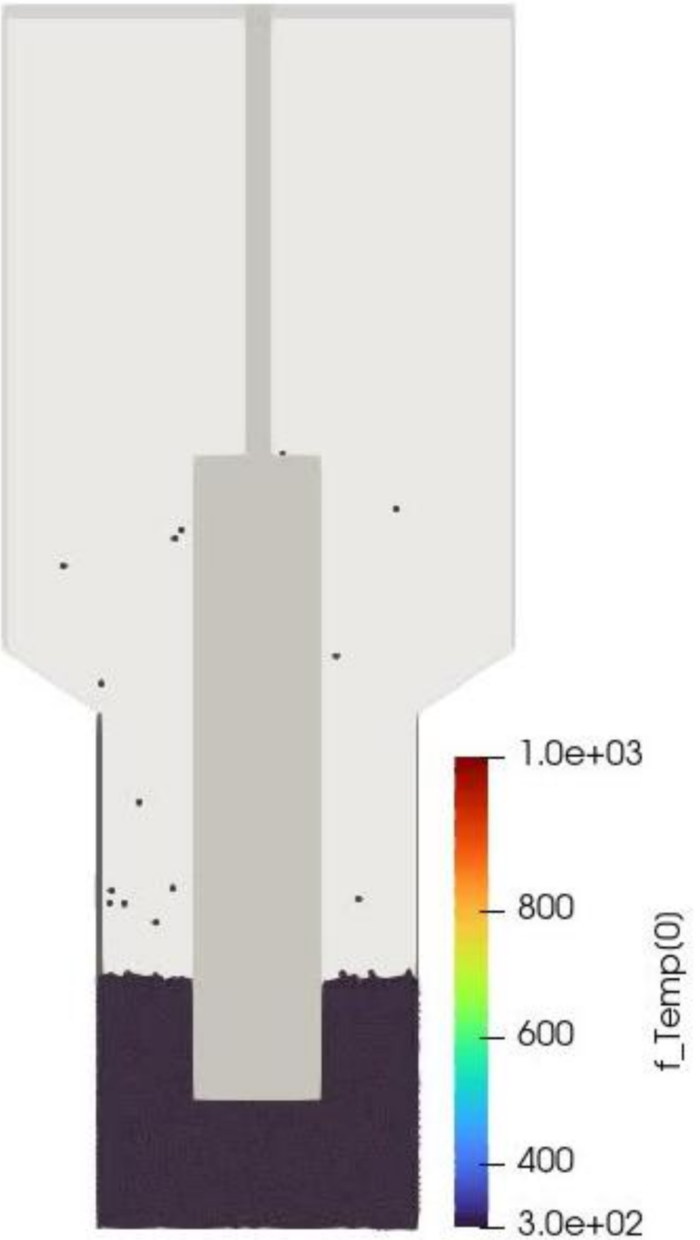
d_p=1mm
P=2500 kg/m^3
N_p= 20k

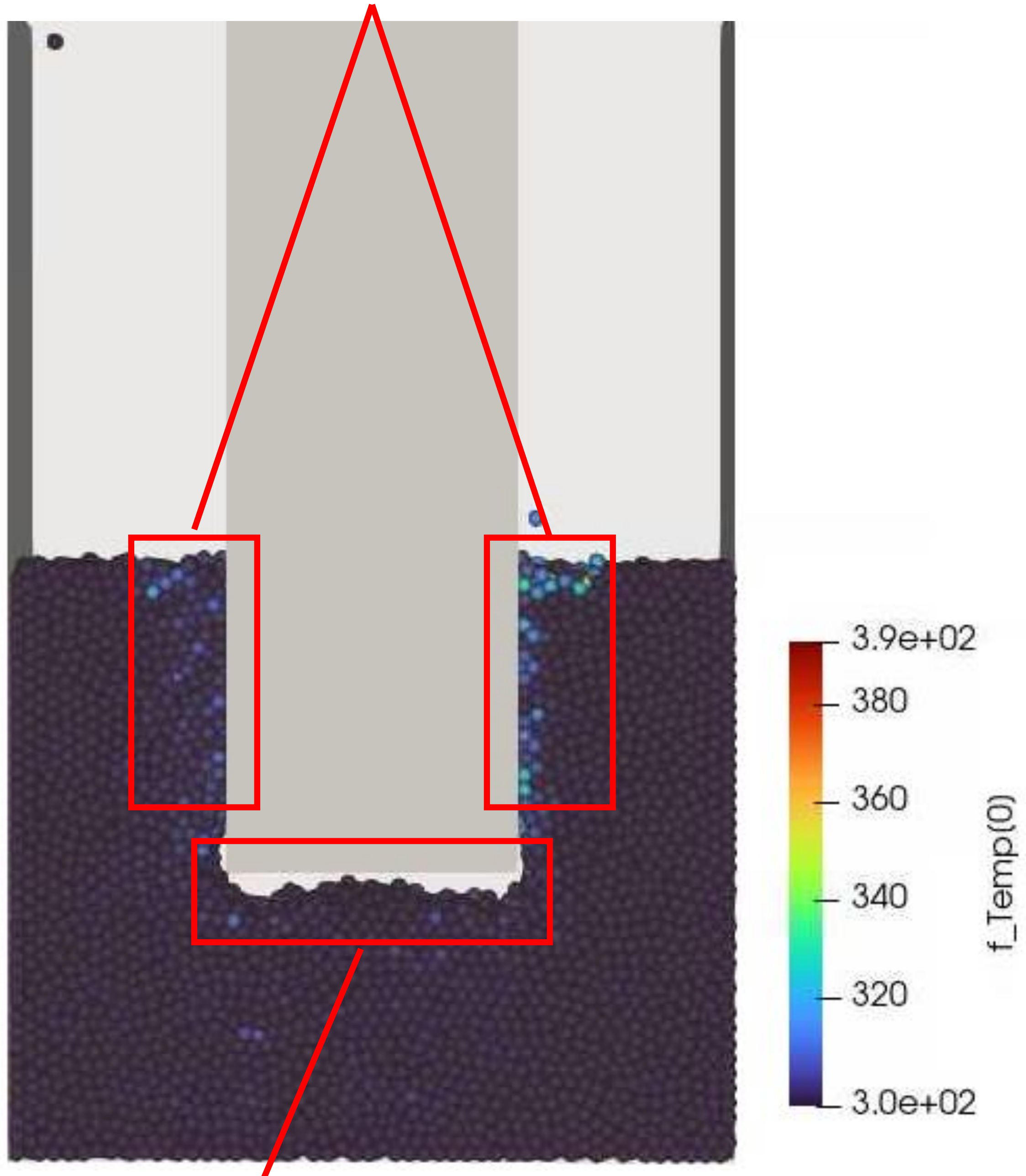
Fluidized-condition

Sides become the primary sources of electricity transfer



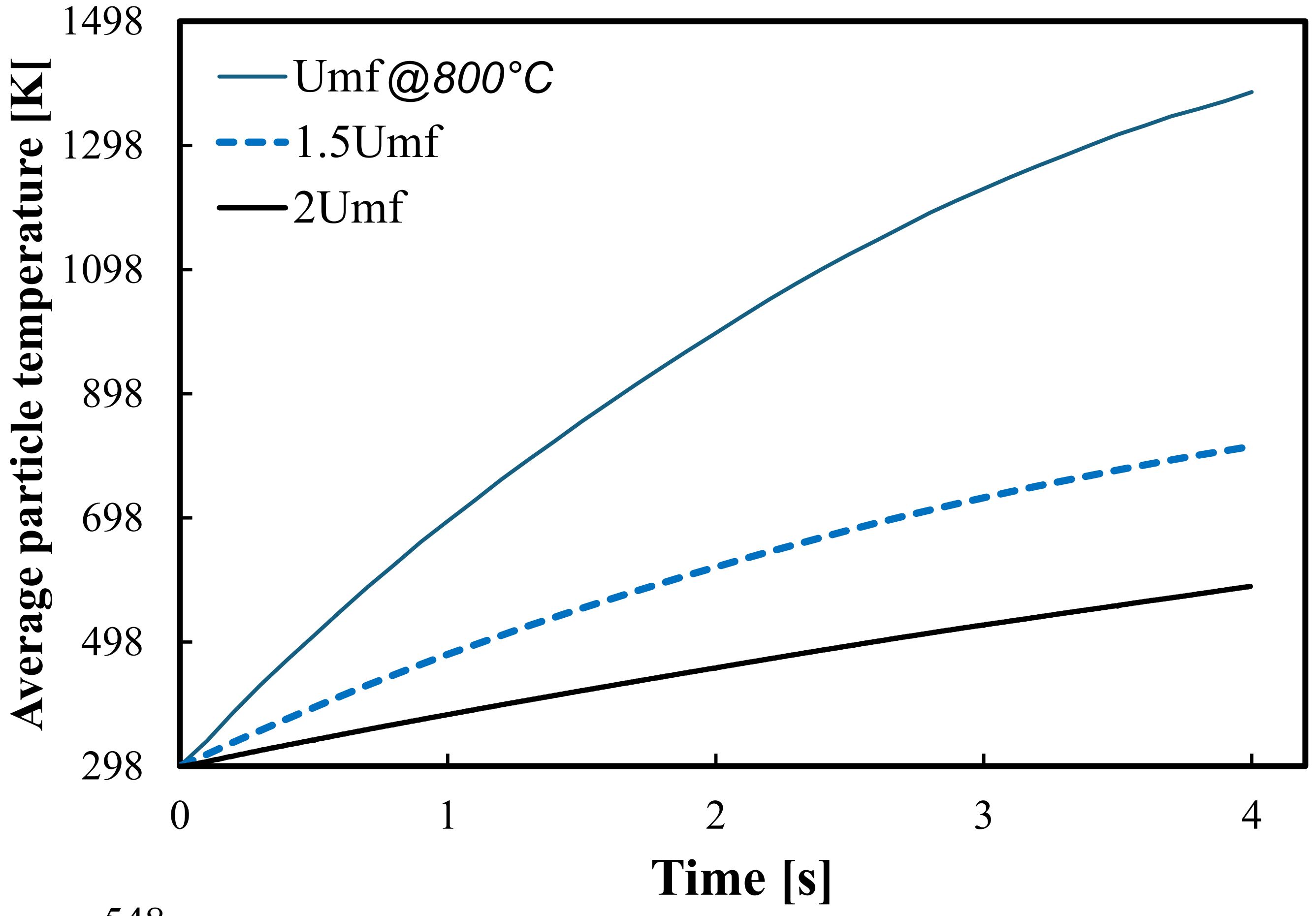
$U=U_{mf@25°C}$

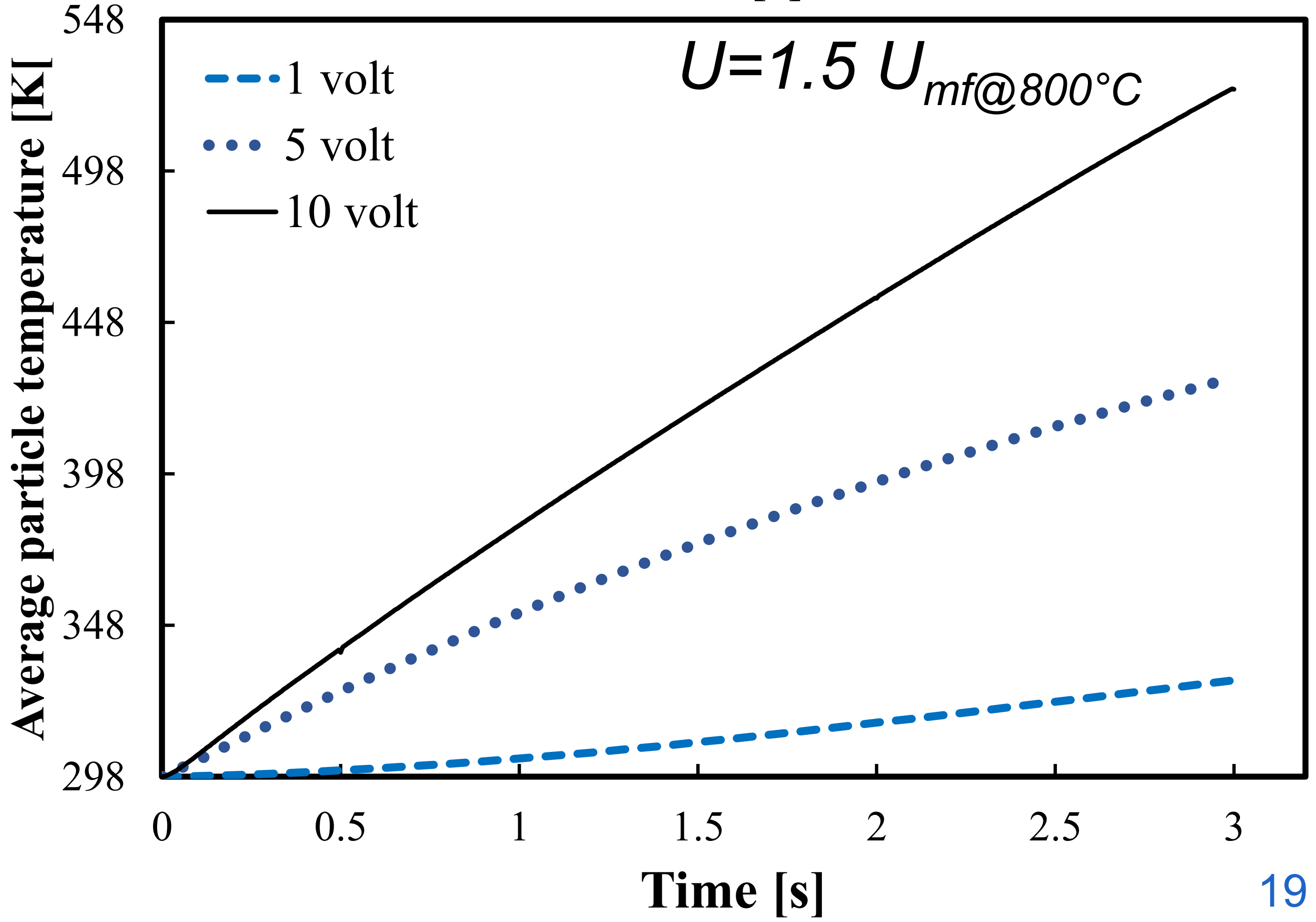
V_{in}=5 volts



Air pocket (bubbles)

Increase of velocity → breakage of clusters





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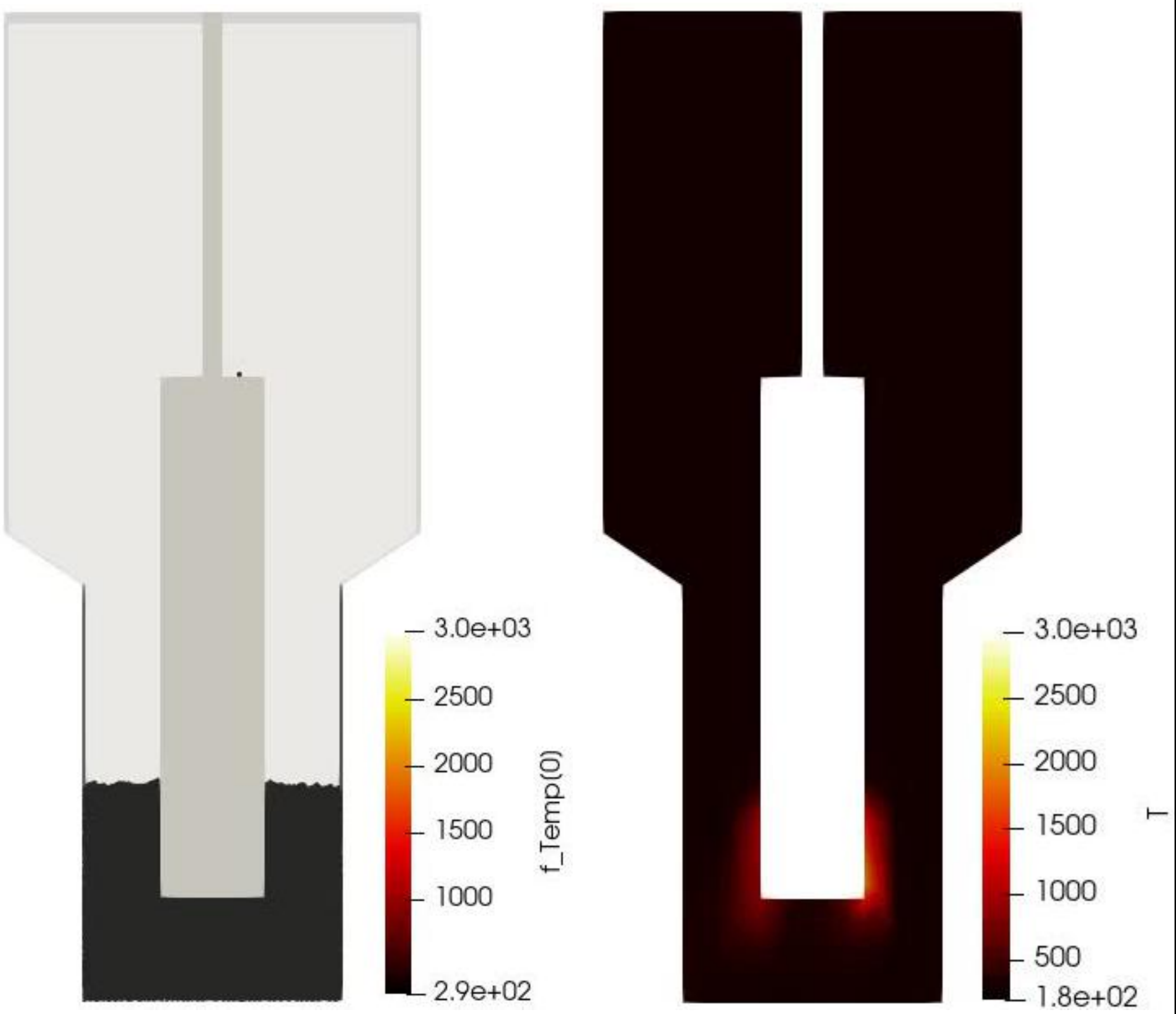
Comparison of Fixed- and Fluidized-conditions

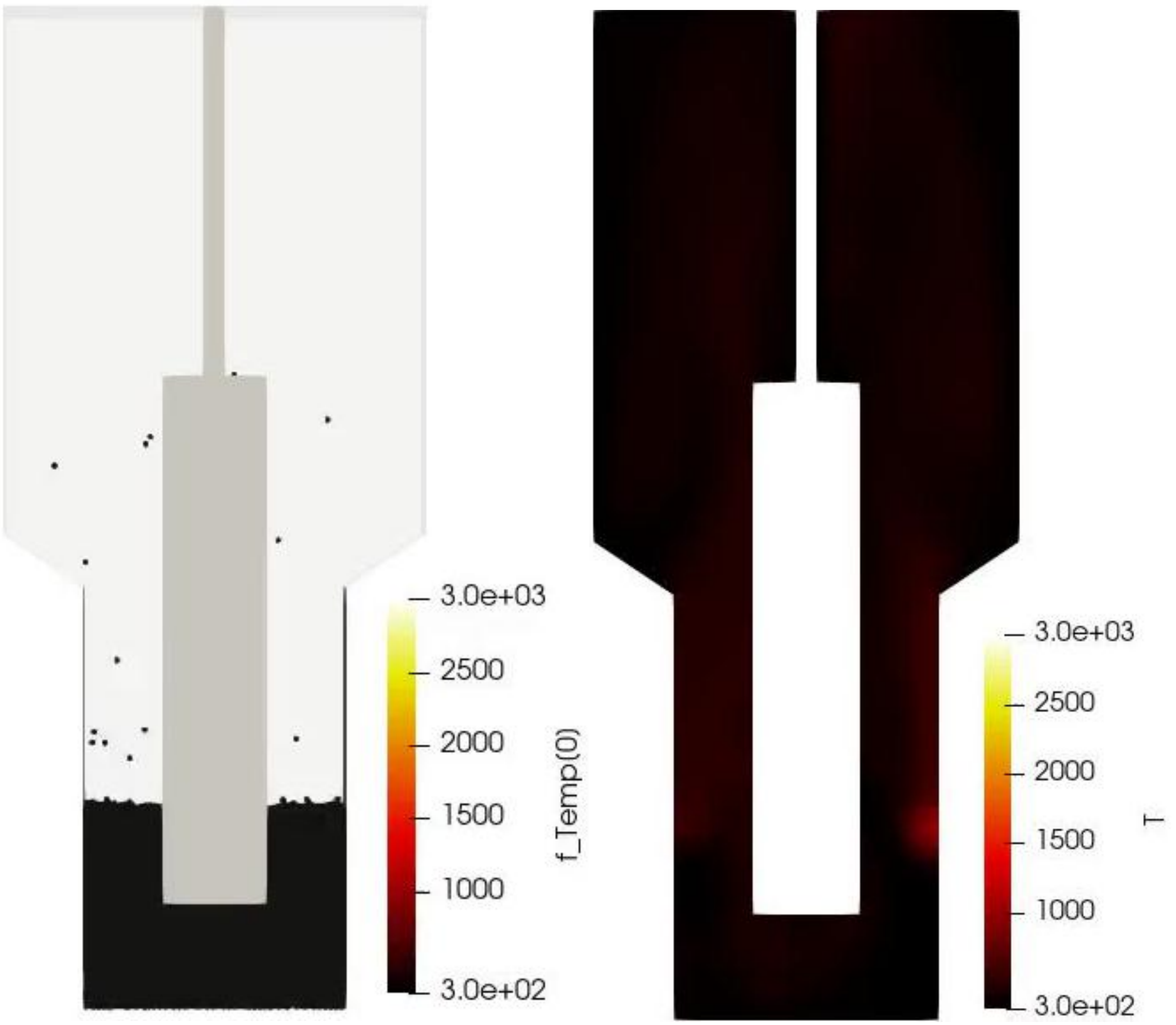
Fixed



Particles *Gas phase*

U=0, V=10 volts

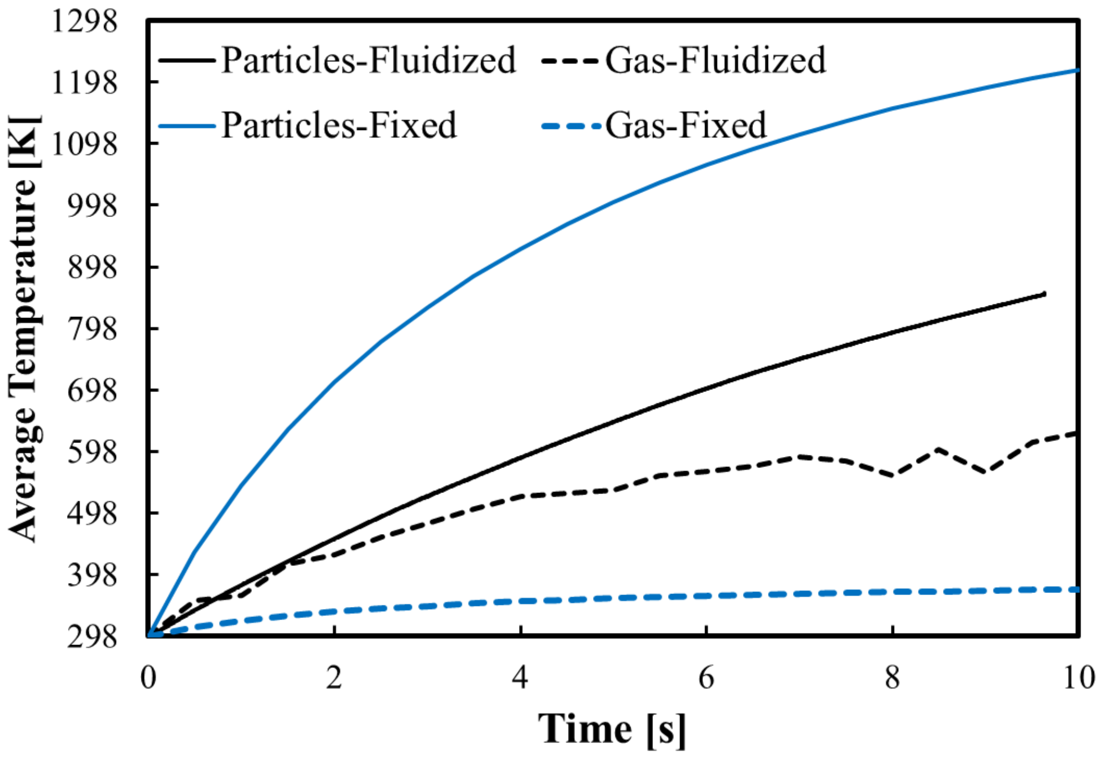
Fluidized



Particles *Gas phase*

U=1.5$U_{mf@800\ °C}$, V=10 volts

Average temperature



- *Higher particle temp for fixed-bed (static-bed)*
- *Higher gas temp for fluidized-bed (higher convection)*

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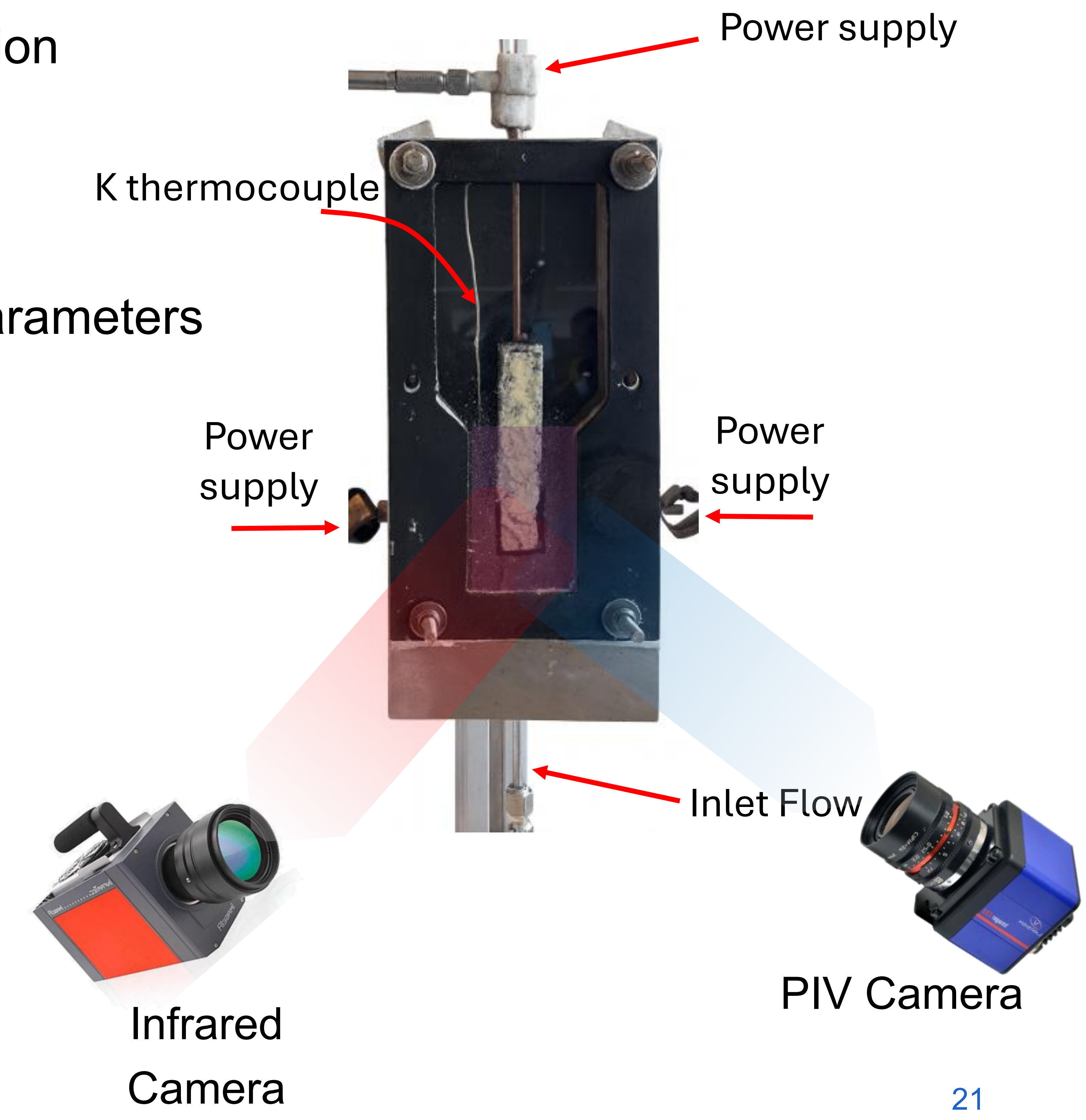
Conclusion and Future works

- Develop an algorithm for modeling electric conduction and joule heating
- Validation with available data in literature
- Chain formation and number of contacts are key parameters to control process

Future works

- Modeling arcs and discharges in bed
- Validation with experimental data of a 2D e-Bed
- Reactor design optimization
- Reactive CFD-DEM in e-Bed



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Yi.Ouyang@ugent.be
Kevin.VanGeem@ugent.be

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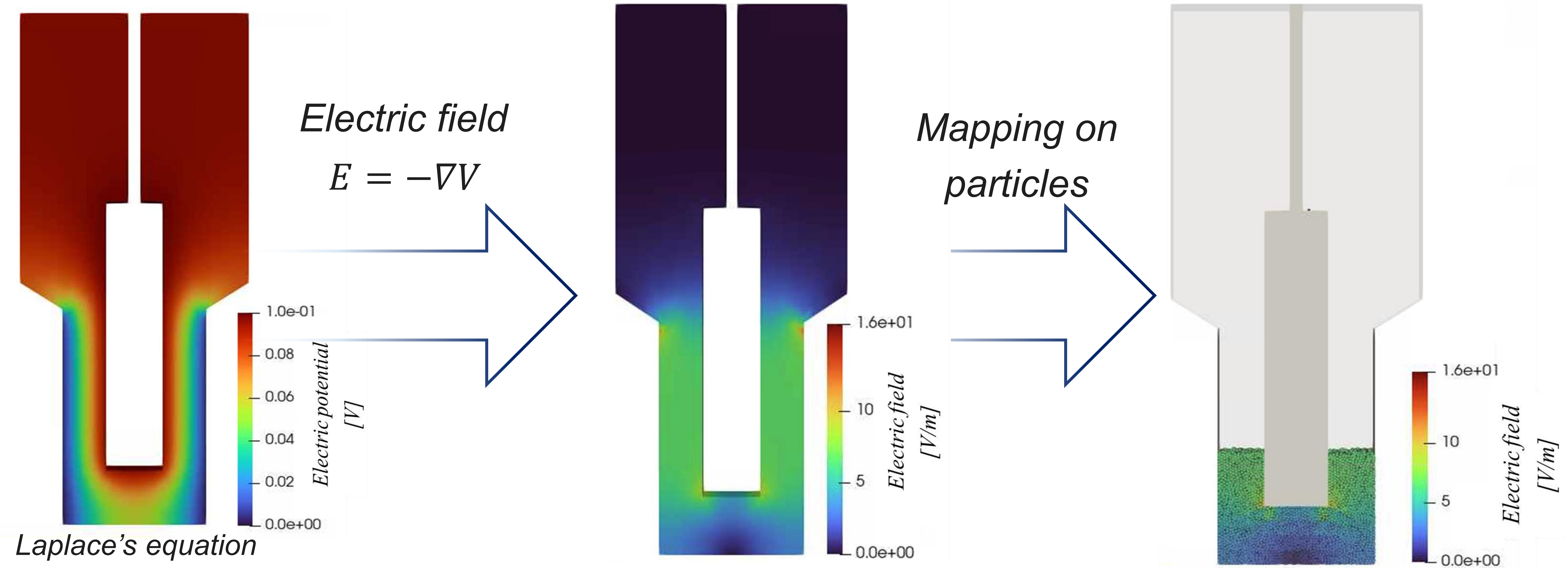
Fluidized-condition



Laplace's equation

$$\nabla^2 V = 0$$

Dipole-dipole force between particles i and j:

$$f_{ij}^{e} = \frac{3}{16}\pi\varepsilon_0^{e}\varepsilon_g^{e} d_p^2 \beta^2 \underline{\boldsymbol{E}}^2 \left(\frac{d_p}{R_{ij}}\right)^4 \left[\left(3\cos^2\theta_{ij} - 1\right)e_r + \left(\sin 2\theta_{ij}\right)e_\theta\right]$$

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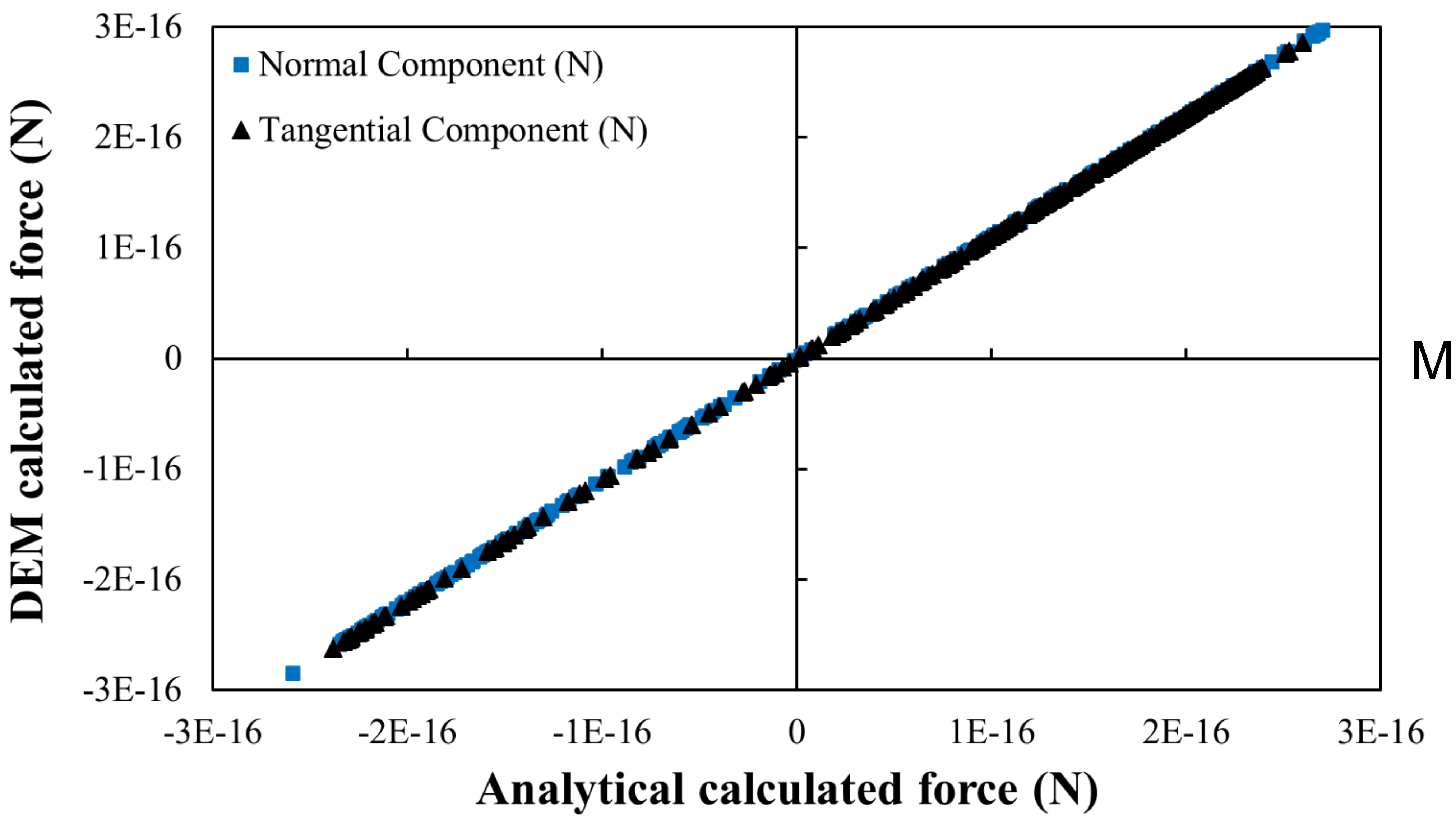
Laplace, Simon. *Traité de mécanique céleste* libraire pour les mathématiques (1825)
Liu, et al., Powder Technology. (2020) https://doi.org/10.1016/j.powtec.2019.11.096

Fluidized-condition



Mean absolute percentage error

%9.13

Dipole-dipole force between particles i and j:

$$f_{ij}^{e} = \frac{3}{16}\pi\varepsilon_0^e\varepsilon_g^e d_p^2\beta^2\underline{E}^2\left(\frac{d_p}{R_{ij}}\right)^4\left[\left(3\cos^2\theta_{ij}-1\right)e_r+\left(\sin 2\theta_{ij}\right)e_\theta\right]$$

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Laplace, Simon. *Traité de mécanique céleste* libraire pour les mathématiques (1825)
Liu, et al., Powder Technology. (2020) https://doi.org/10.1016/j.powtec.2019.11.096

Preliminary experiments

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