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Challenges in Microscale simulation of cycling proccess of CaO hydration and re-hydration in thermochemical heat storage

Introduction

For thermal energy storage in the high temperature range (>250 °C), TCES-concepts based on lime $CaO/Ca(OH)_2$ are promising. The basis is the reversible reaction $CaO + H_2O \leftrightarrow Ca(OH)_2$, which is exothermal for the hydration process and endothermal for the dehydration process. The material has several advantages: widely available and thus cheap, non-toxic, high energy density and useable for high temperature processes. Schmidt et al. [1] use mentioned material for thermochemical energy storage at low vapour pressure in a lab scale reactor in a closed system with indirect Heat Transfer Fluid (HTF). However, after some cycling process of de/re-hydration the powder becomes agglomerates as it can be seen in figure 1.
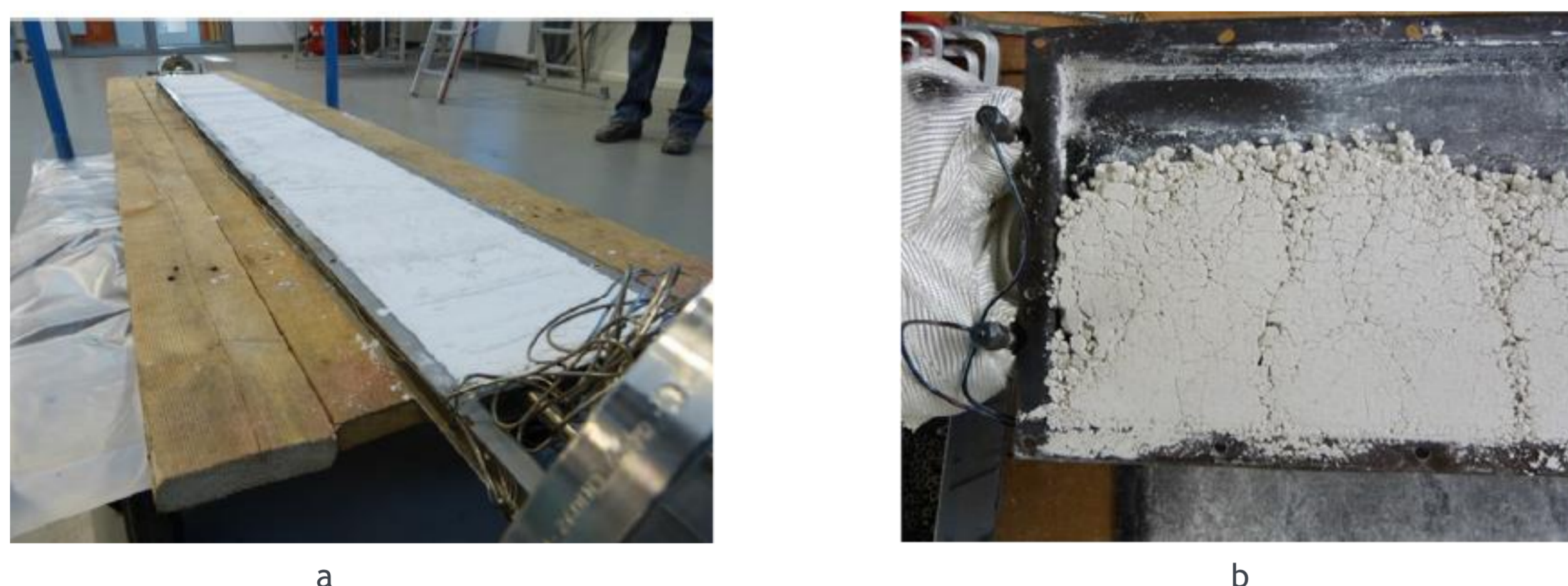
Figure 1. a) Initial bed of powders befor reaction. b) After some cycling reaction process.

Thus, the new structure of the powder bed make it inappropriate for simulation in conventional continuum method. The goal of this research is to conduct micro-scale simulation of this process to find how the structure changes and agglomerates are formed. During this process particles change size and interact with each other and also the steam can exert an external force to them as it can be seen schematically in figure 2.
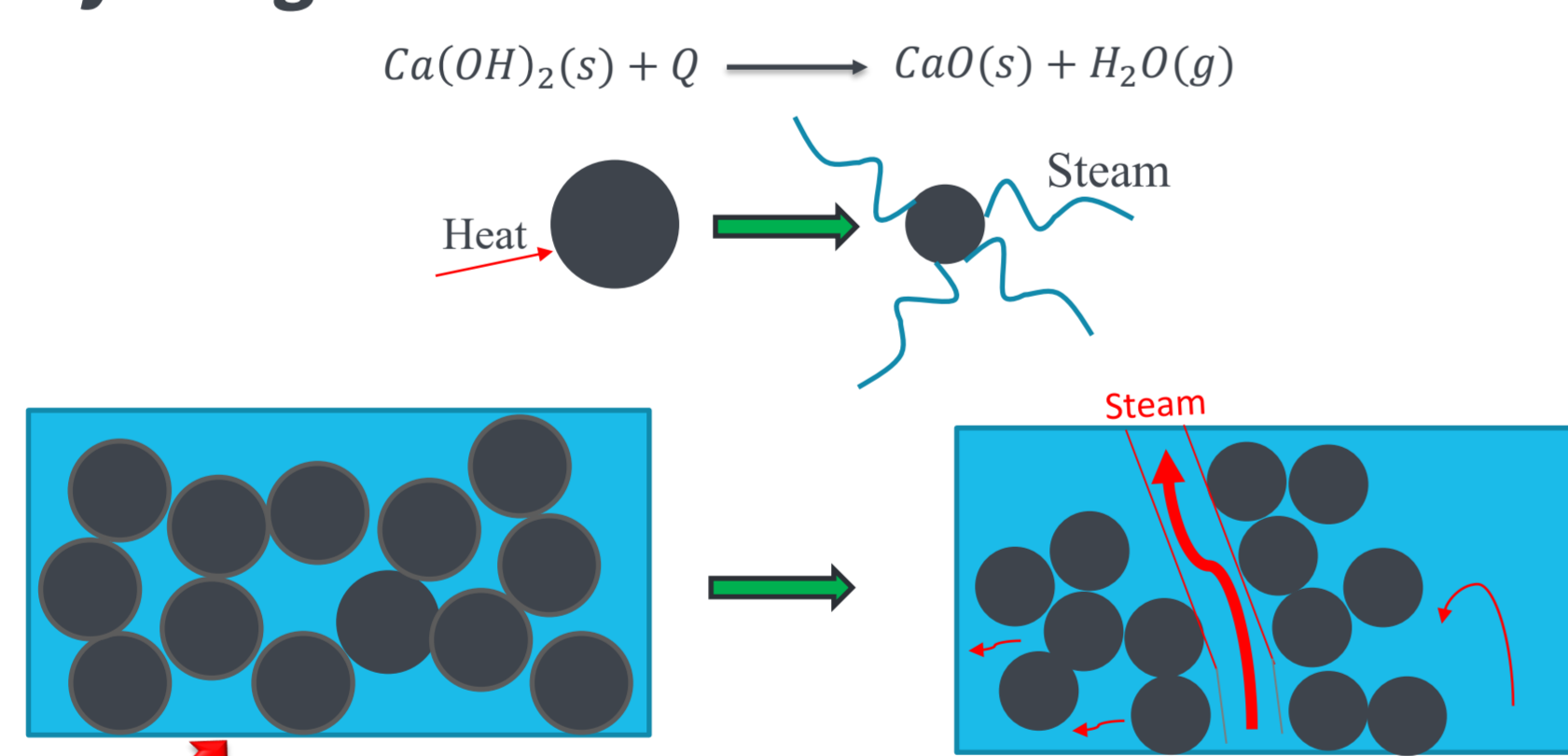
$$Ca(OH)_2(s) + Q \longrightarrow CaO(s) + H_2O(g)$$

Heat, Steam, Steam, Heat

Figure 2. Reaction process Schematically

Numerical Scheme:

Since we are looking for the new position of the particle, the DEM method can be DEM method can be appropriate. In this method , the particle position update based on the newton's second law. Additionally, we consider that forces between particles are similar to spring and dashpot between them.

$$\frac{\partial^2 \vec{r}_i}{\partial t^2} = \frac{1}{m_i}\vec{F_i}(\vec{r}_j, \vec{v}_j, \vec{\varphi}_j, \vec{\omega}_j)$$

Therefore, if we know forces that applied in the particle we can find the new position. We consider the mesoscale model by Luding[2].

The normal and tangential contact force in Luding model has been shown in figure 3.
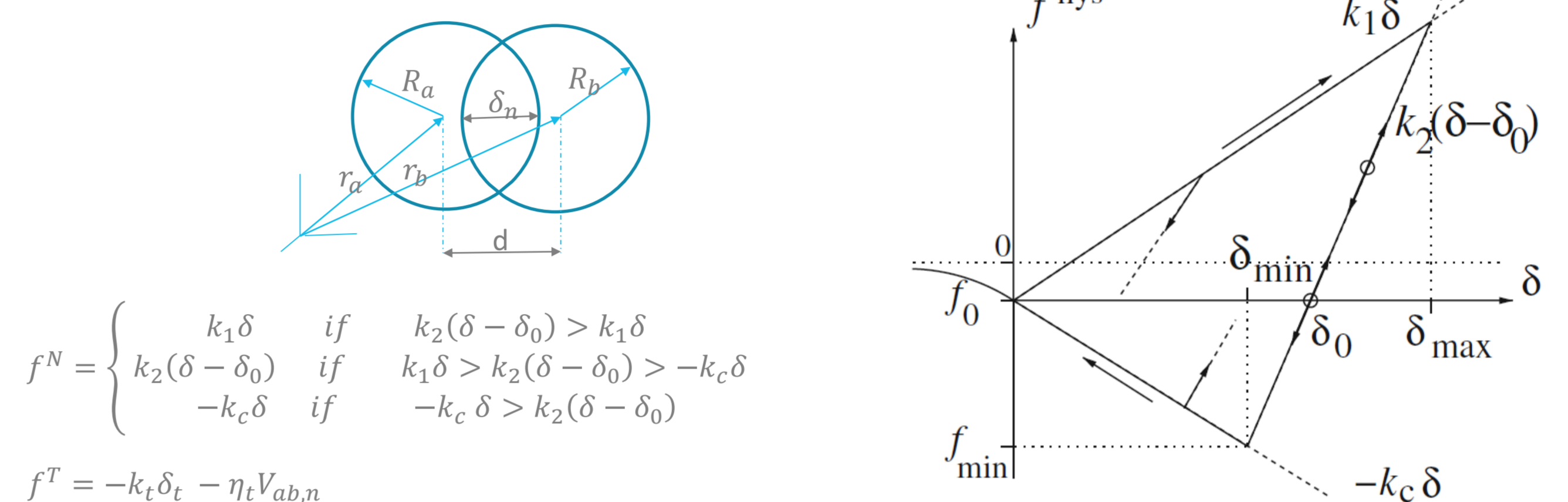
$$f^N = \begin{cases} k_1\delta & if & k_2(\delta - \delta_0) > k_1\delta \\ k_2(\delta - \delta_0) & if & k_1\delta > k_2(\delta - \delta_0) > -k_c\delta \\ -k_c\delta & if & -k_c\delta > k_2(\delta - \delta_0) \end{cases}$$

$$f^T = -k_t\delta_t - \eta_t V_{ab,n}$$

Figure 3. Normal and tangential contact force [2]

Results:

As a first step, we conduct a simple simulation. In this example we consider that particle size linearly change with time. The particle size linearly increases during the hydration and decreases in re-hydration. Additionally, the adhesion force between particles linearly increase with time. The snapshopts of simulation cab be seen in the figure 4.

Timestep = 2,500,000   Timestep = 5,000,000   Timestep = 7,500,000

Timestep = 10,000,000   Timestep = 12,500,000   Timestep = 15,000,000

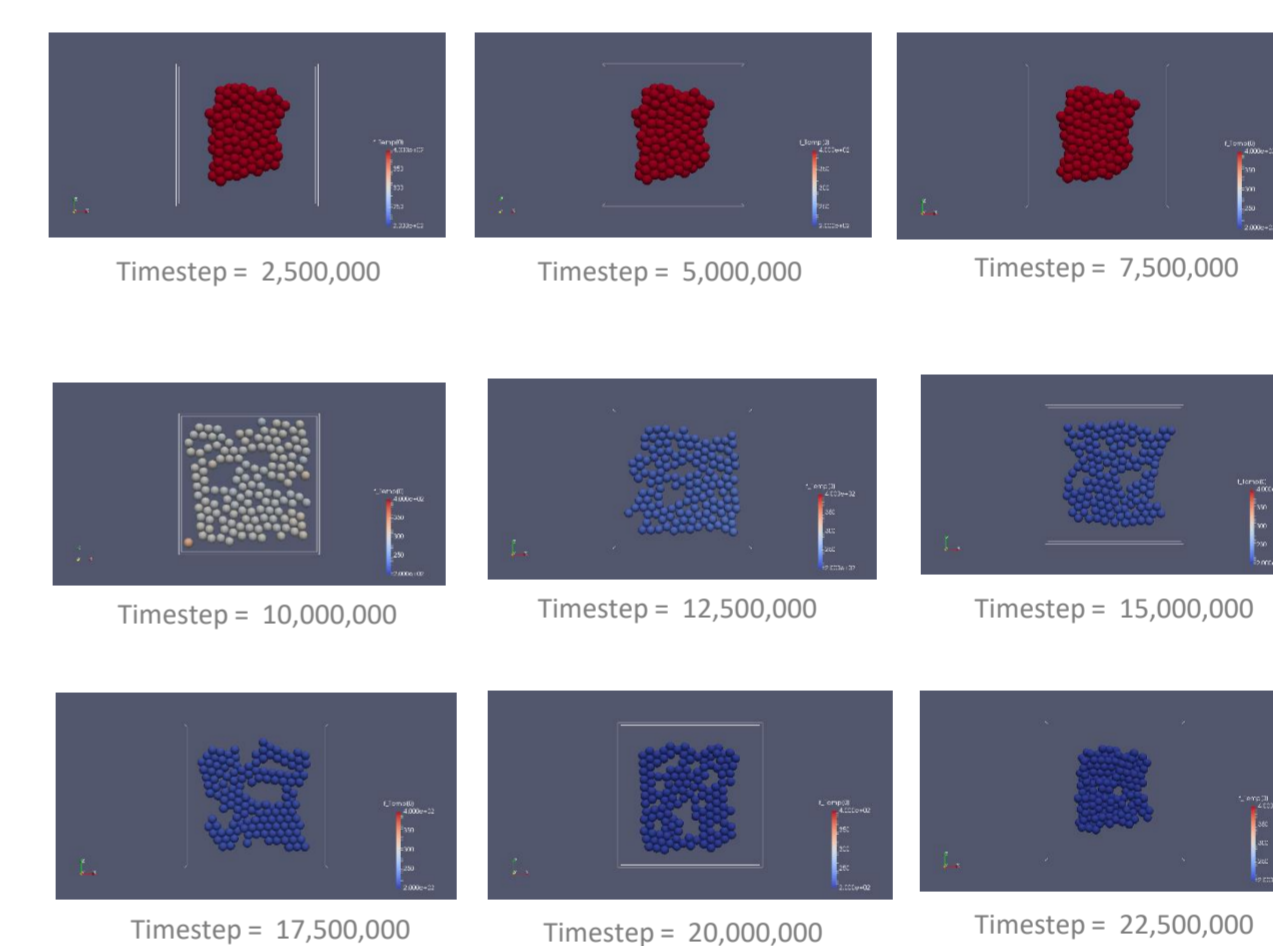Timestep = 17,500,000   Timestep = 20,000,000   Timestep = 22,500,000

Figure 4. Snapshots of simulation. Each time step is $10^{-7}[s]$

Figure 5. shows that how the the number of agglomerates and an agglomerate with maximum number of particles changes during this simulation.
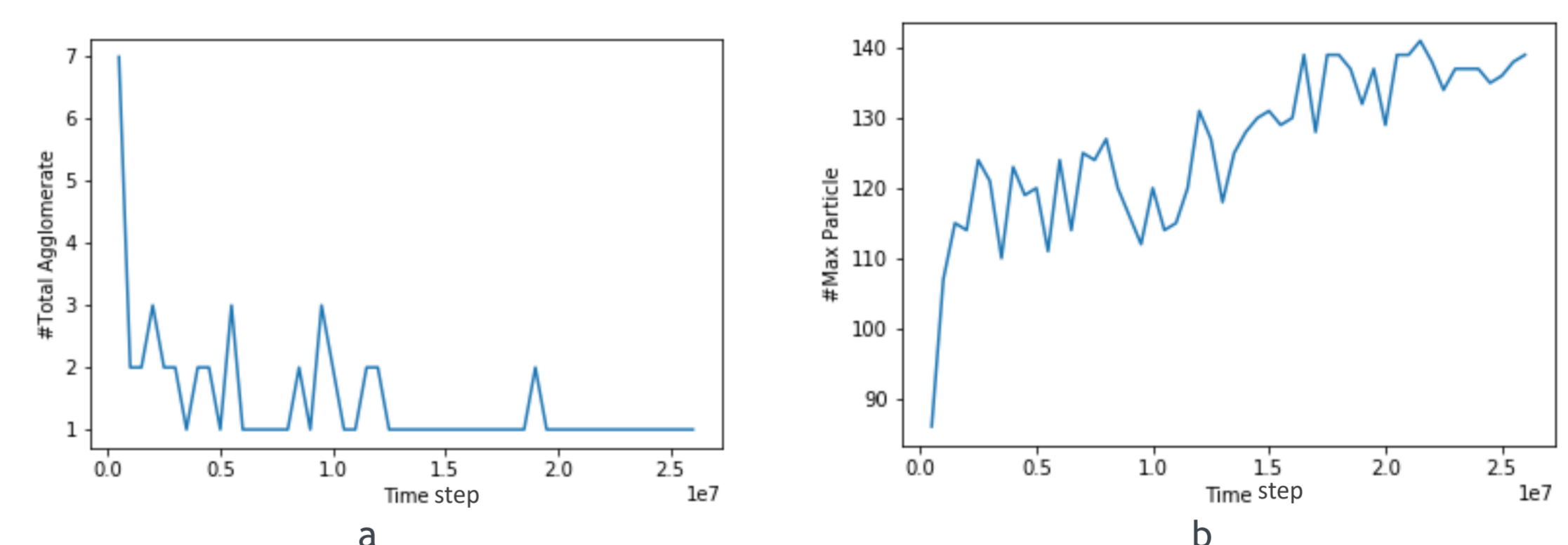
Figure 5. a) Total number of agglomerates. b) An Agglomerate with maximum number of particles.

Outlook:

The model needs to be callibrated with an appropriate experiment. In current model we did not consider fluid force on particle. It can be consider in next steps.

Reference:

1- Power generation based on the Ca(OH) 2 / CaO thermochemical storage system – Experimental investigation of discharge operation modes in lab scale and corresponding conceptual process design, M. Schmidt, M. Linder, 2017

2- Cohesive, frictional powders: contact models for tension, S. Luding, 2008