Attrition Prediction in Chemical Looping Systems

Ronald Breault, Samuel Bayham, Esmail Monazam, Nathan Galinsky

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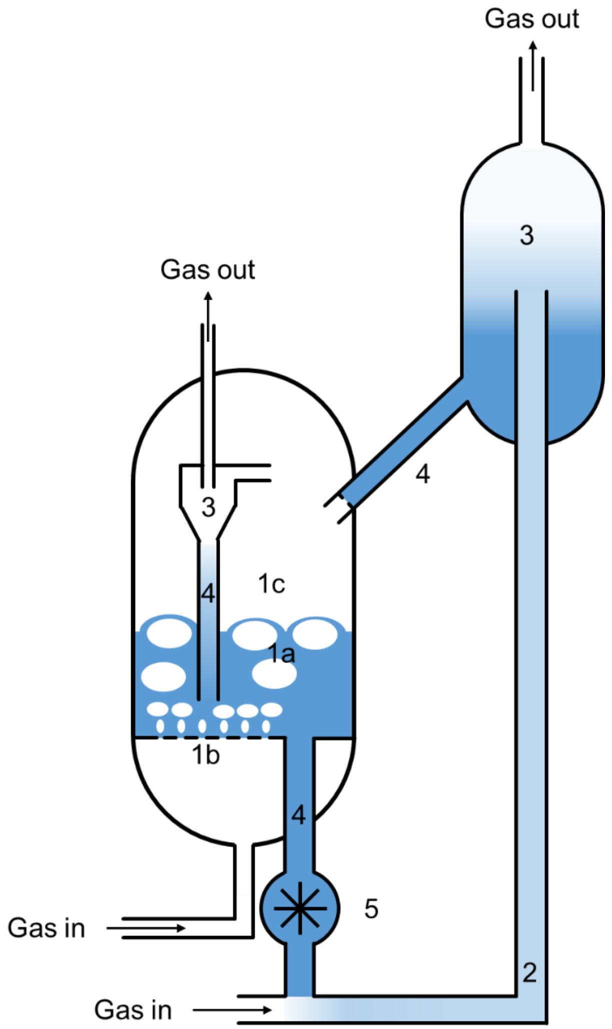
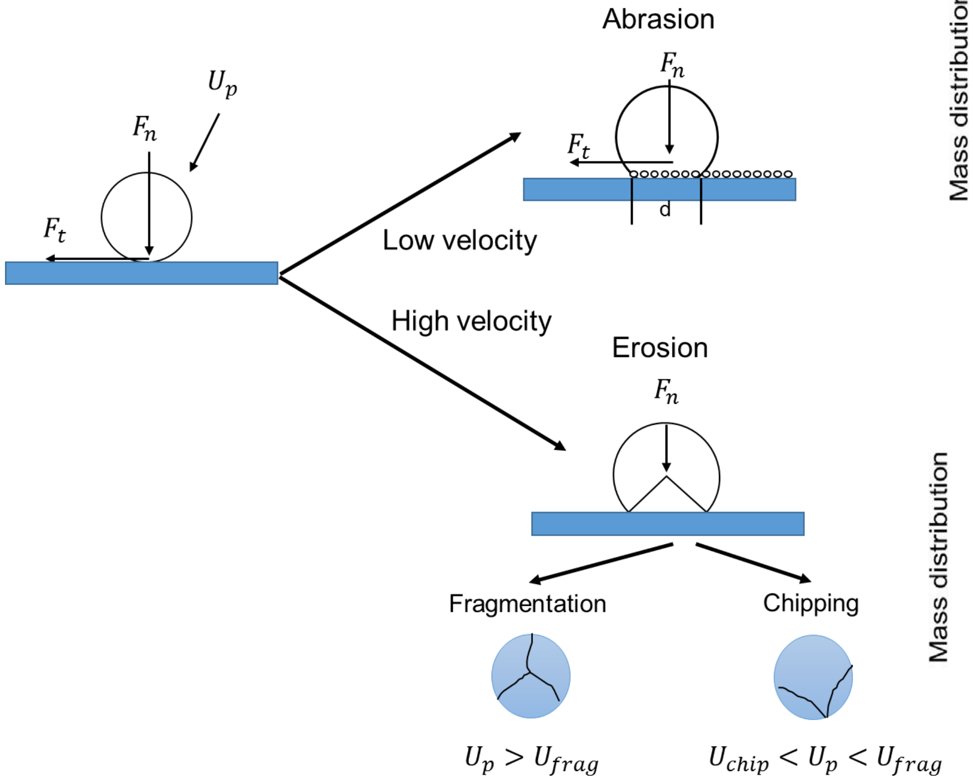
Attrition of Particulate Solids

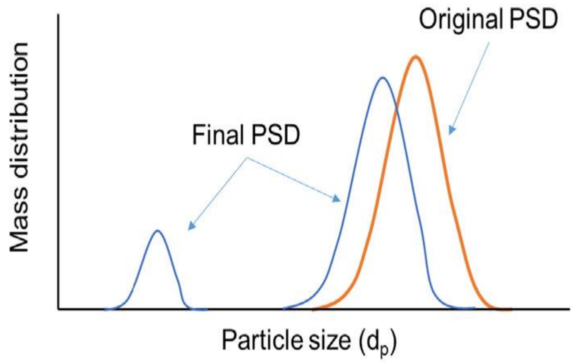
- **Attrition is the unintentional breakdown of solids due to stresses applied**
  - As opposed to comminution, where breakdown is intentional (e.g., coal pulverizer)
- **Three types of stress on the solid:**
  - Thermal:
    - Uneven expansion or contraction of the particle as it is heated or cooled, causing decrepitation
  - Chemical
    - internal stresses that change the lattice structure, weakening particles and produces surface features that can be easily abraded upon application of small external stresses
  - Mechanical
    - Abrasion (low velocity rubbing)
    - Fragmentation/chipping (high velocity impact)

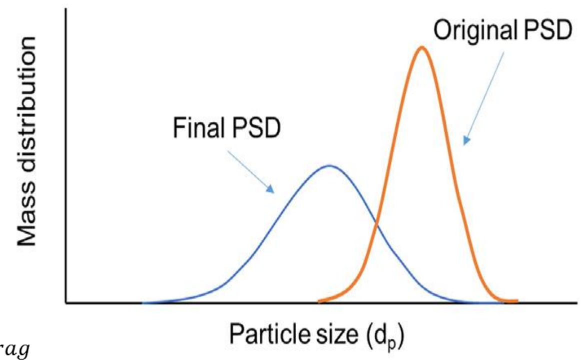


Mechanical Attrition in CFB systems

- The rate of mechanical attrition is based on the velocity range and mode of contact.
- Abrasion is **low velocity** rubbing of particles against surfaces, producing very small fines
- Erosion consist of fragmentation and chipping as a result of **high velocity** impact
  - Does not occur below a certain threshold velocity







Bayham, Samuel C., Ronald Breault, and Esmail Monazam. "Particulate solid attrition in CFB systems–An assessment for emerging technologies." *Powder Technology* 302 (2016): 42-62.

Motivation: Chemical Looping Combustion

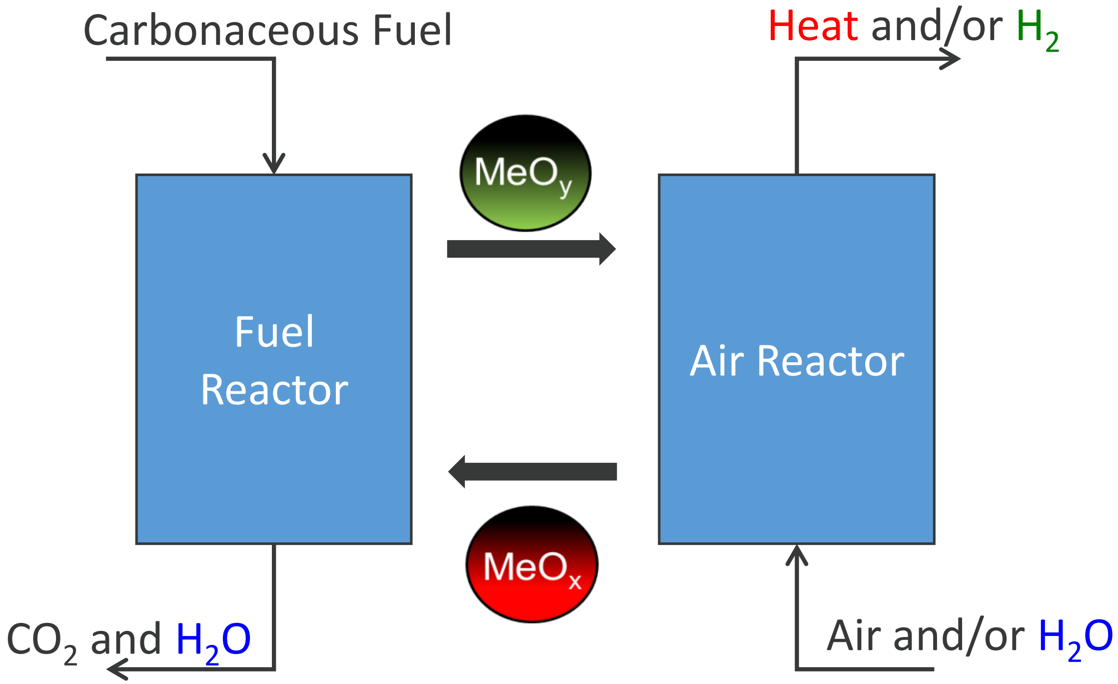
- Chemical Looping Combustion is an advanced oxycombustion technology that utilizes a metal oxide to provide oxygen to the fuel.

Potential advantages:

- CO_2 capture
- No need for cryogenic separation of O_2
- Heat integration between reactors

Key challenges:

- Reactor design
- **Oxygen carrier design and cost**
  - **Favorable economics** of scaled-up process highly dependent on **cost** and **makeup rate** of metal oxide
  - **Makeup rate** dependent on metal oxide **attrition** rate



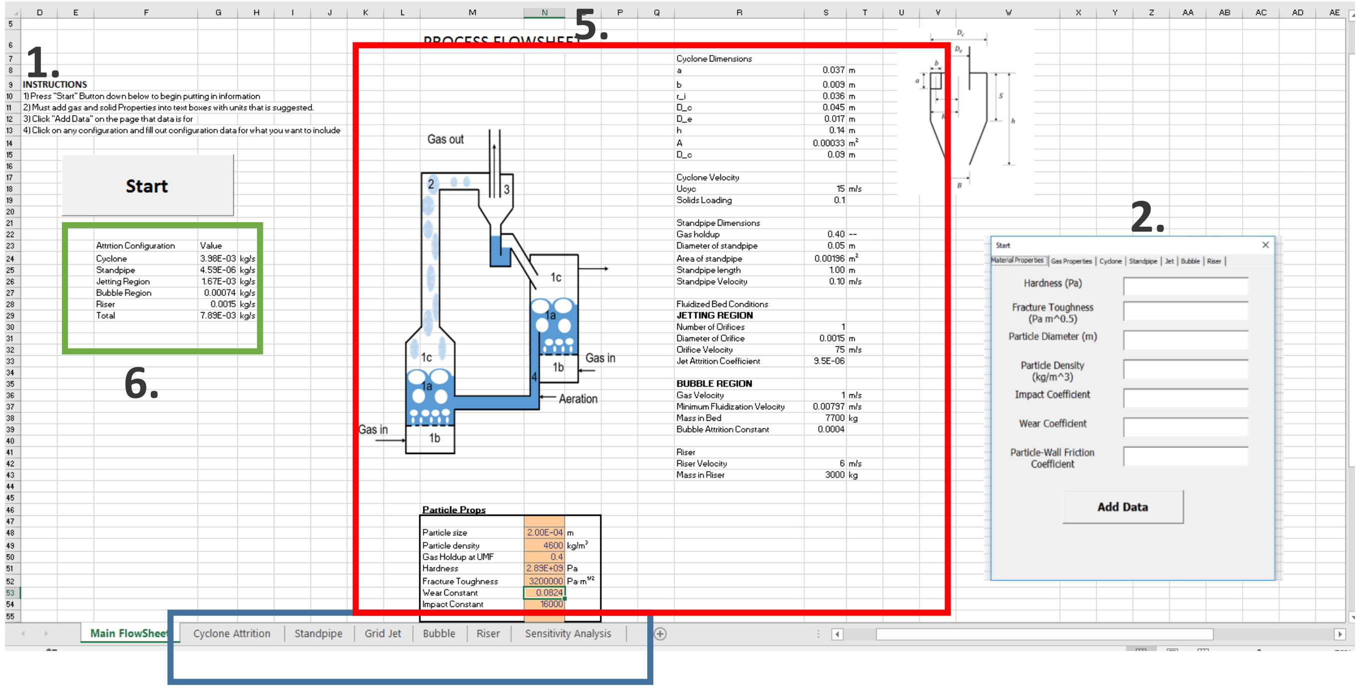
Goal and Approach of Attrition Research at NETL

1. Determine functionality of material parameters relevant to attrition as the carrier progresses through various oxidation and reduction states while thermally cycling.
2. Construct a high temperature attrition unit to validate **spreadsheet model**
   - Solids sampling system with bank of filters that can be switched in and out of service to capture fines as function of time
3. Development of **simple** (population-balance type) model to predict attrition losses based on fundamental erosion and abrasion mechanisms
   - Combine with technoeconomic modeling

- Utilize attrition data from NETL's 50 kW_{th} CLR unit as applicable

Zero-order Spreadsheet Model

- **Developed in Microsoft Excel using VBA**
- **Key Features:**
  1. Instructions on running model
  2. Simple user form input data
  3. Unit Configurations (Fluidized beds, risers, cyclones, standpipes, impactor)
     1. Can choose # of each configuration
  4. Sensitivity Analysis
  5. Key properties for different configurations
  6. Total Attrition rate per configuration



3. and 4.

Mechanical Attrition Models

1) Fluidized bed

- Consists of bubble and jet attrition

$$\dot{m}_{attr,bubble} = m_{bed} C_b (u_g - u_{mf})$$

$$\dot{m}_{attr,jet} = n_{or} C_j d_p \rho_g d_{or}^2 u_{or}^3$$

[Thon and Werther 2009]

2) Standpipe

$$\dot{m}_{attr,sp} = \frac{k}{H} \frac{\rho_s^2 (1 - \epsilon_g) g}{4 f_w} \pi D_s^2 L u_p$$

[Bayham et al. 2016]

3) Cyclone

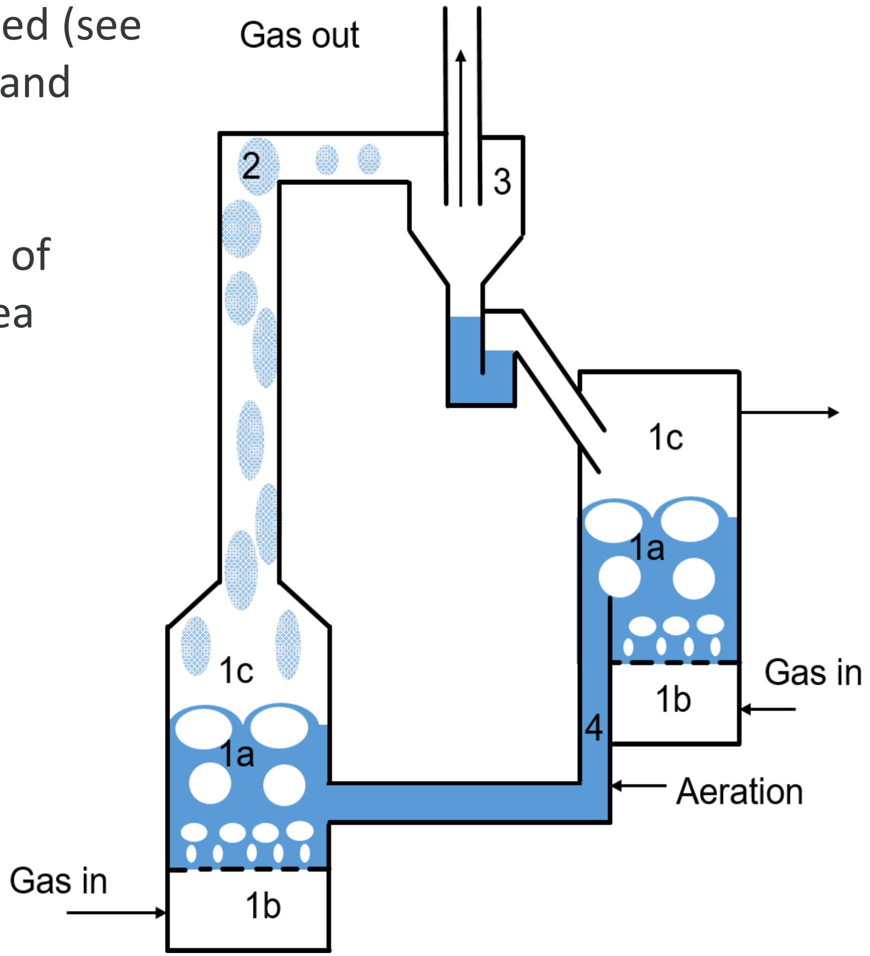
$$\dot{m}_{attr,cyc} = \dot{m}_{c,in} K_{cyc} \mu^{2-m} u_{c,in}^m$$

$$K_{cyc} = 2 \frac{k \rho_s}{H D_c} \left(\frac{\bar{r}_i}{D_c}\right)^2 \frac{\pi (D_c^2 - D_e^2) S}{A} \sqrt{\left[4 \left(\frac{\bar{r}_i}{D_c}\right)^2 + \left(\frac{4A}{\pi (D_c^2 - D_e^2)}\right)^2\right]}$$

[Bayham et al. 2016]

4) Riser- treated as bubbling bed (see 1.) [Thon 2011] and [Werther and Hartge 2004]

5) L-valve- ignored due to lack of model development in this area



Total Attrition: $\dot{m}_{attr,total} = \dot{m}_{attr,jet,i} + \dot{m}_{attr,bubble,i} + \dot{m}_{attr,cyc,i} + \dot{m}_{attr,riser,i} + \dot{m}_{attr,sp,i} + \dot{m}_{attr,valve,i}$

Example Case

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- **Oxygen carrier example is Fe_2O_3/Al_2O_3**
  - Properties such as density are taken from averaging pure components
  - Single unit configurations are used

MATERIAL PROPERTIES		
PROPERTY	VALUE	UNITS
Particle Density (ρ_p)	4600	kg/m^3
Average Particle Size (d_p)	$2.0x10^{-4}$	m
Hardness (H)	$2.89x10^9$	Pa
Wear Coefficient (k)	0.0824	-------
Total Inventory	100	kg

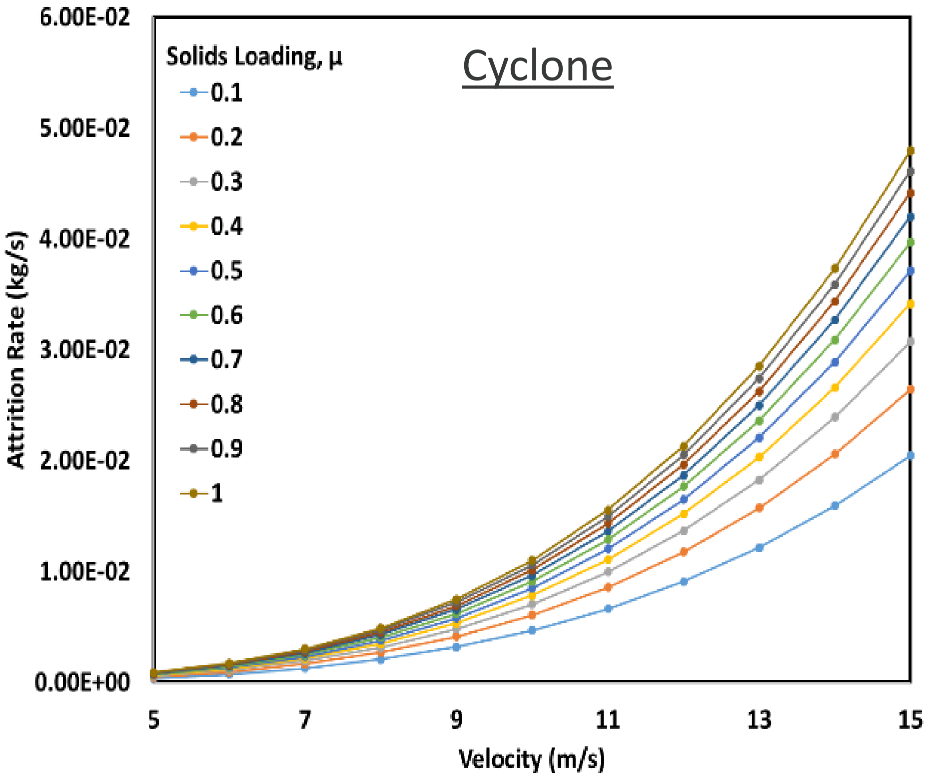
Configurational Parameters	
Standpipe	$\epsilon_g = 0.4$ $f_w = 0.2$ $D_s = 0.05m$ $L = 1m$ $u_p = 0.1 - 0.5m/s$
Cyclone	$D_c = 0.045m$ $D_e = 0.017m$ $\bar{r}_i = 0.036m$ $S = 0.14m$ $A = 3.33x10^{-4}m^2$ $\mu = 0.1 - 1$ $u_{c,in} = 5 - 15m/s$
Jetting Region of Fluidized Bed	$d_{or} = 0.0015m$ $C_j = 0.2s^2/m^3$ $u_{or} = 120 - 200\ m/s$
Bubbling Region of Fluidized Bed	$m_{bed,fuel\ reactor} = 35\ kg$ $m_{bed,air\ reactor} = 20\ kg$ $C_b = 0.00004m^{-1}$ $u_g = 0.1 - 1m/s$
Riser	$u_{g,riser} = 1.5 - 5m/s$

Attrition Rates

CONFIGURATION	VALUE (kg/s)
Standpipe	$3.8x10^{-5}$
Cyclone	$4.69x10^{-3}$
Jetting Region of Fluidized Bed (Fuel Reactor)	$6.2x10^{-3}$
Bubbling Region of Fluidized Bed (Fuel Reactor)	$7.4x10^{-4}$
Jetting Region of Fluidized Bed (Air Reactor)	$6.2x10^{-3}$
Bubbling Region of Fluidized Bed (Air Reactor)	$3.9x10^{-4}$
Riser	$1.5x10^{-3}$
TOTAL	0.0197

- Total attrition rate is approximately 0.02 w.t%/second
- Most of the attrition comes from cyclone and jetting region of the fluidized bed
- Bed inventory is assumed to not effect attrition rate at the jetting region (this needs to be experimentally confirmed and model may be adjusted)
- Riser is likely inaccurate since model for attrition is not fully developed

Sensitivity Analysis



Important Parameters: Solids Loading (µ) and Velocity

- Attrition in cyclones typically written as:

$$r_{attr,cyc} = \frac{\dot{m}_{attr,cyc}}{\dot{m}_{c,in}} = K_{cyc}\mu^{2-m}u_{c,in}^{m}, \text{where m} = 2.5 - 2.63$$

(Reppenhagen and Werther 2000; Bayham et al. 2016)

- µ increases, r_{attr} would decrease
- For this work, the above equation needed to be rearranged for the purpose to adding to other configurational attrition rates which the equation then becomes:

$$\dot{m}_{attr,cyc} = \dot{m}_{c,in}K_{cyc}\mu^{2-m}u_{c,in}^{m} \quad (1)$$

$where\ \dot{m}_{c,in}$ comes from the solid loading µ

$\mu = \frac{\dot{m}_{c,in}}{\rho_f u_{c,in} A}$ Solving for $\dot{m}_{c,in}$ and plugging into (1):

$$\dot{m}_{attr,cyc} = \rho_f A K_{cyc}\mu^{3-m}u_{c,in}^{m+1} \text{ where m} = 2.5 - 2.63$$

- µ increases, $\dot{m}_{attr,cyc}$ would also increase

Future Development of Model

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- Main disadvantage of the mechanical attrition models is the fact that many constants need to be determined **experimentally** (C_{jet}, C_{bubble}, etc.)
  - Solution: Develop mechanical models based only on material properties that are measurable such as hardness, fracture toughness, density, etc., velocities, and hydrodynamics in reactors (work ongoing).
- Implementation of more robust statistical analysis and additional configurations such as impactor attrition.
- Implementation of population balance on solids to be able to combine with technoeconomic models.
- Validate model utilizing 50 kW_{th} CLR unit at NETL

Concluding Remarks

- A simple zero-order spreadsheet model for attrition is developed in Excel and VBA
- An example case using hematite/alumina oxygen carrier is investigated using previously developed mechanical models for attrition in different parts of chemical looping CFB units.
- Future development of attrition models for various configurations are needed.

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