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Applications of tribology and fracture mechanics to determine wear and impact attrition of particulate solids in CFB systems

Ronald W. Breault
National Energy Technology Laboratory, USA, ronald.breault@netl.doe.gov

Samuel C. Bayham
National Energy Technology Laboratory, USA ; Oak Ridge Institute for Science and Education

Esmail R. Monazam
National Energy Technology Laboratory ; REM Engineering Services, USA

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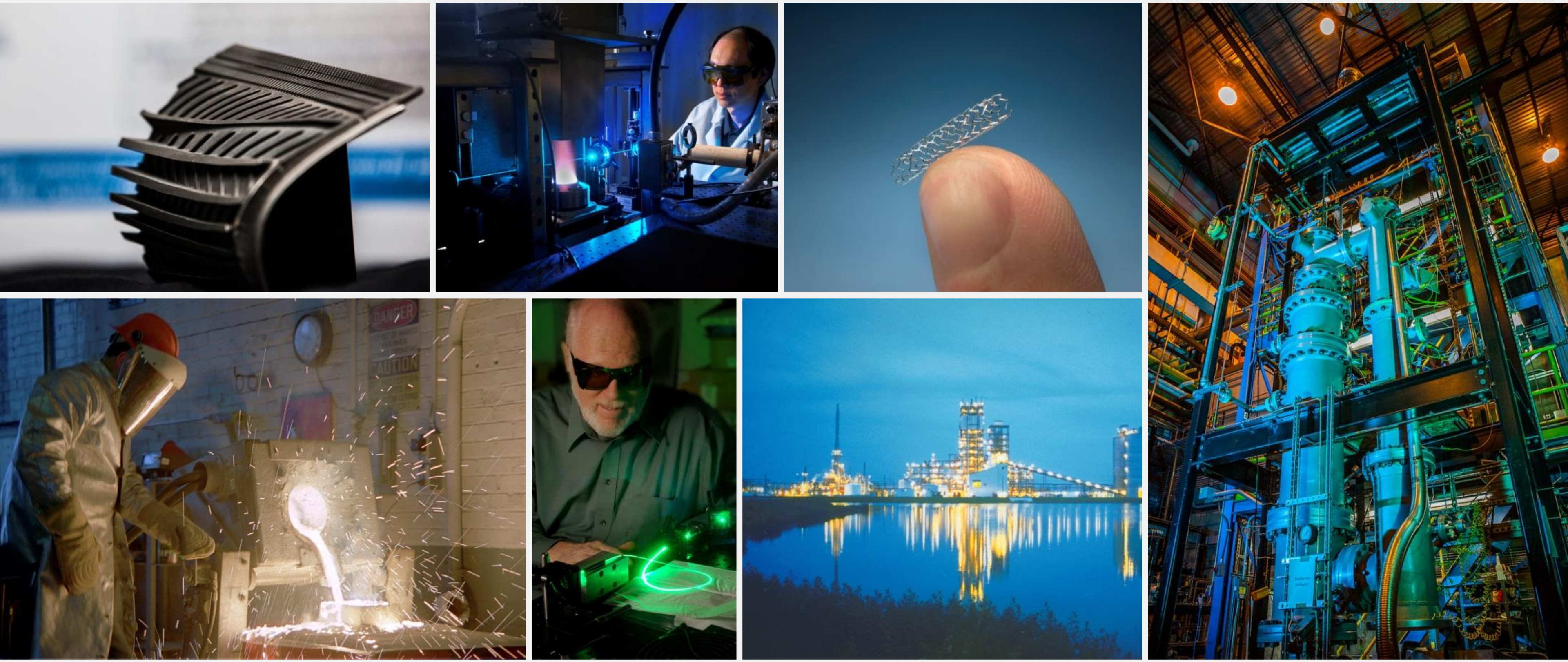
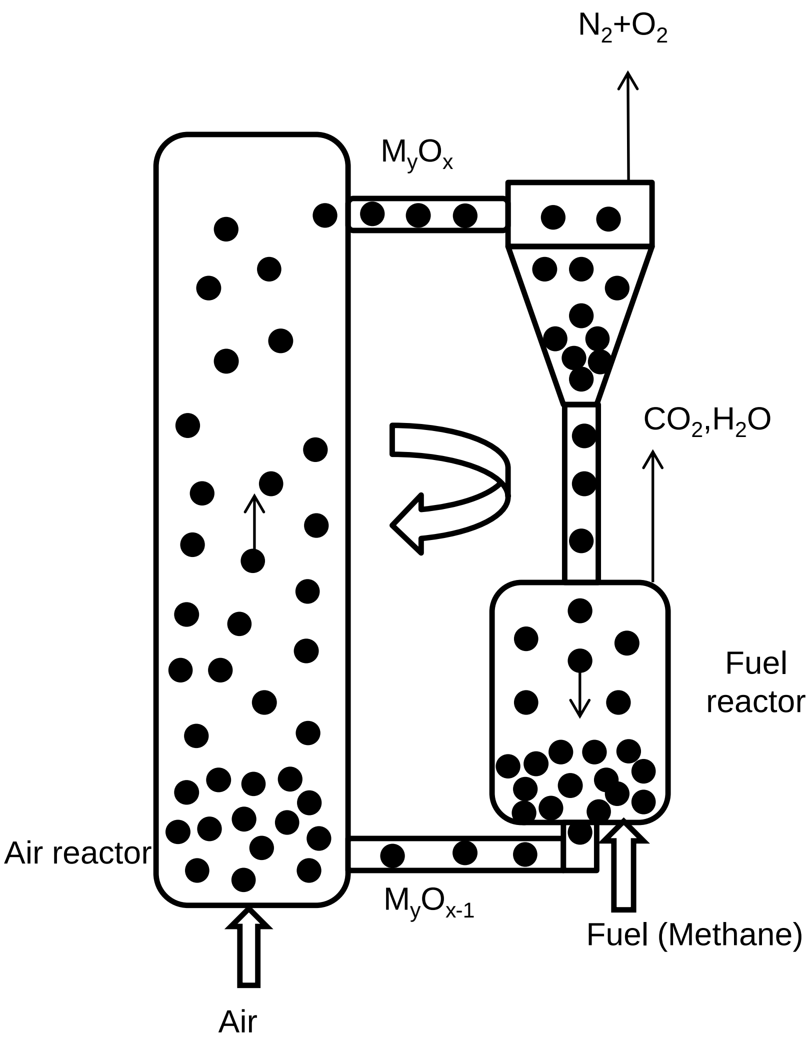


Applications of tribology to determine attrition by wear of particulate solids in CFB systems

Sam Bayham, Ronald Breault, Esmail Monazam

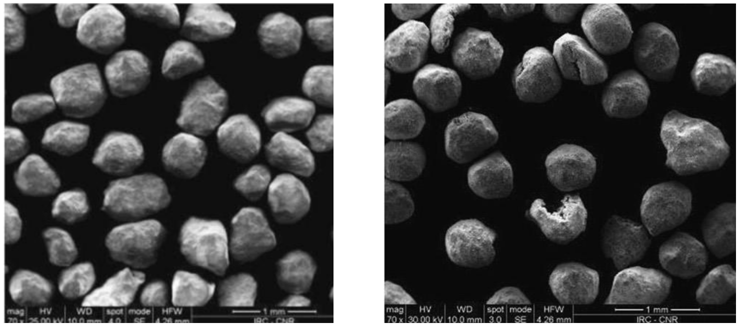
Motivation: Chemical Looping Combustion

- Chemical Looping Combustion is an advanced oxycombustion technology that utilizes a metal oxide to provide oxygen to the fuel.
  - Metal oxide is reduced in fuel reactor and is oxidized in a separate air reactor. The CO_2 is kept separate from the air in the air reactor.
  - Energy is released upon combustion of the reduced metal oxide
- **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

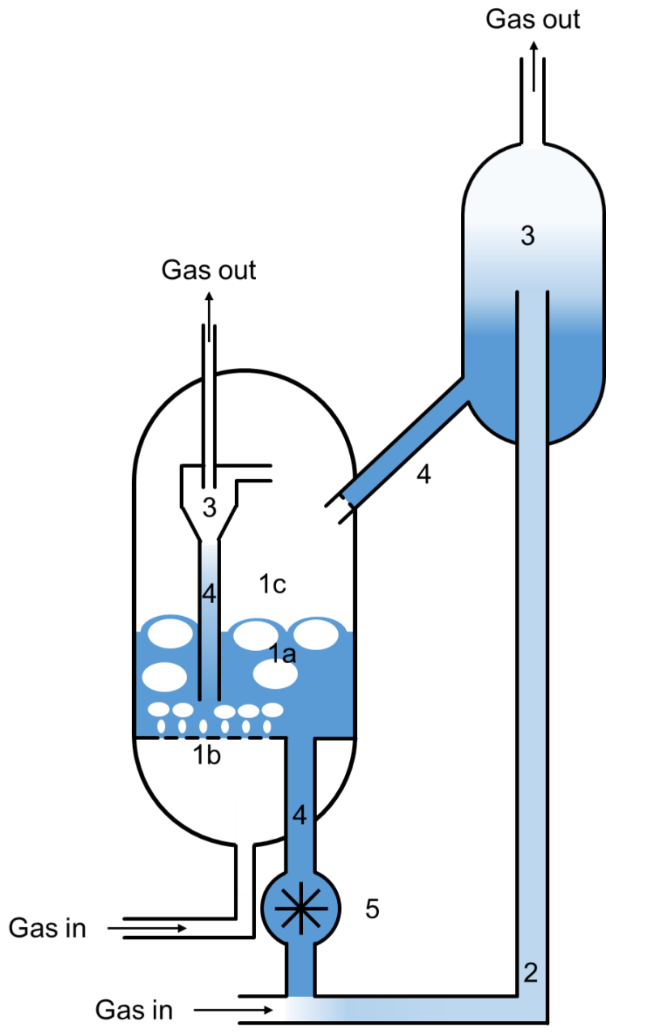
1. Development of **simple** (population-balance type) model to predict attrition losses based on fundamental erosion and abrasion mechanisms for areas such as chemical looping combustion
   - Combine with technoeconomic modeling
2. Determine functionality of material parameters relevant to attrition as the carrier progresses through various oxidation and reduction states while thermally cycling.
   - Avoid methods that produce a semi-quantitative "index" value
   - Attempt to find ways of determining attrition rate based on unique material properties



T.A. Brown et al. / Chemical Engineering Science 71 (2012) 449–467

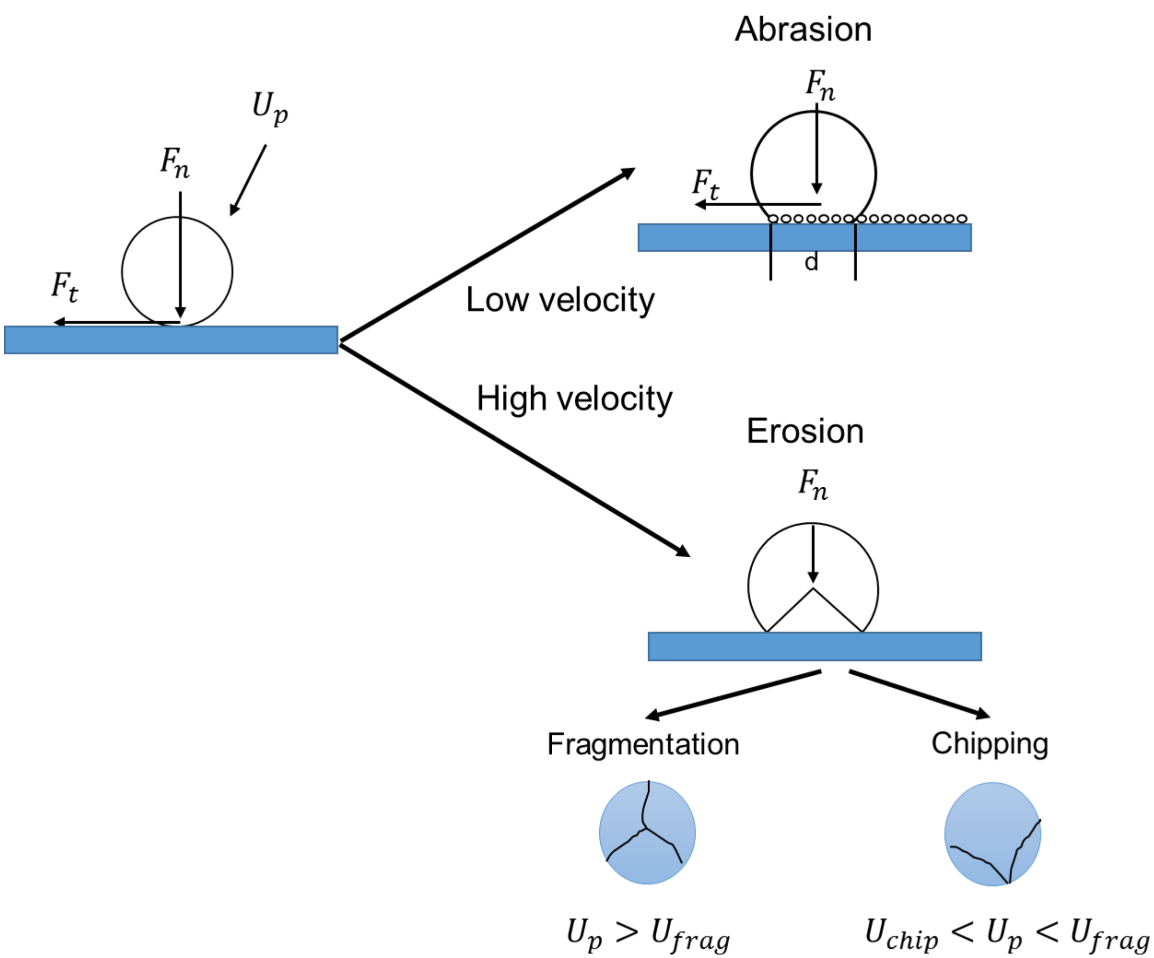
Attrition of particulate solids

- **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



Traditional mechanical attrition models

Steady State Models

Jet attrition (Werther & Xi, 1993): $\dot{m}_{attr,jet} = C_{jet} n_{or} d_{or}^2 U_{or}^3$

Bed/bubble attrition (Ray et al., 1987): $\dot{m}_{attr,bed} = C_{bed} m_{bed} (U_g - U_{mf})$

Cyclone attrition (Reppenhagen & Werther, 2000): $\dot{m}_{attr,cyc} = \frac{C_{cyc} \dot{m}_{solids} U_{in}^2}{\sqrt{\mu_c}}$

Equations based on energy transfer method

These models capture the functionality of system parameters on attrition, but the attrition constant is difficult to know without running experiments at the required scale.

$$C_{\text{jet}} = \frac{\pi}{8} \frac{\eta_{j,abr}}{\sigma_p S_{mi}}$$

σ_p = Surface free energy (**measurable**)

S_{mi} = Specific surface energy of fines (**measurable**)

$\eta_{j,abr}$ = Energy transfer efficiency from jet to particle surface creation (**difficult to predict!**)

Alternative approach to attrition modeling

Develop attrition models based on *fundamental material properties* as well as basic abrasion and erosion models.

Particulate wear: Archard's equation

$$\text{Volume worn} = \frac{kPL}{H}$$

Fragmentation: Ghadiri equation

$$\begin{pmatrix}\text{Volume fragmented} \\ \text{from mother particle}\end{pmatrix} = \alpha \frac{\left(\rho_P U_p^2 d_p H\right)}{K_c^2}$$

Given knowledge of the **forces** and **sliding distances** on the particles in the CFB system, the extent of attrition can be deduced if the following material properties are known.

Parameter	Defined as	How obtained
H	Material hardness	Material property test
K_c	Crack toughness	Material property test ($K_c = \phi\sigma\sqrt{a}$)
α and k	Fragmentation and wear constants	Attrition experiments with controlled conditions

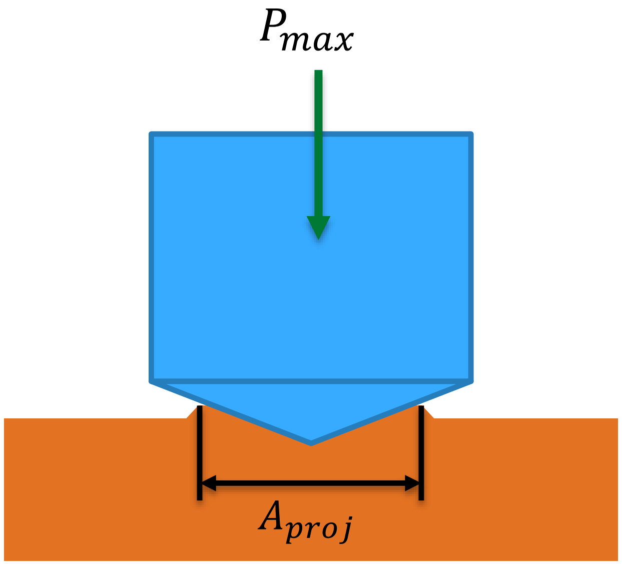
NEEDS: Particle Properties - α, H, K_c, k

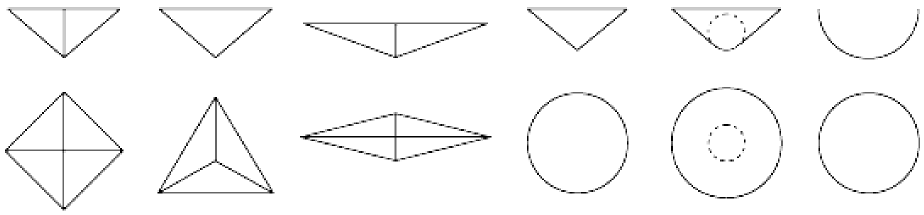
Parameter determination: Hardness

- **<u>Hardness</u>**: Defined as the resistance to localized plastic deformation
- Determined by applying a known load to a shaped indenter and measuring the projected area A_{proj}
- Hardness has units of *pressure* (Pa)

$$H = \frac{P_{max}}{A_{proj}} [=] \frac{N}{m^2}$$

- Examples of hardness testing for non-particulate samples:
  - Brinell, Rockwell, Vickers, Knoop
- Hardness is usually greater than the material yield stress (e.g., $H \approx 3\sigma_y$) due to the surrounding material constraining motion of the indented material

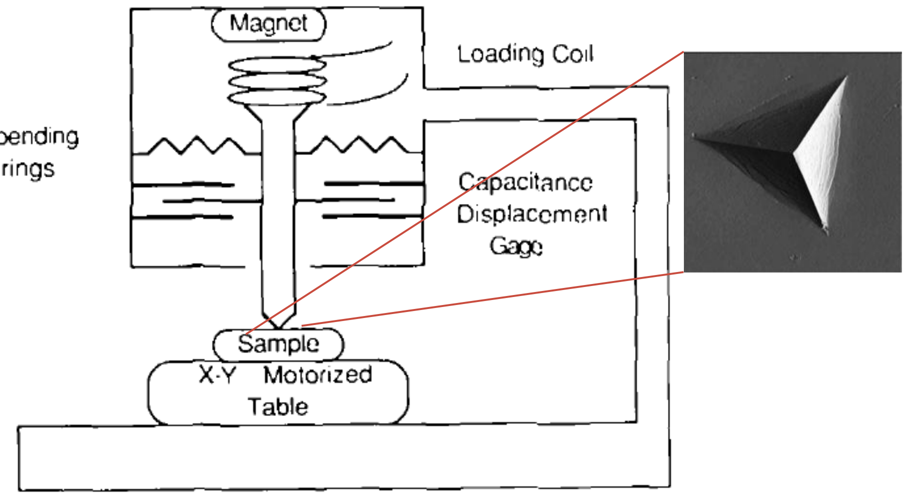




Ortiz, C. "Theoretical aspects of nanoindentation", Lecture notes, 2007. http://ocw.mit.edu/courses/materials-science-and-engineering/3-052-nanomechanics-of-materials-and-biomaterials-spring-2007/lecture-notes/lec22.pdf

Parameter determination: Nanoindentation

- Hardness and fracture toughness are easy to obtain for non-particulate materials, ***but what about small particles?***
- Nanoindentation common technique to ascertain
  - Young's modulus (E)
  - hardness (H) and
  - fracture toughness (K_c)
- Ability to perform on small particles (100 microns) at high temperatures under oxidizing or reducing conditions



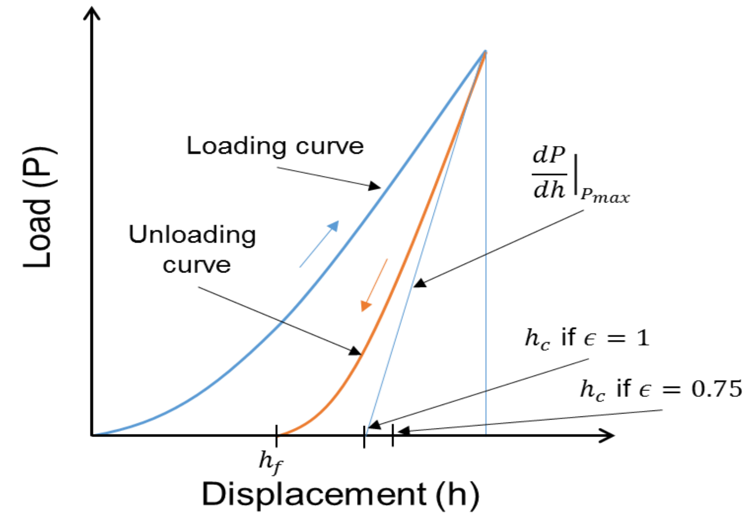
Doerner, M.F.; Nix, W. D. *J. Mater. Res.* 1 (1986), 601-609

$$H = \frac{P_{max}}{A(h_c)}$$

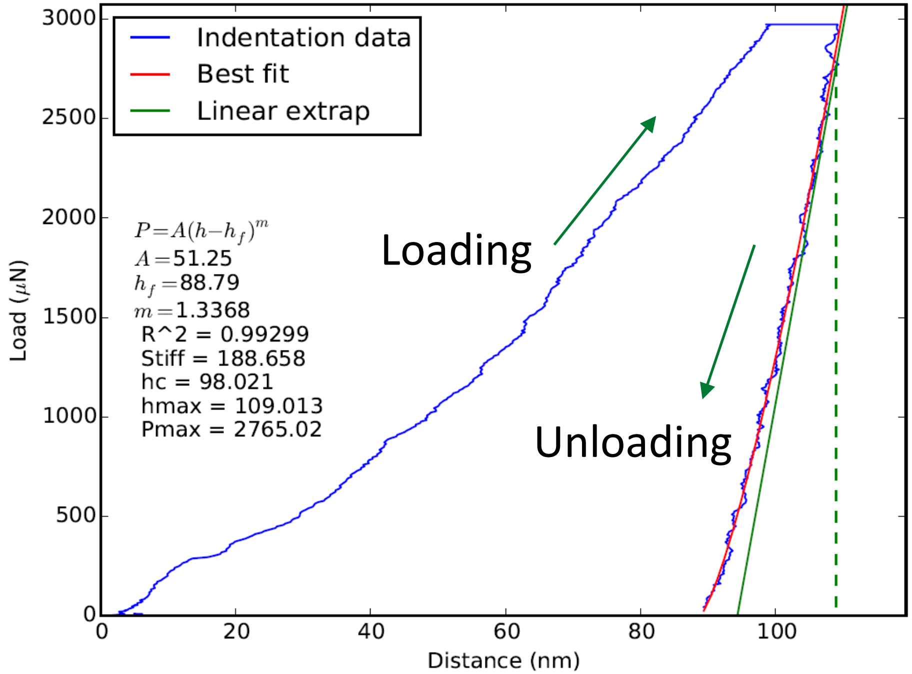
P_{max} = Maximum load
h_c = actual depth of probe in material
$A(h_c)$ = calibrated function of depth

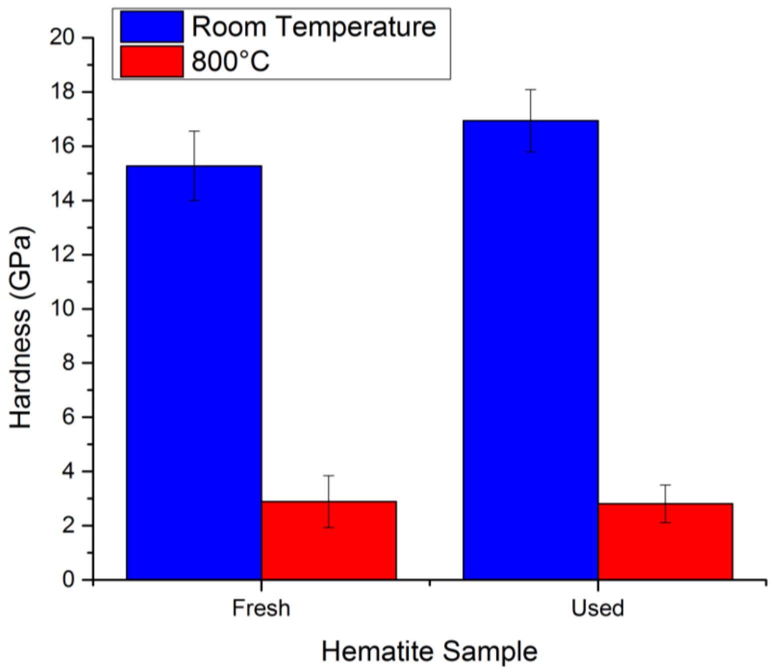
$$K_c = 0.016\sqrt{\frac{E}{H}}\frac{P_{max}}{c^{\frac{3}{2}}}$$

c = size of crack
E = Young's modulus
H = Hardness



Nanoindentation of hematite oxygen carrier





- Hematite tested at room temperature and at 800°C
- Hardness significantly greater at room temperature than at 800°C
- Data courtesy of Hysitron Inc., Minneapolis, MN.

Temperature	24°C	800°C
β (average) (-)	1.59±0.16	1.41±0.16
ω (average) ($\mu N/nm^{\beta}$)	7.48±3.53	47.84±24.54
Young's Modulus (GPa)	216.7±15.3	198.6±49.1
Hardness (GPa)	15.27±1.28	2.89±0.96

Example 1: Simple standpipe model

- Starting with Archard's wear equation, and applying it to Janssen's standpipe model, the following equation can be derived for the wear rate

$$\sigma_z = \frac{\rho_B g D_s}{4 f_w K_{pr}}\left(1 - e^{-\frac{4 f_w K_{pr}}{D_s} z}\right)$$

Large z/D ratio

$$F_r = K_{pr}\sigma_z(\pi D_s L)$$

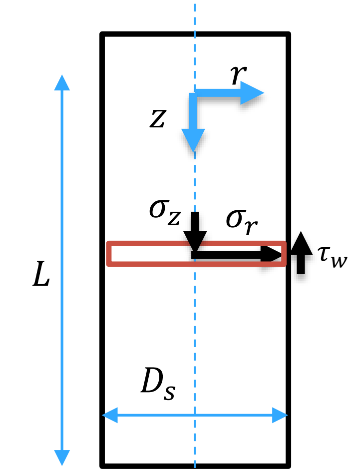
$$\frac{dV}{ds} = \frac{k}{H} F_r$$

Take time derivative of both sides

$$\frac{dV_w}{dt} = \frac{k}{H}\frac{\rho_B g D_s}{4 f_w}\pi D_s L \frac{ds}{dt}$$

$$\dot{m}_{sp,attr} = \rho_s \frac{dV_w}{dt}$$

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



K_{pr} =ratio of principal stresses for the powder in passive stress mode

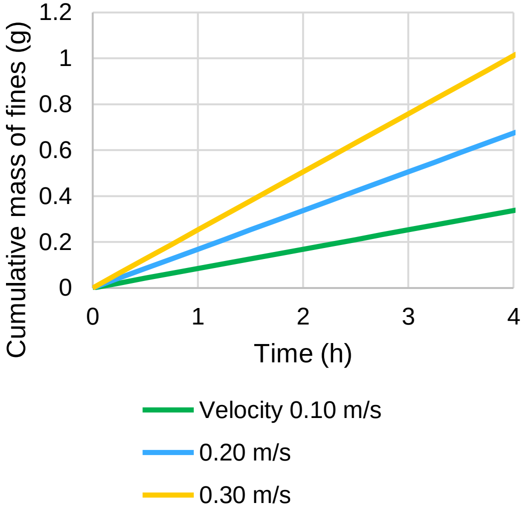
Example 1: Simple standpipe model

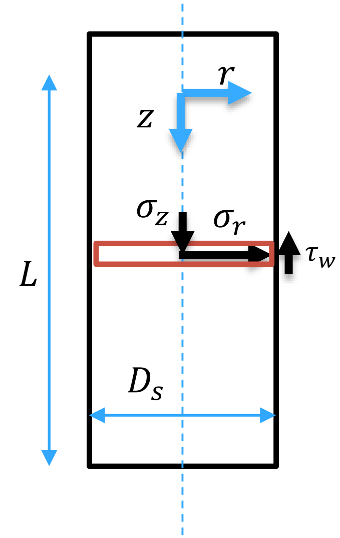
- Parametric effects on standpipe abrasion model

$$\dot{m}_{attr} = \frac{k}{H}\left(\frac{\rho_s^2(1-\epsilon_g)gD_s}{4f_w}(\pi D_s L)\right)U_s$$

D_s = Standpipe diameter
L = Standpipe length
U_s = Solids velocity
g = Acceleration of gravity

Standpipe attrition





Parameter	Measurement Technique
Wear constant (k)	Standpipe experiment
Hardness (H)	Nanoindentation (Hysitron)
Particle-wall friction coefficient (f_w)	Annular shear cell, Jenike shear box, angled plate, or literature
Particle Density (ρ_s)	He Pycnometer
Gas holdup (ϵ_g)	Back calculate from bulk density of powder

Example 2: Cyclone

The normal force experienced by the particle is based on centrifugal force

$$F_i = \frac{2m_i u_t^2}{D_c}$$

The differential wear volume for a single particle traveling a differential distance

$$dV_i = \frac{k}{H} F_i ds$$

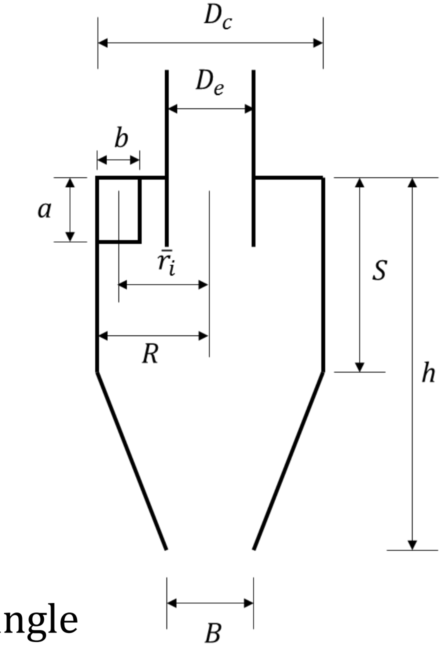
The path length traveled by a particle

$$ds = \sqrt{u_t^2 + u_z^2} dt$$

$$u_t = \frac{2u_{c,in}\bar{r}_i}{D_c}$$

$$u_z \approx \frac{4u_{c,in}A}{\pi(D_c^2 - D_e^2)}$$

k = Wear constant
H = Hardness
ds = Distance traveled
dV_i = Single particle wear volume
F_i = Normal force on particle
u_t = Tangential velocity at wall
u_z = Axial velocity at wall



Integrate over the particle residence time

Wear rate for single particle

$$V_i = \frac{km_i}{H} K_{geo} u_{c,in}^2$$

$$K_{geo} = \frac{2\pi(D_c^2 - D_e^2)S}{AD_c}\left(\frac{\bar{r}_i}{D_c}\right)^2 \sqrt{\left(\frac{2\bar{r}_i}{D_c}\right)^2 + \left(\frac{4A}{\pi(D_c^2 - D_e^2)}\right)^2}$$

Example 2: Cyclone

k = Wear constant
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ds = Distance traveled
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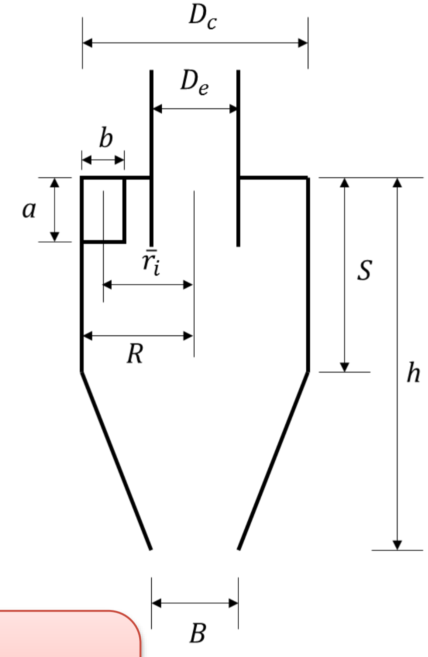
u_t = Tangential velocity at wall
u_z = Axial velocity at wall



Wear rate for single particle

$$V_i = \frac{km_i}{H} K_{geo} u_{c,in}^2$$

$$\frac{dV}{dt} = V_i \frac{dN}{dt} \approx V_i \frac{\dot{m}_s}{m_i}$$

Multiply both sides by the particle density to get mass attrition rate

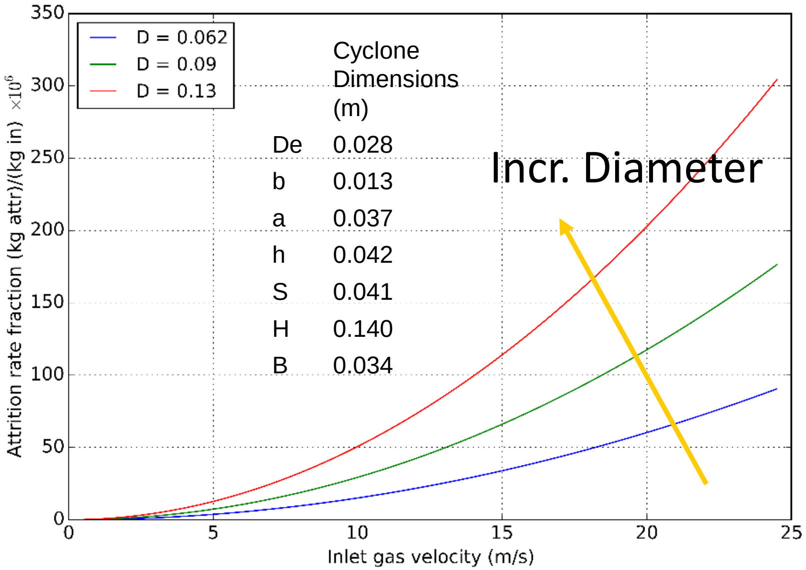
$$\dot{m}_{attr} = K_{cyc} \dot{m}_{c,in} u_{c,in}^2$$

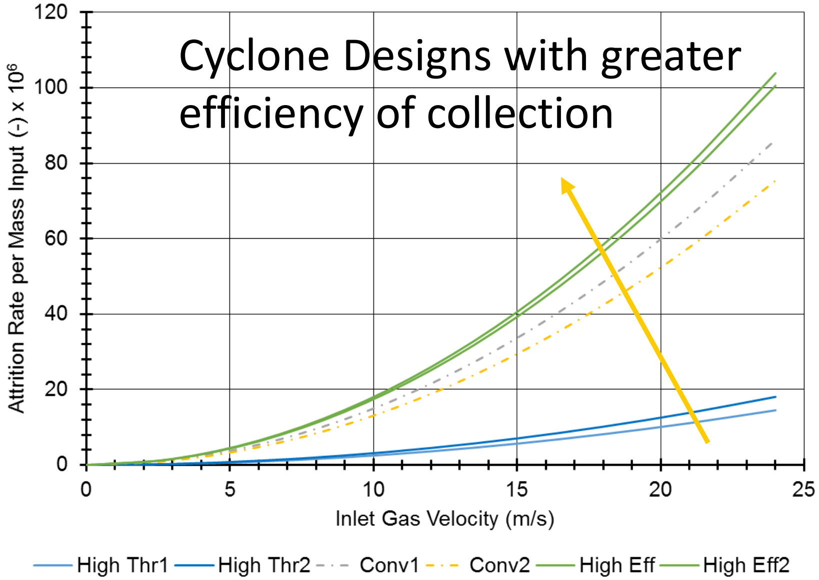
The total attrition rate is the product of the wear volume per pass times the number of particles passing per time

$$K_{cyc} = K_{geo} K_{matl} \qquad K_{matl} = \frac{k\rho_s}{H}$$

$$K_{geo} = \frac{2\pi(D_c^2 - D_e^2)S}{AD_c} \left(\frac{\bar{r}_i}{D_c}\right)^2 \sqrt{\left(\frac{2\bar{r}_i}{D_c}\right)^2 + \left(\frac{4A}{\pi(D_c^2 - D_e^2)}\right)^2}$$

Functionality of Cyclone Abrasion Equation





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

$$K_{cyc} = K_{geo} K_{matl} \qquad K_{matl} = \frac{k\rho_s}{H}$$

$$K_{geo} = 2\frac{\overline{r_i}^2}{D_c^3}\frac{\pi(D_c^2 - D_e^2)S}{A}\sqrt{4\left(\frac{\overline{r_i}}{D_c}\right)^2 + \left(\frac{4A}{\pi(D_c^2 - D_e^2)}\right)^2}$$

Cyclone Model and Data from Literature

Data from: Reppenhagen, J.; Werther, J. Catalyst attrition in cyclones. *Powder Technol.* ***113*** *(2000) 55-69.*

- Data from all loadings fits well to the expression below

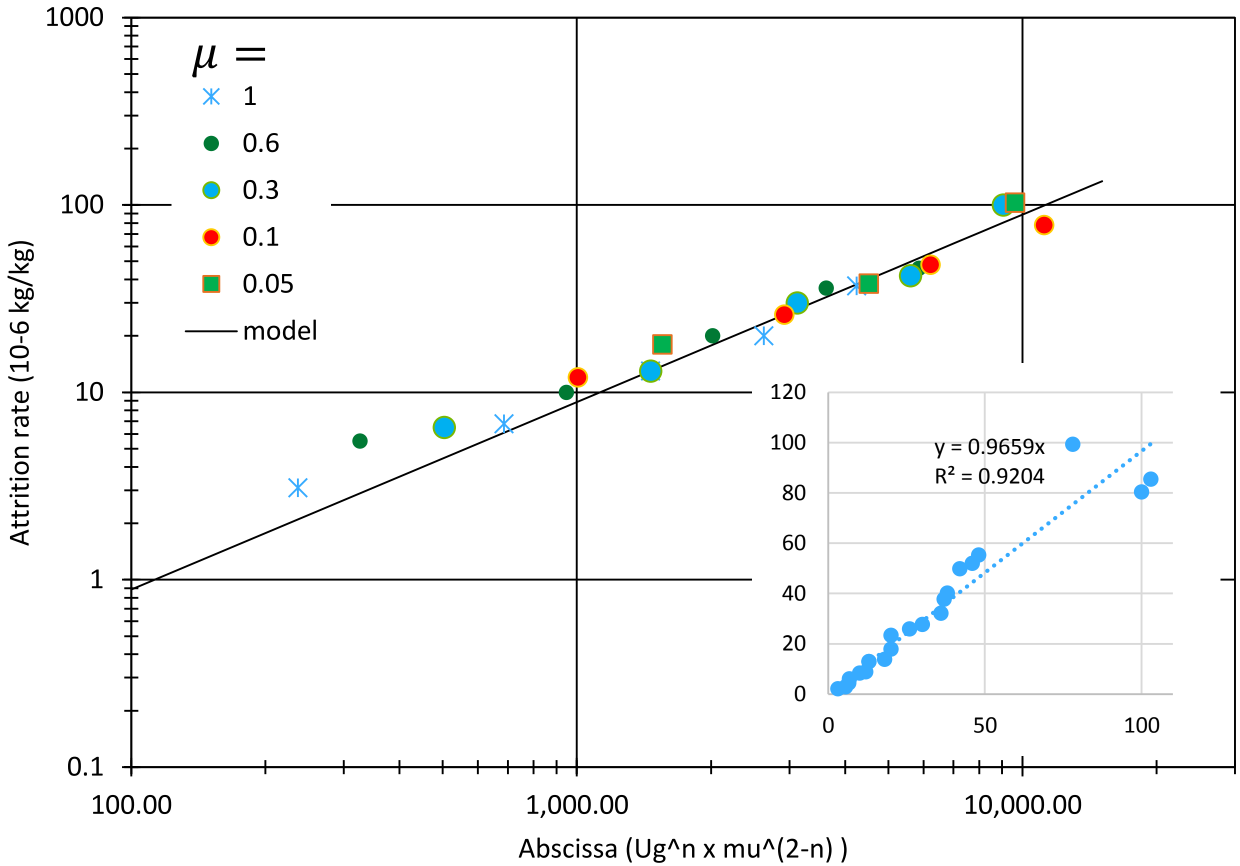
$$\dot{m}_{attr} = C\dot{m}_{c,in}\mu^n u_{c,in}^2$$

$$\mu = \frac{\dot{m}_{c,in}}{\rho_f u_{c,in} A}$$

C = material and efficiency constant

Compare to equation derived by Reppenhagen and Werther [1]

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



Best fit constant K_{cyc}	8.88×10^{-3}
Best fit constant n	2.6
Effective wear coefficient: $k' = k \cdot k_\mu$	6.04×10^{-4}

[1] *Reppenhagen, J.; Werther, J. Powder Technol.* ***113*** *(2000) 55-69.*

Concluding remarks

- This presentation focuses on the need for mathematical modeling and offers recommendations on how to model the attrition process for fields such as chemical looping combustion, whose economics are highly dependent on attrition and makeup rate of solid oxygen carrier.
- Many attrition expressions exist for different areas of the CFB but are dependent on constants that are unknown.
- Modeling approach at NETL: Develop modeling scheme based on material properties and wear/fragmentation rate laws
- Validate model using data from high-temperature attrition unit and 50 kW_{th} Chemical Looping Combustion unit at NETL

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