A simple shell model for the break-up of agglomerates in turbulent flows

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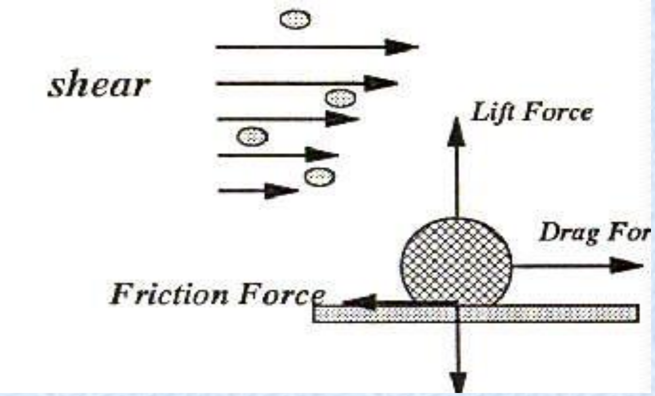
Outline

- Escape of particles from potential wells
  - Role of the turbulence
  - Removal rate
  - Rock n roll model
- Characterising agglomerates
- Shell model for breakup
- Prediction versus experimental results
  - ARTIST experiment

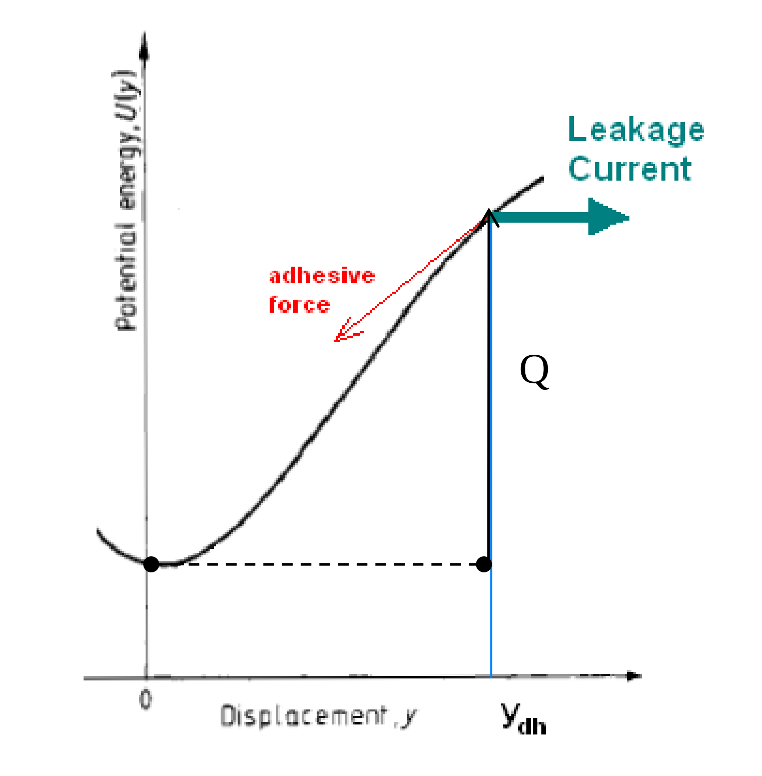
Escape of particles from potential wells



particle resuspension

$$p = \omega \exp - Q / 2\langle PE \rangle$$

- *p, the resuspension rate constant*
- *ω , the typical frequency of vibration,*
- *Q height of adhesive potential well,*
- *<PE> average potential energy of particle in the well.*



Particle escape from potential well

Rock'n'Roll Model (Reeks & Hall, 2001)

Fraction remaining after 1 sec and resuspension rate:

$$f_R(t) = \int_0^\infty e^{-p(f_a')t} \varphi(f_a') df_a'$$

$$\Lambda(t) = \int_0^\infty p(f_a') e^{-p(f_a')t} \varphi(f_a') df_a'$$

$$p = \frac{\omega_0}{2\pi} \exp\left(-\frac{k(f_a - \langle F \rangle)^2}{\langle f^2 \rangle (1+\eta)} \right)$$

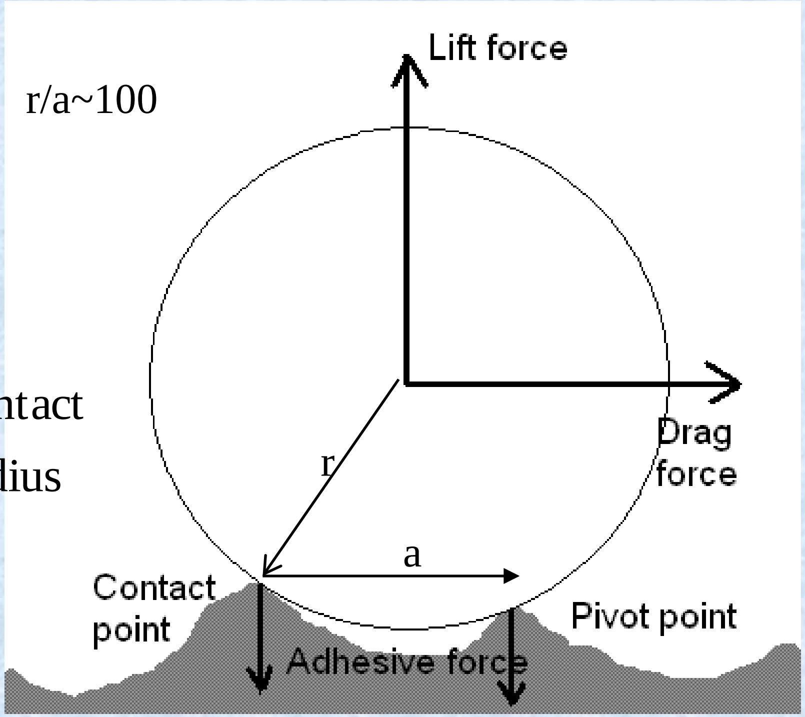
f_a = adhesive force F_a = adhesive for perfect contact

$F_a = 3\pi\gamma r$, γ = surface energy, r = particle radius

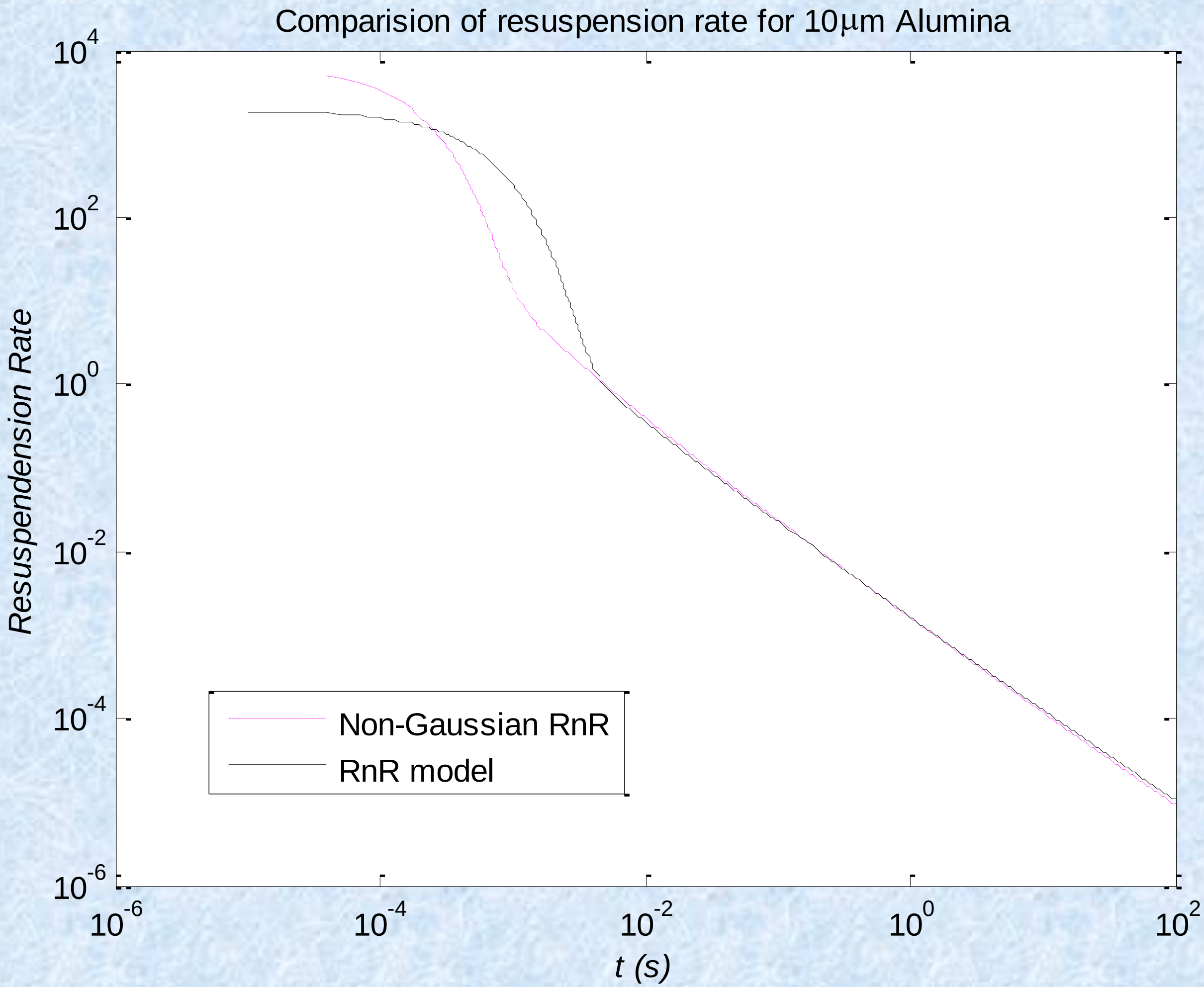
$f_a' = f_a / F_a$; $\varphi(f_a')$ Lognormal distribution

Biasi *et al.* (2001) $\langle f_a' \rangle = 0.016 - 0.0023 r^{0.545}$

$\sigma_a' = 1.8 + 0.136 r^{1.4}$, r in microns



Short and long term removal rates



Mehanism for Agglomerate breakup

- Rupture
  - Break-up into fragments -daughter agglomerates
  - simialr to particle removal from a surface
    - Threshold for aerodynamic forces based on strength of agglomerate
    - Continues until agglomerates reaches a minimum size
    - Usually 3 or 4 daughter fragments
- Erosion
  - Lower aerodynamic forces than rupure
  - Much slower than breakup due to rupture
  - Onion peeling mechanism
  - Use of kinetic / stochastic models

Characterising an Agglomerate

For a fractal agglomerate, the number of primary particles within the agglomerate is given by:

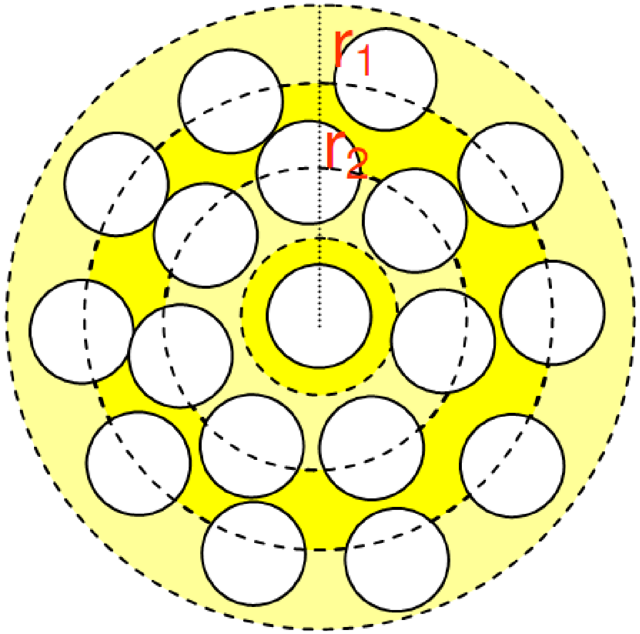
$$N_P = k_o \left(R_c / r_p\right)^{d_f}$$

$k_o \approx 0.42 d_f - 0.22$ in the range $1.50 \le d_f \le 2.75$

d_f is the fractal dimension.

R_c is the collision or outer radius

r_p is the primary particle radius



volume fraction of the particle

$$\phi = \frac{V_m}{V_P}$$

V_m is the material volume
V_p is the volume of the particle the material and void volume

$$\phi(r) = k_o \frac{d_f}{3} \left(\frac{r}{r_p}\right)^{d_f - 3}$$

Characterising agglomerate

The average thickness of the l-th shell $\overline{\Delta r_l}$ will depend upon the volume fraction and the distribution of particles sizes within each shell. It is given by

$$\overline{\Delta r_l} = \left(\frac{v_p}{\phi(R_{l+1})}\right)^{1/3}$$

The l-th shell outer radius is then defined as:

$$R_l = r_p + \sum_{i=1}^{l} \overline{\Delta r_i}$$

And the radius of the l-th shell which is half way between the outer and inner radii of the shell is then:

$$r_l = \frac{1}{2}\left(R_l + R_{l+1}\right)$$

The number of particles in the k-th shell is given by:

$$\overline{n_{pl}} = N_p(r_{l+1}) - N_p(r_l)$$

Equations for the breakup rate

p(ξ) is the rate constant for removal of particles from an adhesive potential well characterised by ξ

The total removal rate of particles being an integration over a broad range of adhesive potential , i.e. values of ξ due to a distribution of particle sizes, microscale roughness and flow exposure

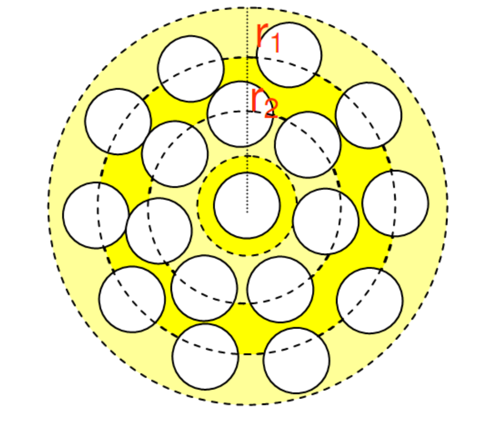
The removal rate of particles from any given shell/layer depends upon the rate at which particles are are exposed to the flow by removal of particles from the shell above

If $n_i(\xi,t)\, d\xi$ is the number of particles in the layer *i* with adhesive and flow parameters between ξ, $\xi + d\xi$, with pdf $\psi(\xi)$

$$\frac{\partial n_i(\xi,t)}{\partial t} = -p(\xi)n_i(\xi,t) + \psi(\xi)\int_0^\infty p(\xi')n_{i-1}(\xi',t)d\xi'$$

coverage coefficient =1

$$= -p(\xi)n_i(\xi,t) + \psi(\xi)\Lambda_{i-1}(t)$$

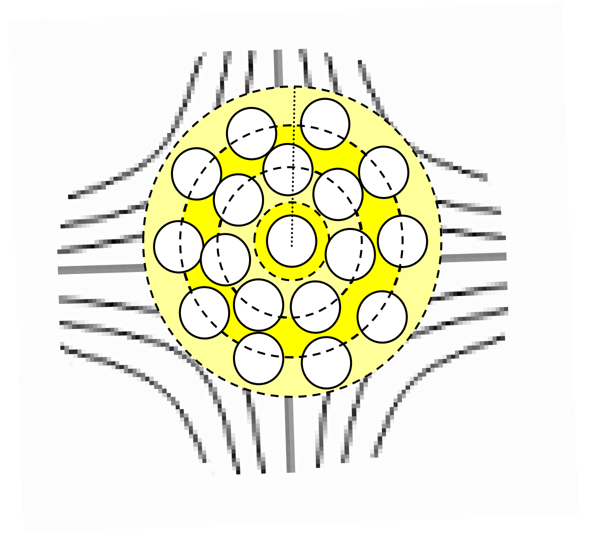


rms fluctuating drag force

RMS flow velocities in the radial (longitudinal) and azimuthal (lateral) directions for

$$\sqrt{\overline{v_r^2}} = \sqrt{\overline{v_\theta^2}} = \left(\overline{\dot{\gamma}^2}\right)^{1/2} r/\sqrt{2}$$

rms radial drag force $\sigma^2 = \frac{1}{2}\overline{\dot{\gamma}^2}\beta_\tau^2 r^2,$



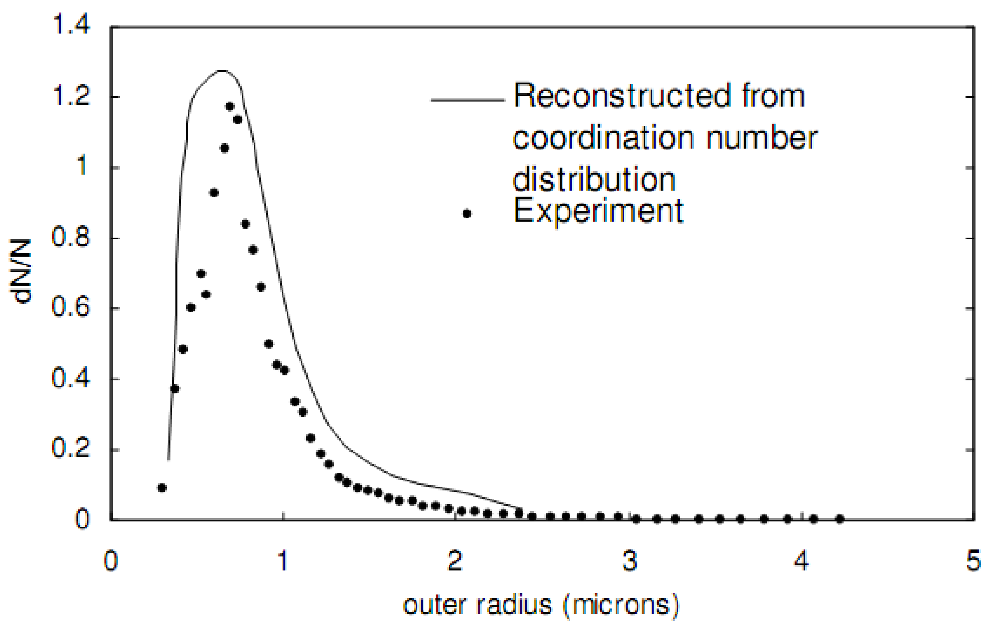
The adhesive force f_a is selected from a lognormal distribution

$$\varphi\left(f_a^{'}\right) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{f_a^{'}\ln\sigma_a^{'}}\right)\exp\left(-\frac{1}{2}\left[\frac{\ln\left(f_a^{'}/\overline{f_a^{'}}\right)}{\ln\sigma_a^{'}}\right]^2\right)$$

$f_a^{'}$ is normalized by the Van der Waals force F_a between 2 spheres in perfectly smooth contact, which is, according to Equation (2.53), $F_a = \frac{3}{2}\pi\Gamma_a r_a$ and reduced by a factor of the order 100 due to the roughness of the contact

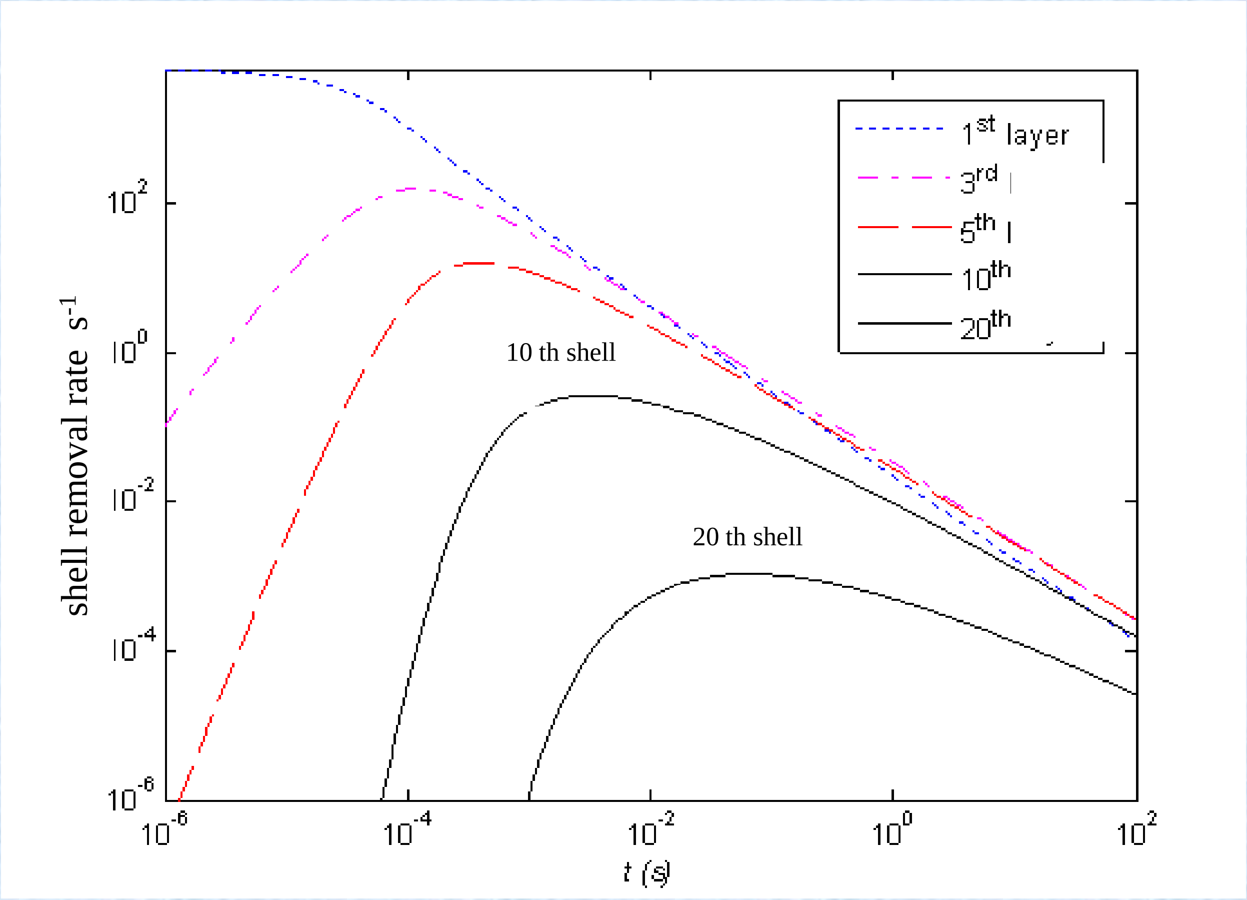
Distribution of clusters within agglomerate

Figure 8.3: Fragment Size distribution obtained experimentally compared to the reconstructed fragmen size distribution based on the coordination distribution

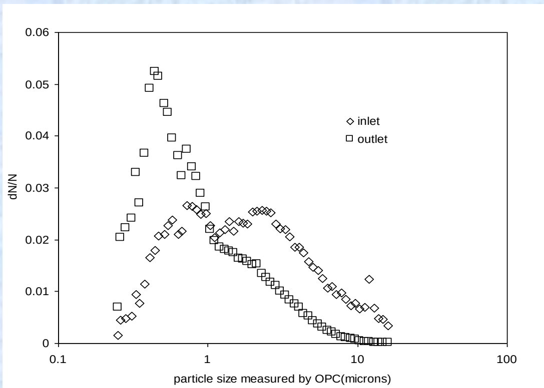


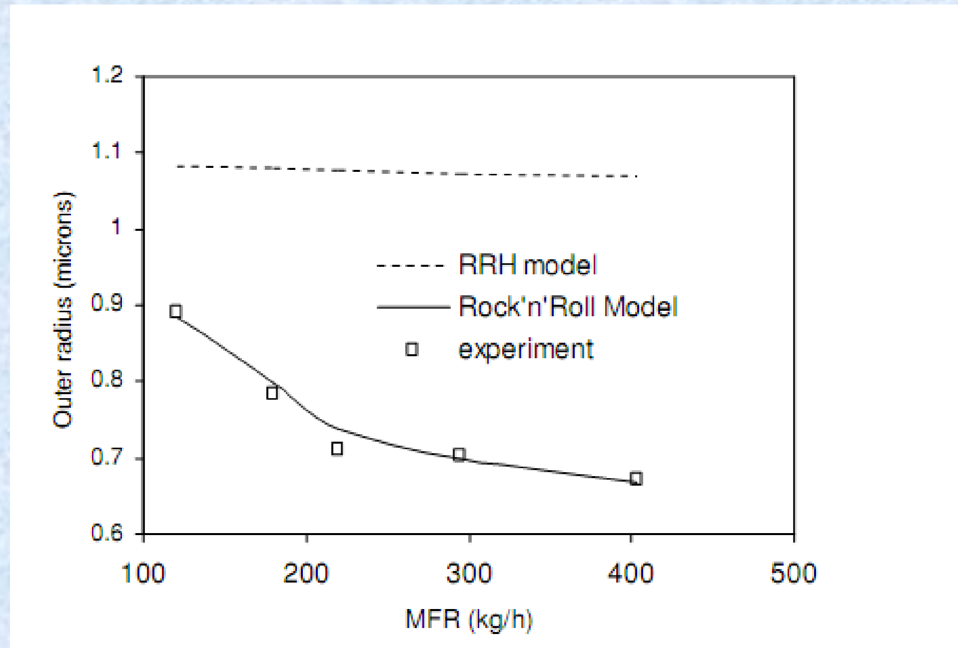
Agglomerates are fragments 48% triplets, 22% quartets, 25% quintets, ..

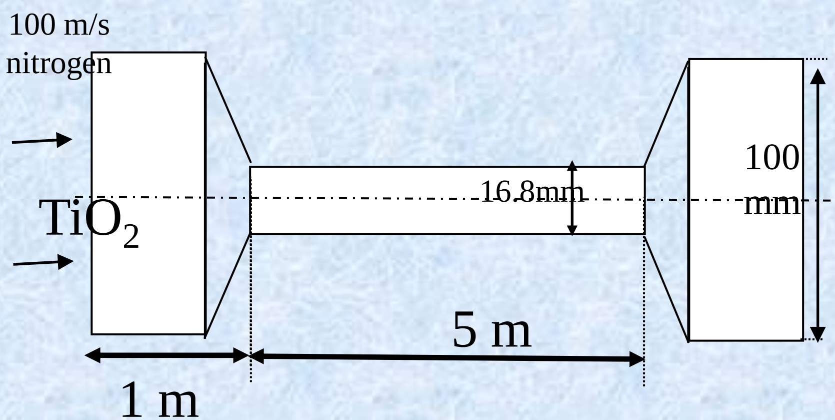
Shell removal removal rates



experimental results and model predictions







reduction factor of the adhesive forces~500.

(r/a) is ~ 100

spread of the adhesive forces ~10

Summary & conclusions

- Model for agglomerate break up
  - Analogous to removal of a particles from surfaces in turbulent boundary layers
    - Escape of particles from adhesive potential wells
    - Motion driven by fluctuating aerodynamic forces/ moments
      - Rock and roll about surface asperities
  - Shell model similar to multilayer resuspension
    - removal particles from any shell/leer rate limited by removal of particles from the layer above
  - Future developments
    - DNS of flows within agglomerates
    - Calculation of forces on individual primary particles