The Development and Application of Kinetic Models for the Resuspension of Small Particles in Turbulent Boundary Layers

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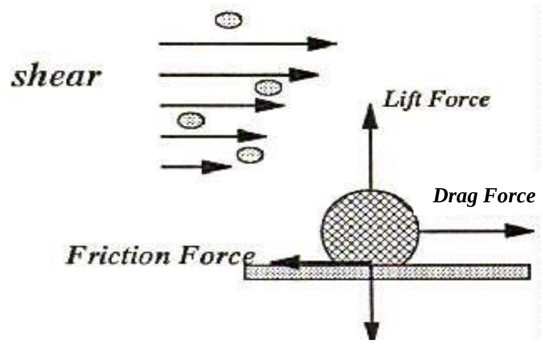

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Background

- Important in a range of environmental and industrial processes
  - Clean air technology,
  - Dust storms on Earth and Mars (wave of darkening)
  - Spreading of pollen and crops diseases by fungal spores
- Release of radioactive particles in a nuclear accident
  - Focus on resuspension particles < 5microns in size
  - principle adhesive forces – Van der Waals intermolecular forces
- Import of safety assessment of nuclear reactors
  - Development and validation of computer codes

Kinetic Models for Resuspensiosn

- ❑ Stochastic models which take account of the role of turbulence in particle resuspension
- ❑ Focus on resuspension rates as well as fraction resuspension
- ❑ Calculation of a rate constant for resuspension
  - analogous to the rate constant for desorption of molecules from a surface $\omega e^{-E/kT}$ (relationship to kinetic theory)
  - Computational very efficicient compared to simulation (particle tracking)
  - Ideally suited for incorporation into severe accident codes e.g. SOPHAEROS -> ASTEC

History and Motivation

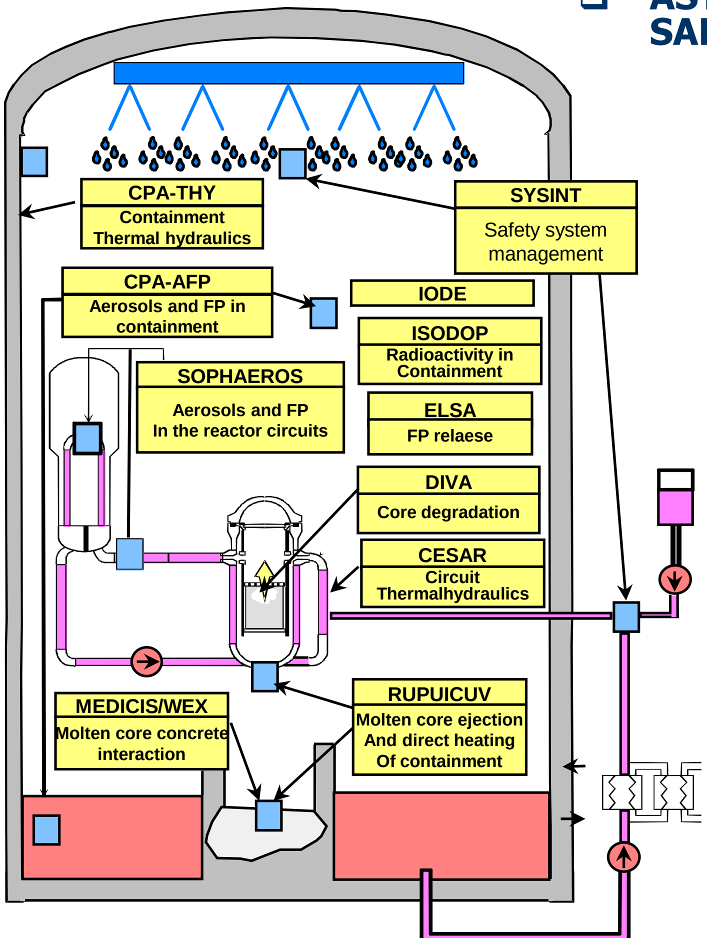
- Radioactive particles released in severe accidents
  - PWRs - steam spikes (primary circuit), hydrogen deflagration (containment)
  - AGRS dropped stringer –accident
  - HTRs Accumulation of contaminated dust in the coolant circuit – loss of coolant accident (LOCA)
  - International Thermonuclear Experimental Reactor (ITER)

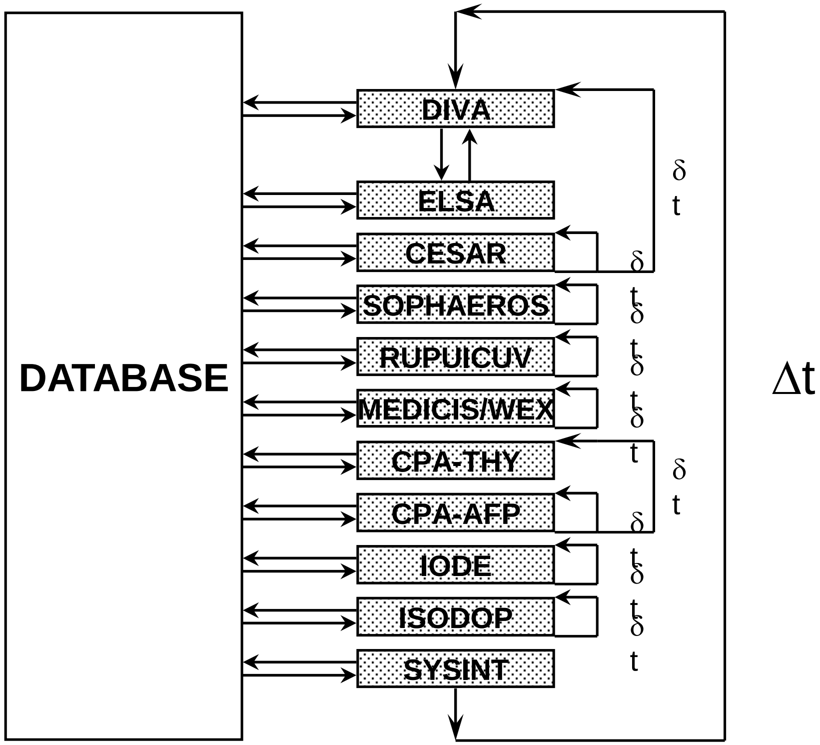
    Accumulation of contaminated dust in the vacuum vessel

    Coolant-water-ingress or Loss of vacuum accident (LOVA)
- SARNET
  - Development of SA Codes / Sophaeros
  - IRSN

ASTEC

- ❑ **ASTEC integrates the technical knowledge in SARNET**

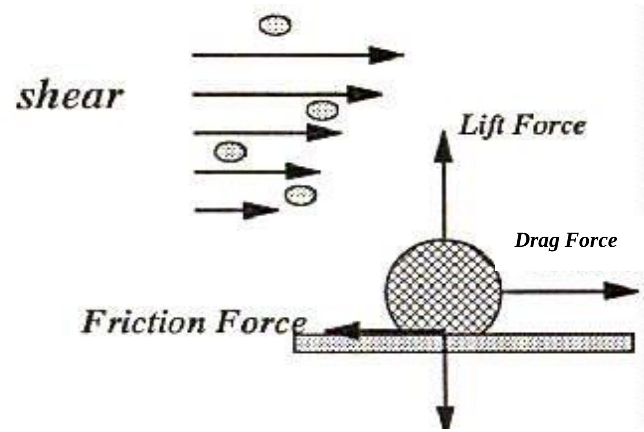




OUTLINE

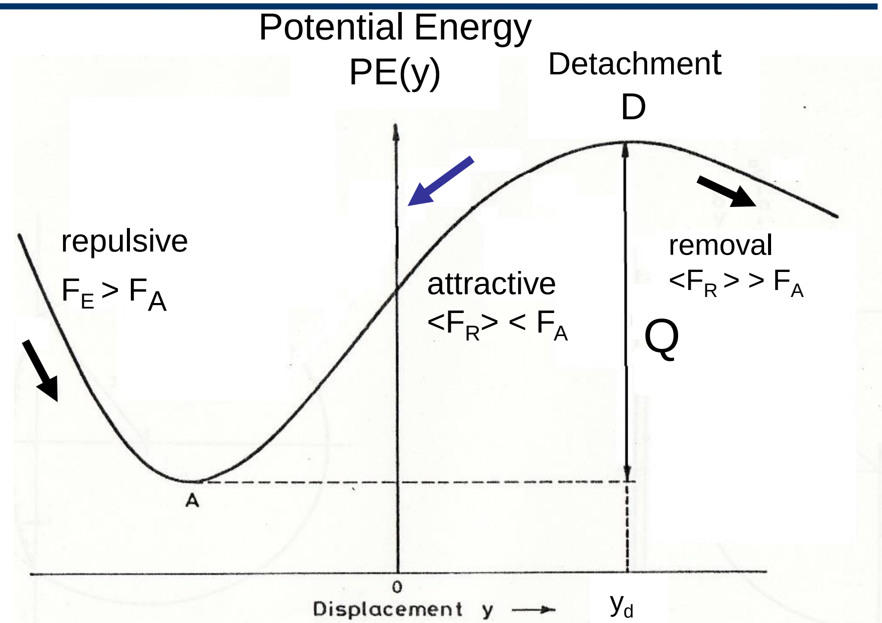
- Early model RRH model
  - Escape of particles from surface adhesive potential well
  - Role of adhesive and aerodynamic removal forces
  - Mechanisms for removal
    - Quasi static
    - Energy accumulation
- Rock n roll Model
- Decay of gas-borne radioactive in a reactor circuit
- Model improvements based non-Gaussian removal forces
- Extension resuspension from multilayer deposits

Reeks Reed & Hall Kinetic Model (1987)



$$\ddot{y} + \beta\,\dot{y} + \omega_n^{\,2} y = m^{-1} f_R(t)$$

very stiff lightly damped harmonic oscillator



particle surface adhesive potential well diagram

$F_R = \langle F_R \rangle + f_R(t)$; mean $\langle F_R \rangle$; fluctuating $f_R(t)$

ω_n = natural frequency of oscillations

$$p = n \exp\left(- \frac{Q}{2\langle \mathrm{PE} \rangle} \right)$$

Resonant energy transfer /energy accumulation

$$p = n \exp\left(-\frac{Q}{2\langle \mathrm{PE} \rangle}\right)$$

- *p* is the rate constant for removal s^{-1}
- *n* typical frequency of the deformation with potential
- Q the height of potential barrier (depends on difference of adhesive removal forces)
- <PE> average Potential Energy in well

$$\eta = \frac{\pi}{2\beta}\,\omega\,\widehat{E}_R(\omega_n)$$

- Resonant energy contribution contribution
- β damping constant
- E_R normaled energy spectrum of $f_R(t)$

$$p = n \exp\left(-\frac{1}{2}\frac{\left(f_a - \langle F_R \rangle\right)^2}{\langle f_R{}^2 \rangle (1+\eta)}\right) \quad ; \quad n = \frac{\omega_n}{2\pi}\frac{\left(\eta + \langle \dot{f}_R{}^2 \rangle / \langle f_R{}^2 \rangle \omega_n{}^2\right)^{1/2}}{\eta + 1}$$

adhesive force $f_a = \frac{3}{2}\pi\gamma r$ (JKR, γ = surface energy, r = radius of curvature)

$\eta \to 0$ quasi static $\qquad$ $\eta >> 1$ resonant energy transfer

$$p = \frac{1}{2\pi}\langle \dot{f}_R{}^2 \rangle / \langle f_R{}^2 \rangle \exp\left(-\frac{1}{2}\frac{\left(f_a - \langle F_R \rangle\right)^2}{\langle f_R{}^2 \rangle}\right) \quad ; \quad p = \frac{\omega_n}{2\pi}\exp\left(-\frac{1}{2}\frac{f_a{}^2}{\langle f_R{}^2 \rangle}\right)$$

Influence of surface micro roughness

- Particle surface adhesive force

$$f_a = \tfrac{3}{2}\pi\gamma r_a \text{ JKR } r_a = \text{asperity radius, } r'_a = \frac{r_a}{r}$$

- Distribution of adhesive forces

$$\varphi(r'_a) = \frac{1}{\sqrt{2\pi}}\frac{1}{r'_a}\frac{1}{\ln\sigma'_a}\exp\left(-\frac{\left[\ln(r'_a/\bar{r}'_a)\right]^2}{2(\ln\sigma'_a)^2}\right)$$

$\overline{r'_a} \sim 0.01$ reduction in adhesion for smooth contact

$\sigma'_a \sim 4$

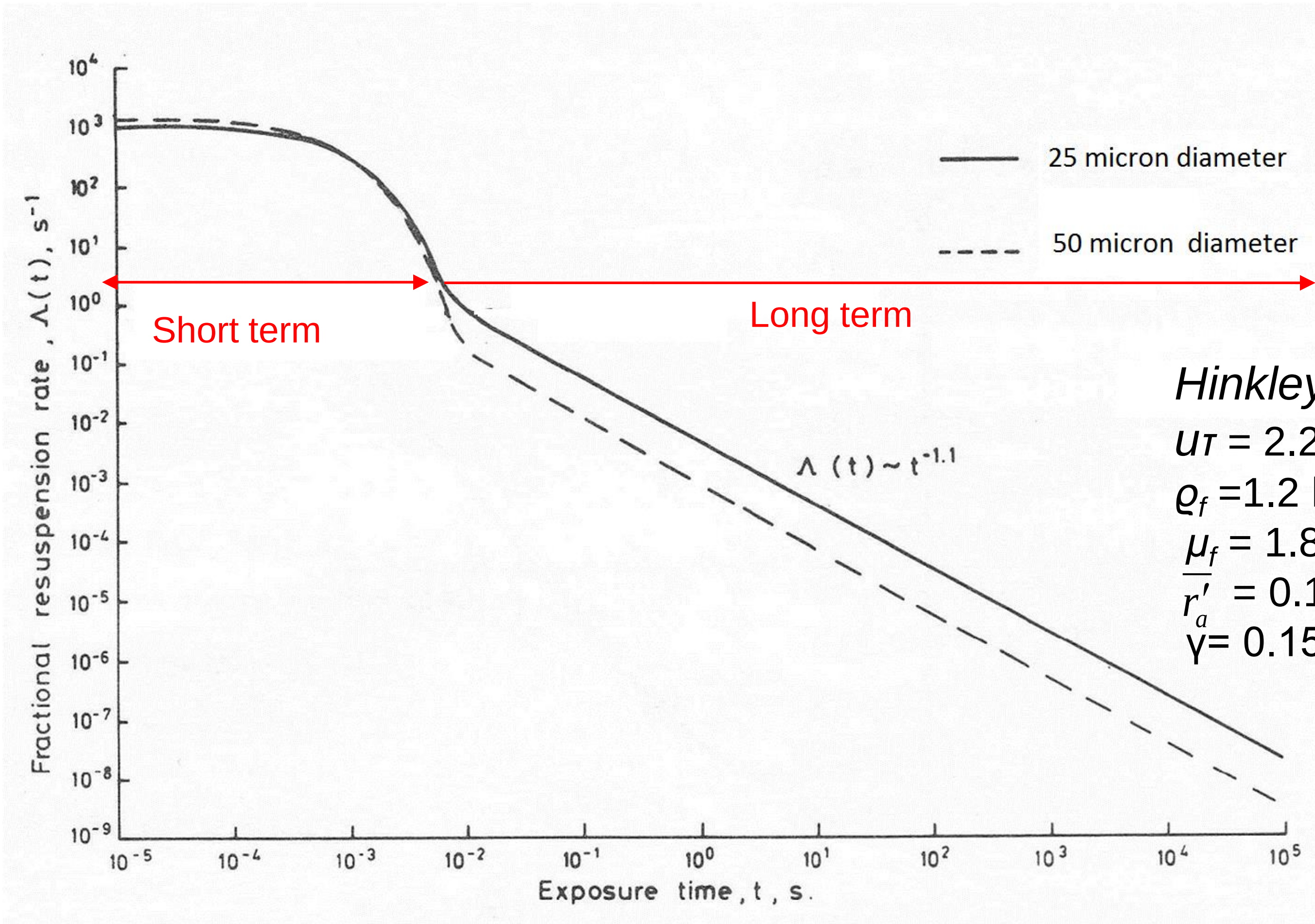
- Fraction remaining after resuspension

$$f_R = \int_0^\infty e^{-p(r'_a,t)}\varphi(r'_a)\,dr'_a$$

- Fractional resuspension rate

$$\Lambda(t) = \int_0^\infty p(r'_a)e^{-p(r'_a)t}\varphi(r'_a)\,dr'_a$$

Short and Long term Resuspension Rate



Hinkley B CAGR gas flow

u_τ = 2.2 m s^{-1}

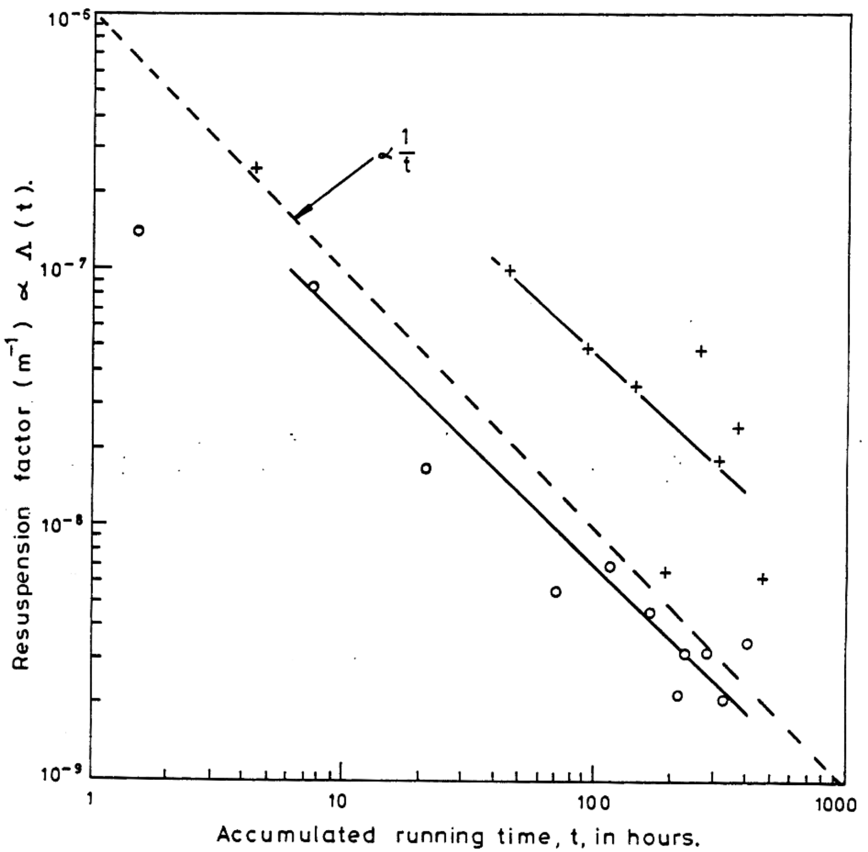
ϱ_f =1.2 kg m^{-3}

μ_f = 1.82 x 10-5 kg $m^{-1}s^{-1}$

$\overline{r_a'}$ = 0.1 ; σ_a=4

γ= 0.15 Jm^{-2}

Measurements of resuspension factor



Silt from grass at wind speeds of 5m/s o 10m/s + in a wind tunnel Garland 1979

Hall's measurements of Lift Force

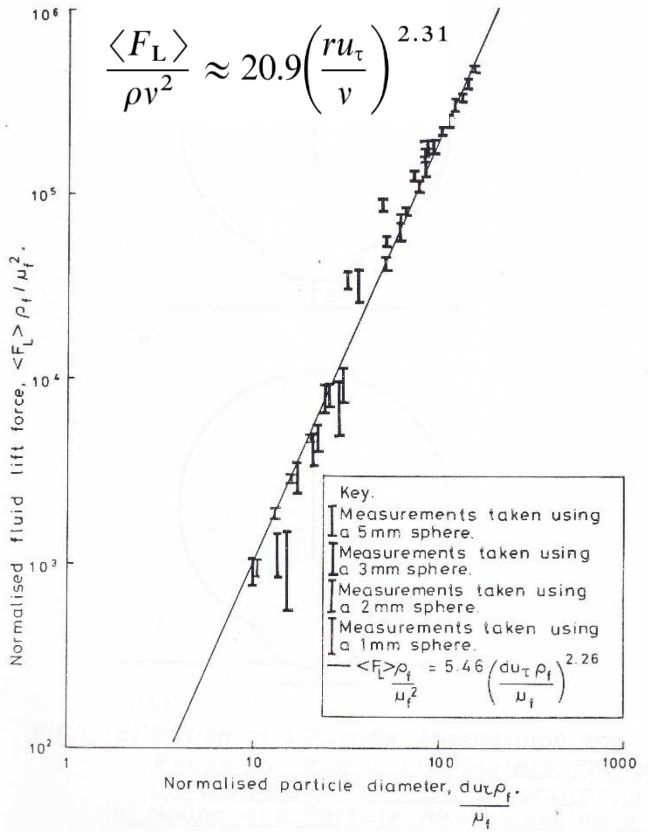


FIG.1. The Mean Lift Force $\langle F_L \rangle$ on a Sphere Near to a Surface in Turbulent Flow.

$$\hat{E}(n) = \left(\frac{\nu}{u_\tau^2} \right) E^+(n^+).$$

$$E^+(n^+) = 58.06, \quad n^+ \leqslant 0.0054,$$

$$E^+(n^+) = 0.0812(n^+)^{-1.26}, \quad 0.0054 < n^+ < 0.104,$$

$$E^+(n^+) = 0.0000173(n^+)^{-5.}, \quad n^+ \geqslant 0.104.$$

$$\chi(P_0) = \tfrac{9}{2} K^{2/3} r_a^{1/3} P_1^{1/3} \left(\frac{P_1 + P_0}{5P_1 + P_0} \right),$$

$$K = \frac{4}{3} \left(\frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2} \right)^{-1}$$

$$P_1 = P_0 + 3\pi\gamma r_a + [6\pi\gamma r_a P_0 + (3\pi\gamma r_a)^2]^{1/2},$$

$$\frac{(\langle \dot{f}^2 \rangle / \langle f^2 \rangle)^{1/2}}{2\pi} = 0.00658 \left(\frac{u_\tau^2}{\nu} \right),$$

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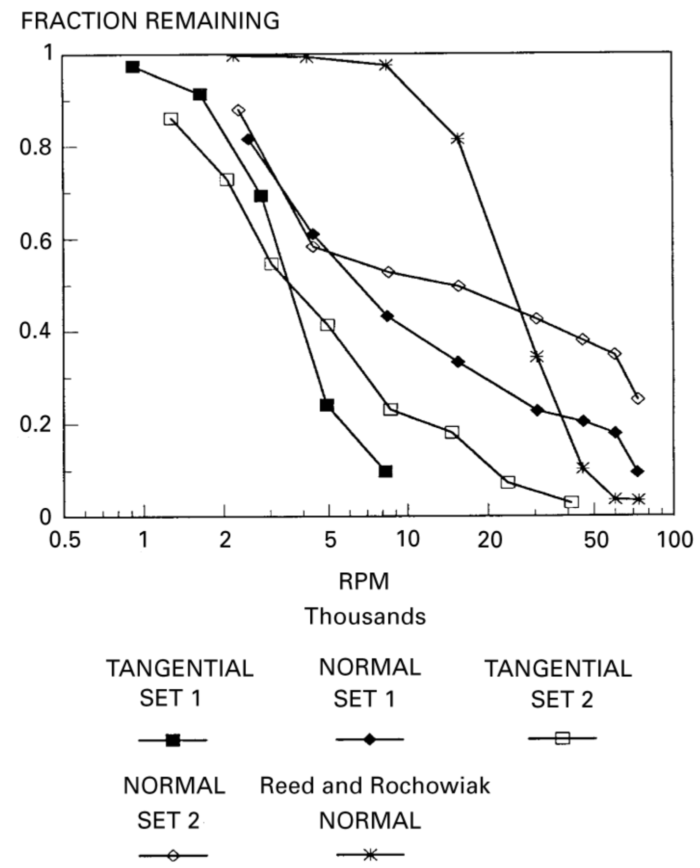
Measurements of adhesion

Table 2
Fitted values for the adhesive force distribution

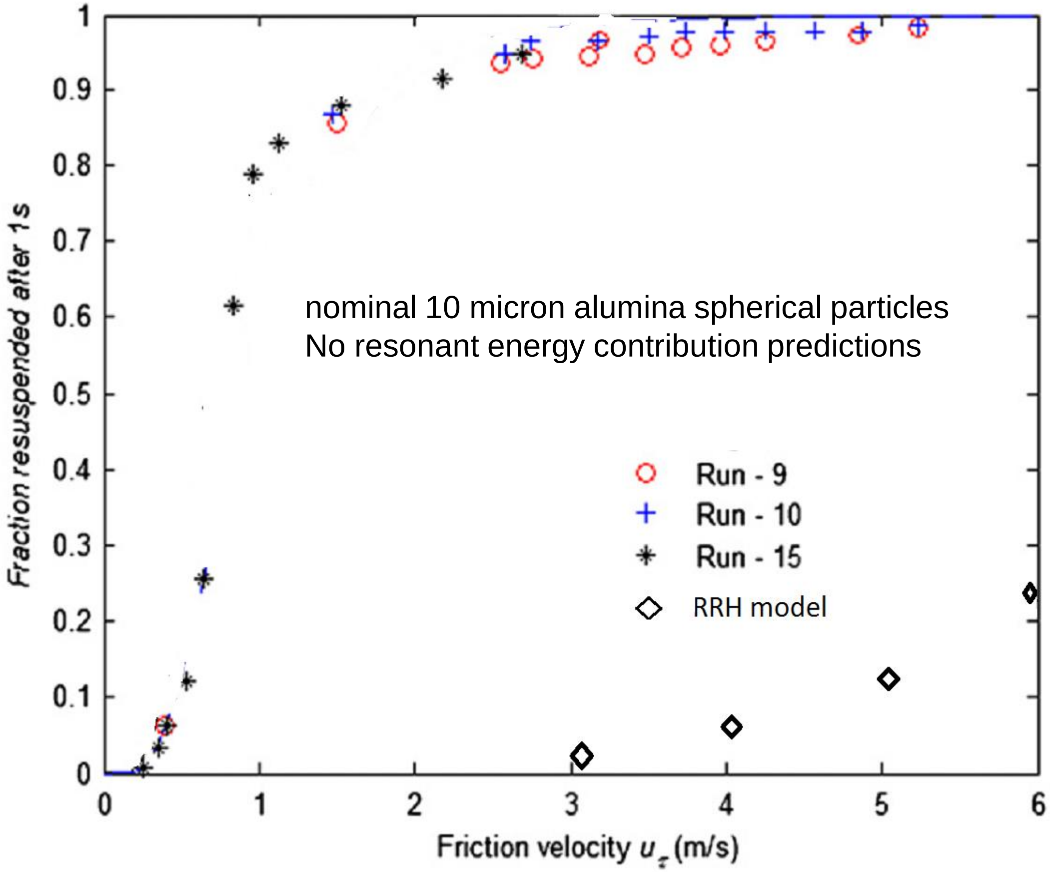
Particle	Force	Measurement	Spread σ_a	Reduction
10 μm alumina	Normal	Set 1	49	592
10 μm alumina	Normal	Set 2	208	56
10 μm alumina	Normal	Reed and Rochowiak (1988)	2.55	37
10 μm alumina	Tangential	Set 1	10.4	848
10 μm alumina	Tangential	Set 2	2.95	1053
20 μm alumina	Normal		78	56
Graphite	Normal		489	1.55
Graphite	Tangential		19	16

Material properties required to calculate particle resuspension using the RRH model

Material	Graphite	Alumina
Interfacial surface energy, Jm^{-2}	0.15	0.56
Substrate density (steel), Kg m^{-3}	7830	7830
Substrate Young's modulus, Pa	2.1×10^{11}	2.1×10^{11}
Particle Young's modulus, Pa	2.0×10^{10}	3.5×10^{11}
Substrate Poissons ratio	0.29	0.29
Particle Poissons ratio	0.3	0.3
Particle density, Kg m^{-3}	2300	1600



Resuspension measurements / model predictions



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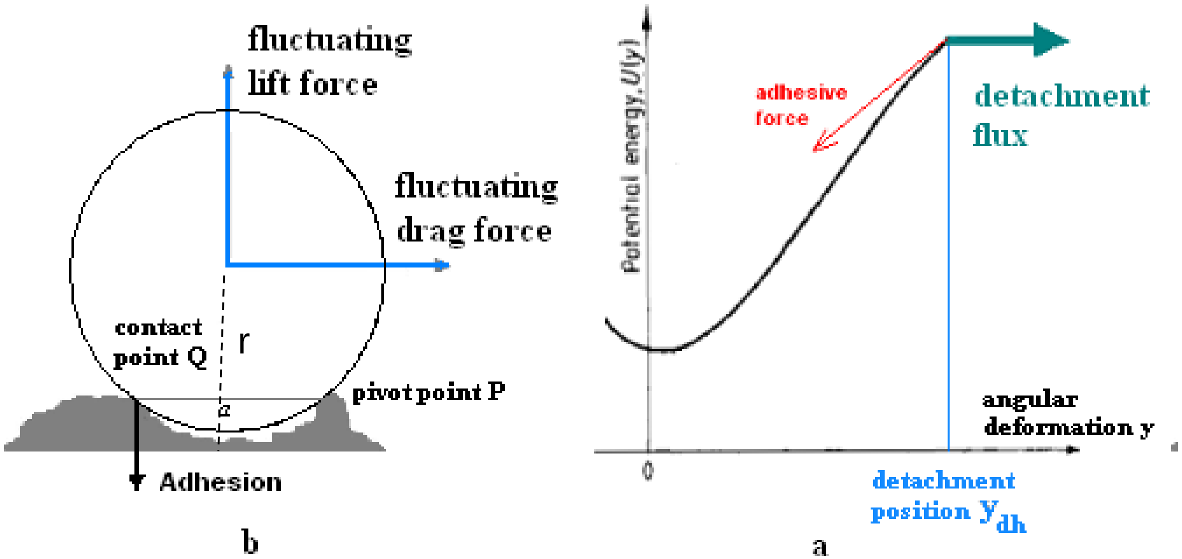
Rock’n’Roll model for particle resuspension



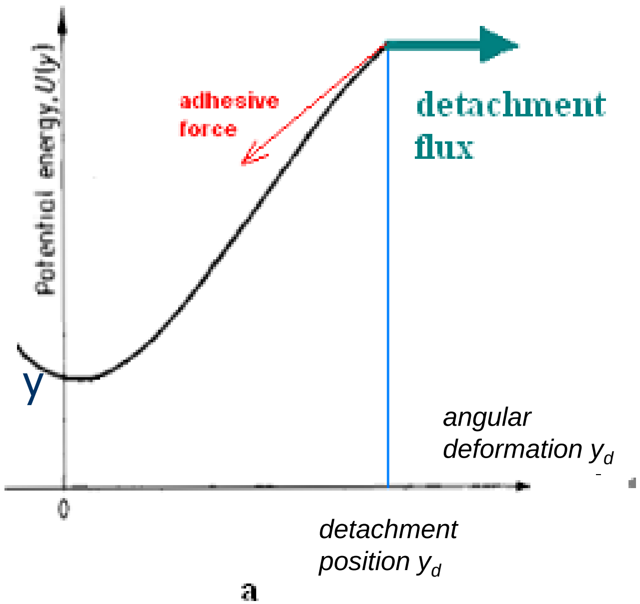
$$\Gamma = \frac{a}{2}F_L + rF_D \quad \Rightarrow \quad F = \frac{1}{2}F_L + \frac{r}{a}F_D$$

$$\underbrace{\langle F \rangle}_{\text{mean}} + \overbrace{f(t)}^{\text{fluctuating}} + F_A(y) = 0$$

At the point of detachment (y_{dh}) the adhesive ‘pull off’ force $f_a = -F_A$ at (y_{dh}),

$$f_{dh} = f_a - \langle F \rangle$$

Rate constant for Rock'n'Roll model



rate constant $p = \dfrac{\int_0^{\infty} vW(v, y_d)dv}{\int_{-\infty}^{\infty}\int_{-\infty}^{y_d} W(v, y)dydv}$

number of particles released per sec
/ number of particles attached to surface

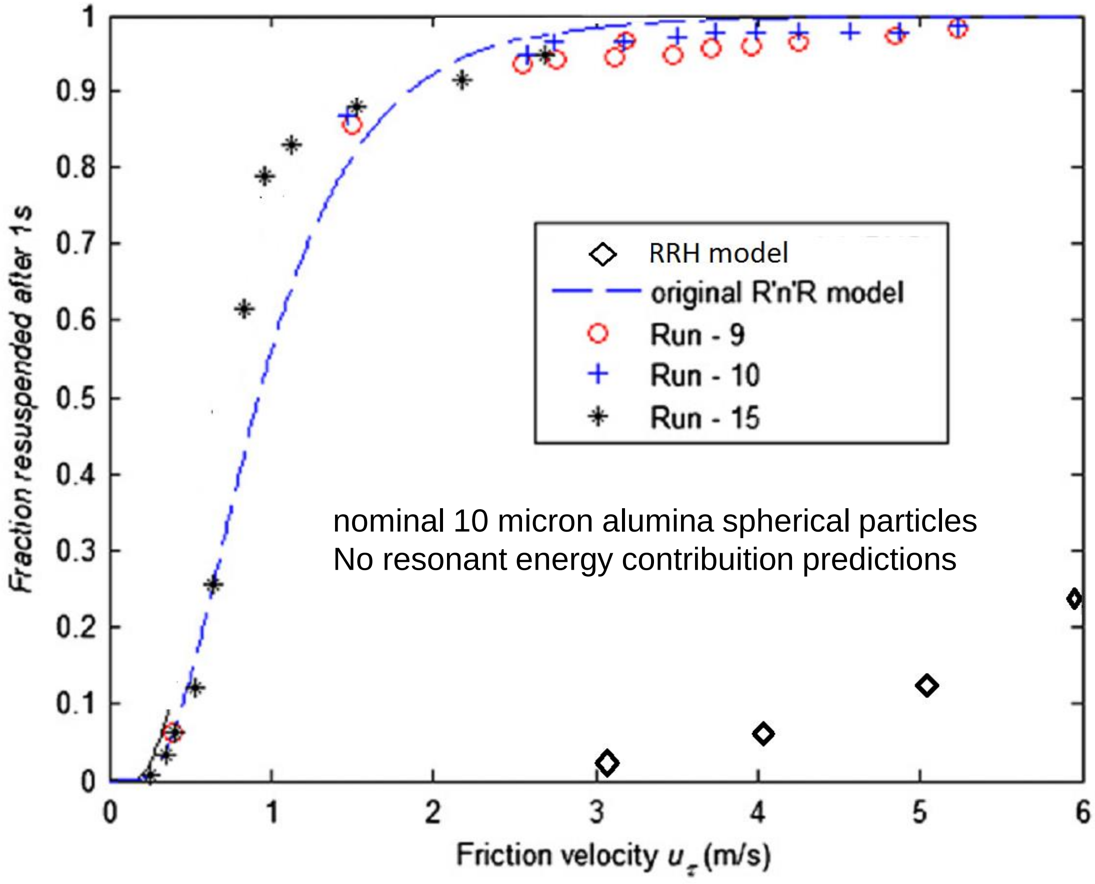
$$y(t) = \psi(f) \text{ and so } \dot{y}(t) = \dot{f}\psi'(f)$$

$$p = \frac{\int_0^{\infty} \dot{f}W(f_d, \dot{f})d\dot{f}}{\int_{-\infty}^{\infty}\int_{-\infty}^{f_d} W(f, \dot{f})dfd\dot{f}}$$

Gaussian statistically independent pdf

$$W(f,\dot{f}) = 2\pi\sqrt{\langle f^2\rangle\langle \dot{f}^2\rangle}\exp\left(-\frac{f^2}{2\langle f^2\rangle}\right)\exp\left(-\frac{\dot{f}^2}{2\langle \dot{f}^2\rangle}\right) \longrightarrow p = \frac{1}{2\pi}\underbrace{\sqrt{\frac{\langle \dot{f}^2\rangle}{\langle f^2\rangle}}}_{\omega}\exp\left(-\frac{f_d{}^2}{2\langle f^2\rangle}\right)\Bigg/\frac{1}{2}\left[1+erf\left(\frac{f_d}{\sqrt{2\langle f^2\rangle}}\right)\right]$$

Resuspension measurements / model predictions



Decay of particle concentration in a recirculating flow

❑ CAGR reactor coolant circuit

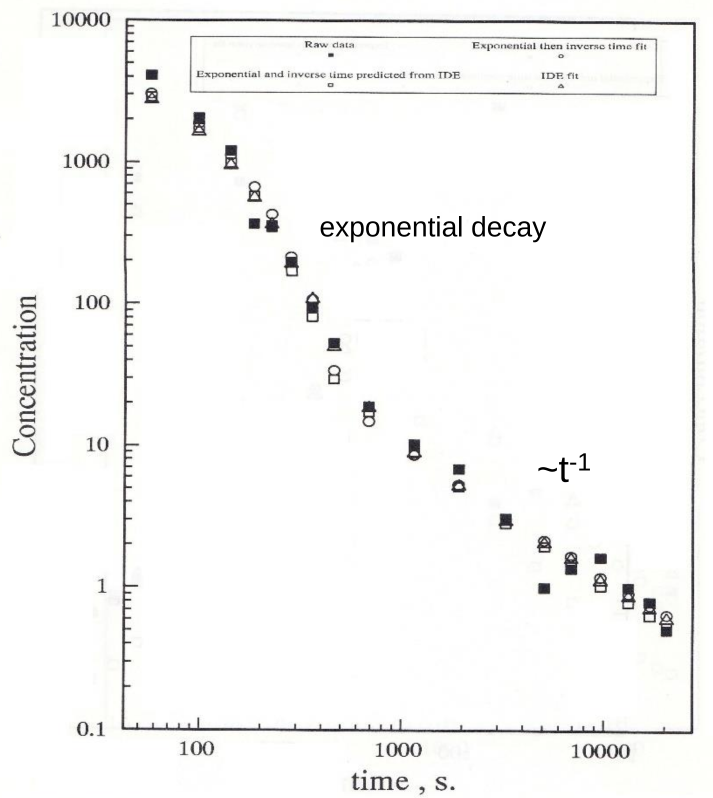


FIGURE 11 The variation in concentration of 40µm graphite particles in Hinkley Point B at full flow.

$$\frac{\partial C}{\partial t} = -(\lambda_A k_A + \lambda_B k_B)C(t) + \lambda_A k_A \int_0^t \Lambda(t-s)C(s)ds + S(t),$$

$$\Lambda(t) = \frac{\xi}{t^{\epsilon}},$$

$$\frac{\partial C}{\partial t} = -\alpha_{AB}C(t) + \alpha_A \int_0^{t-t_c} \frac{\xi C(s)ds}{(t-s)^{\epsilon}} + S(t),$$

where

Reeks-Hall IDF Equation

$$C(t) \sim \frac{\Gamma(\epsilon)\Gamma(2-\epsilon)\sin[(\epsilon-1)\pi]\alpha_A \xi}{\pi(\epsilon-1)\left[\alpha_{AB} - \alpha_A \xi \int_{t_c}^{\infty} \frac{ds}{(s+t_0)^{\epsilon}}\right]^2} t^{-\epsilon}$$

Biasi Correlations adhesive force distribution

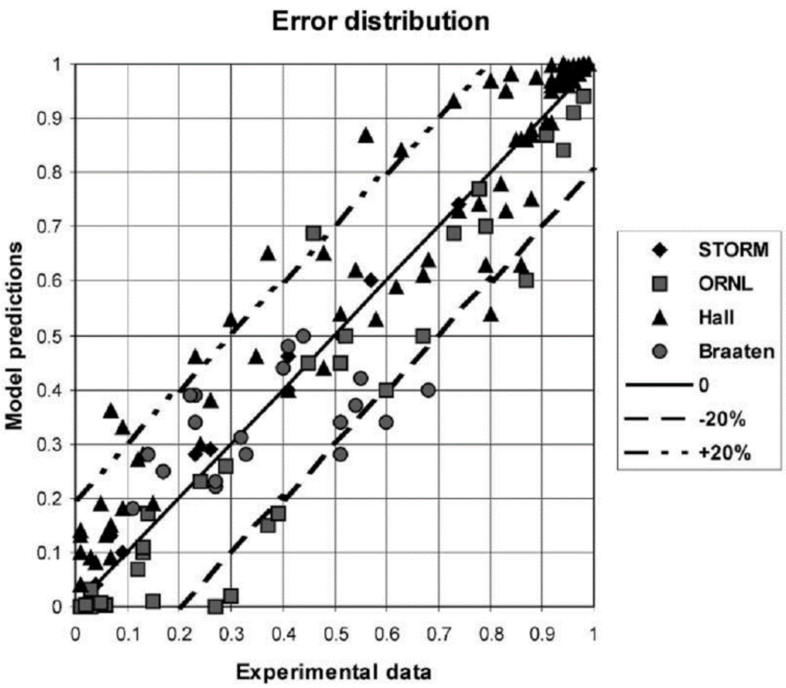


Fig. 18. Error distribution of model predictions of the fraction of resuspended particles.

$$\varphi(r_a') = \frac{1}{\sqrt{2\pi}}\frac{1}{r_a'}\frac{1}{\ln\sigma_a'}\exp\left(-\frac{\left[\ln(r_a'/\bar{r}_a')\right]^2}{2(\ln\sigma_a')^2}\right) \quad \bar{r}_a' \;\&\; \sigma_a'$$

geometric mean $\bar{r}_a' = 0.016 - 0.0023r^{0.545}$

geometric spread $\sigma_a' = 1.8 + 0.136r^{1.4}$

Non- Gaussian removal forces

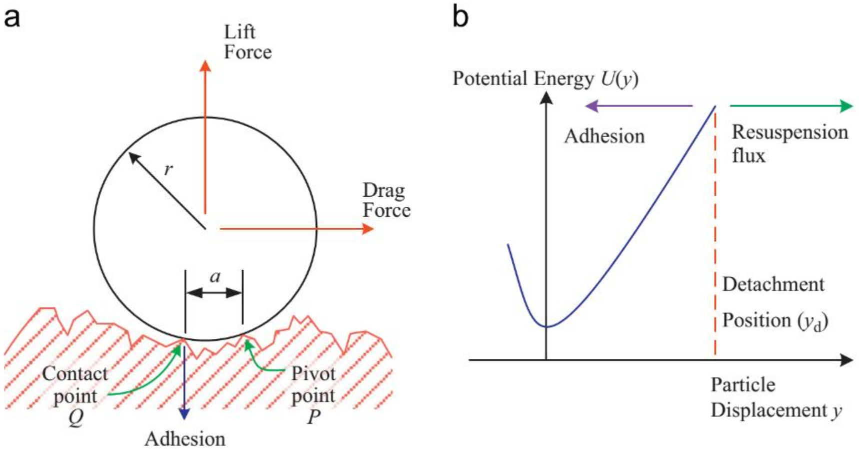


Fig. 1. Particle couple system (a) and potential well (b).

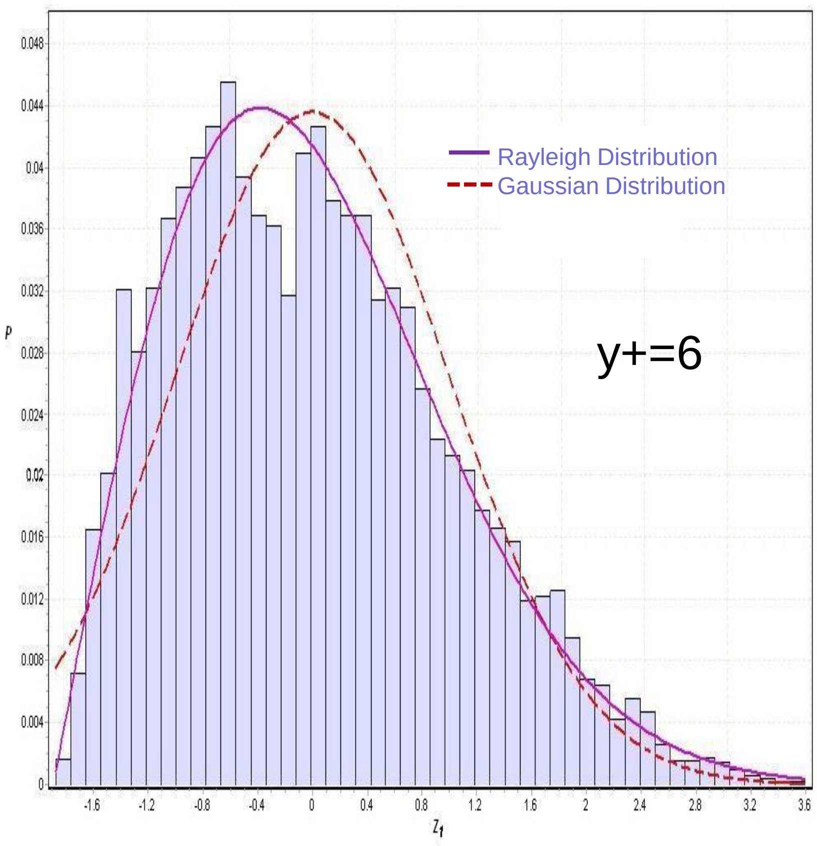
$$p = \int_0^\infty vP(y_d, v)\,dv \Big/ \int_{-\infty}^{\infty}\int_{-\infty}^{y_d} P(y,v)\,dy\,dv$$

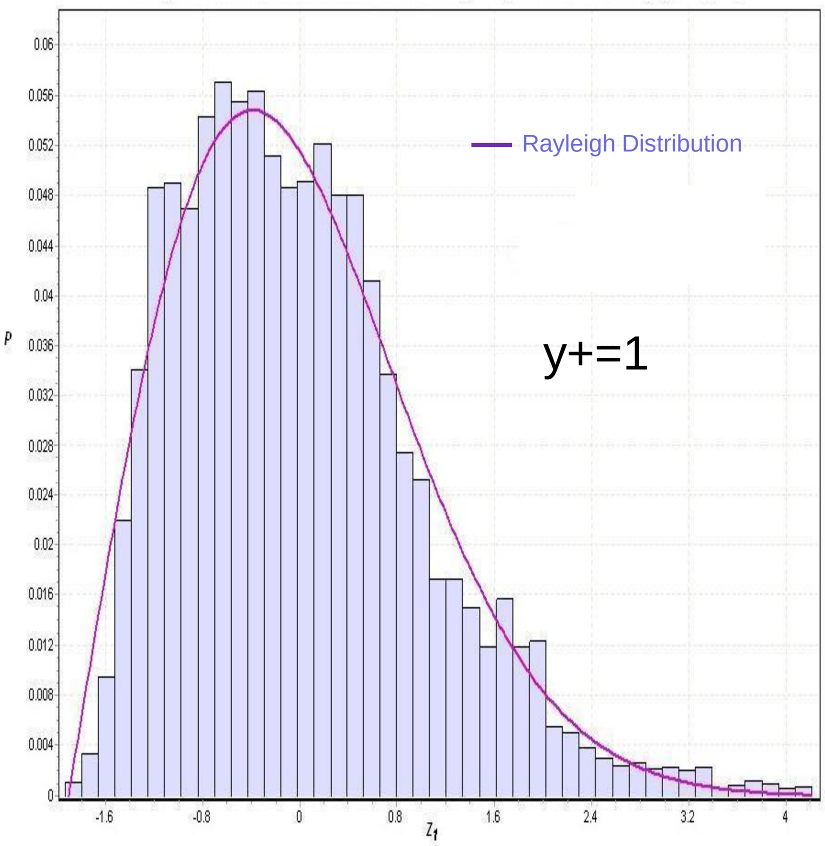
$$f_a(y) + f(t) = 0$$

$$y(t) = \psi(f) \text{ and so } \dot{y}(t) = \dot{f}\psi'(f)$$

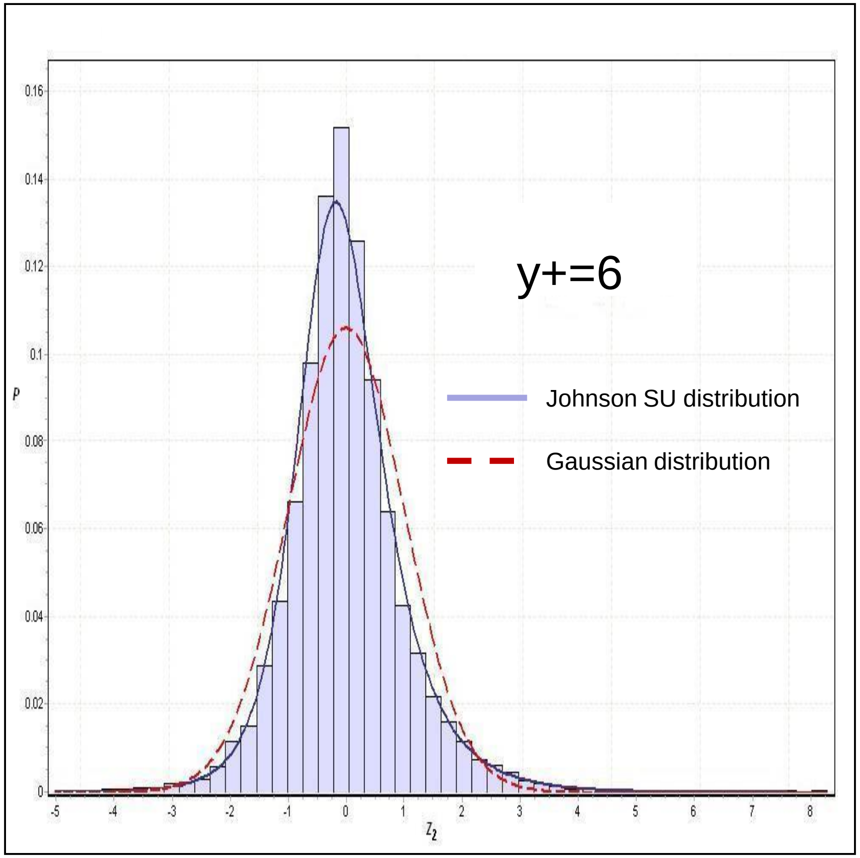
$$p = \int_0^\infty \dot{f}P\left(f_d, \dot{f}\right)d\dot{f} \Big/ \int_{-\infty}^{\infty}\int_{-\infty}^{f_d} P\left(f, \dot{f}\right)df\,d\dot{f}]$$

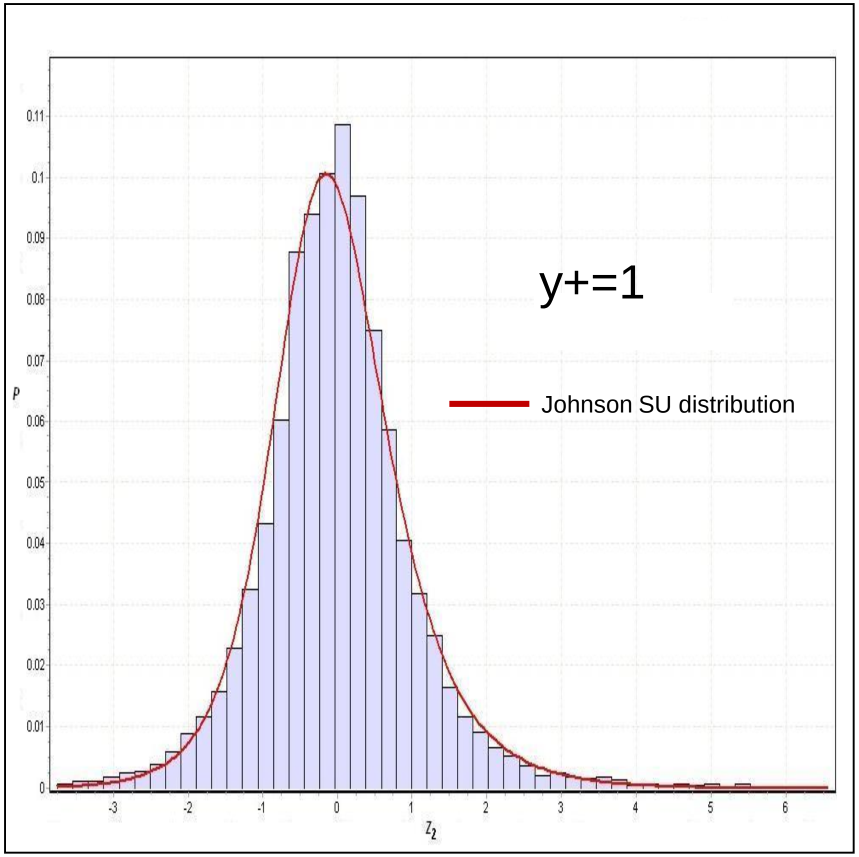
Distributions of $z_1 = f / \langle f^2 \rangle^{1/2}$ from DNS data





Distributions of $z_2 = \dot{f} / \left\langle \dot{f}^{\,2} \right\rangle$ from DNS data





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Resuspension rate constant, p

Joint distribution of fluctuating aerodynamic force and its derivative

$$z_1 = \frac{f}{\sqrt{\langle f^2 \rangle}} \quad z_2 = \frac{\dot{f}}{\sqrt{\langle \dot{f}^2 \rangle}}$$

$$P\,(z_1, z_2) = \frac{z_1 + A_1}{A_2^{\,2}} \exp\left[-\frac{1}{2}\left(\frac{z_1 + A_1}{A_2}\right)^2\right] \cdot \frac{B_1}{B_2\sqrt{2\pi}\sqrt{z^2+1}} \exp\left[-\frac{1}{2}\left(B_3 + B_1 \ln\left(z + \sqrt{z^2+1}\right)\right)^2\right]$$

where A_1, A_2, B_1, B_2, B_3 and B_4 are all constants depending on y^+.

$$z = \frac{z_2 - B_4}{B_2}$$

$$p = B_{\dot{f}}\,\omega \frac{z_{dh} + A_1}{A_2^{\,2}} \exp\left[-\frac{1}{2}\left(\frac{z_{dh} + A_1}{A_2}\right)^2\right] \Big/ 1 - \exp\left[-\frac{1}{2}\left(\frac{z_{dh} + A_1}{A_2}\right)^2\right] \qquad \text{Modified}$$

$$p = \frac{1}{2\pi}\,\omega \exp\left(-\frac{1}{2} z_{dh}^{\,2}\right) \Big/ \frac{1}{2}\left[1 + erf\left(\frac{1}{\sqrt{2}} z_{dh}\right)\right] \qquad \text{Original R'n'R Model}$$

$$\omega = \sqrt{\langle \dot{f}^2 \rangle / \langle f^2 \rangle} = \omega^+ \frac{u_\tau^{\,2}}{\nu}\ ;\ z_{dh} = \left(f_a - \langle F \rangle\right) / \langle f^2 \rangle^{1/2};\ z_a = f_a / \langle f^2 \rangle^{1/2}; B_{\dot{f}} = \phi(B_1, B_2 B_3 B_4)$$

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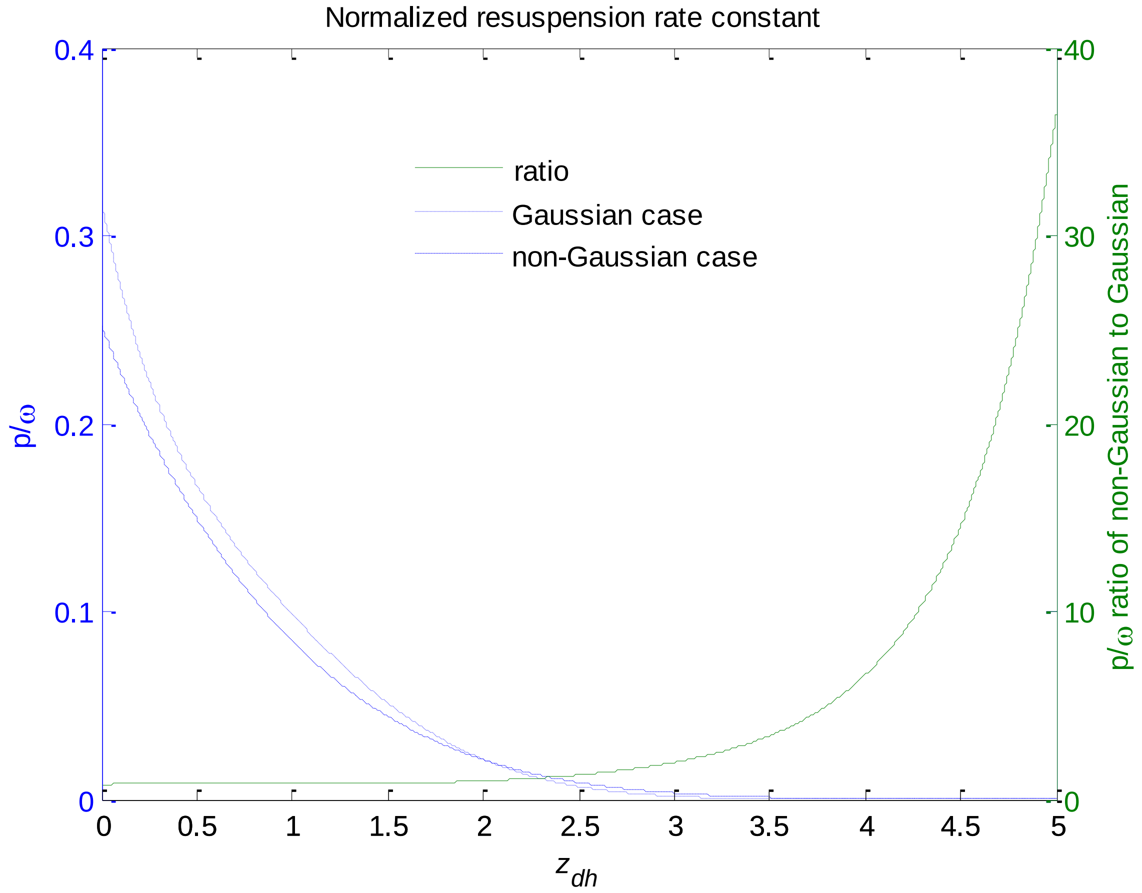
Table of resuspension rate parameters

DNS	B_{fdot}	A_1	A_2	ω^+	$f_{rms} = \langle f^2 \rangle^{1/2} / \langle F \rangle$
$y^+ = 6$	0.358568	1.83605	1.478360	0.12714	0.346
$y^+ = 2$	0.351181	1.75990	1.431301	0.13126	0.365
$y^+ = 0.6$	0.346911	1.78475	1.446609	0.15203	0.366
$y^+ = 0.1$	0.343658	1.81256	1.463790	0.16419	0.366

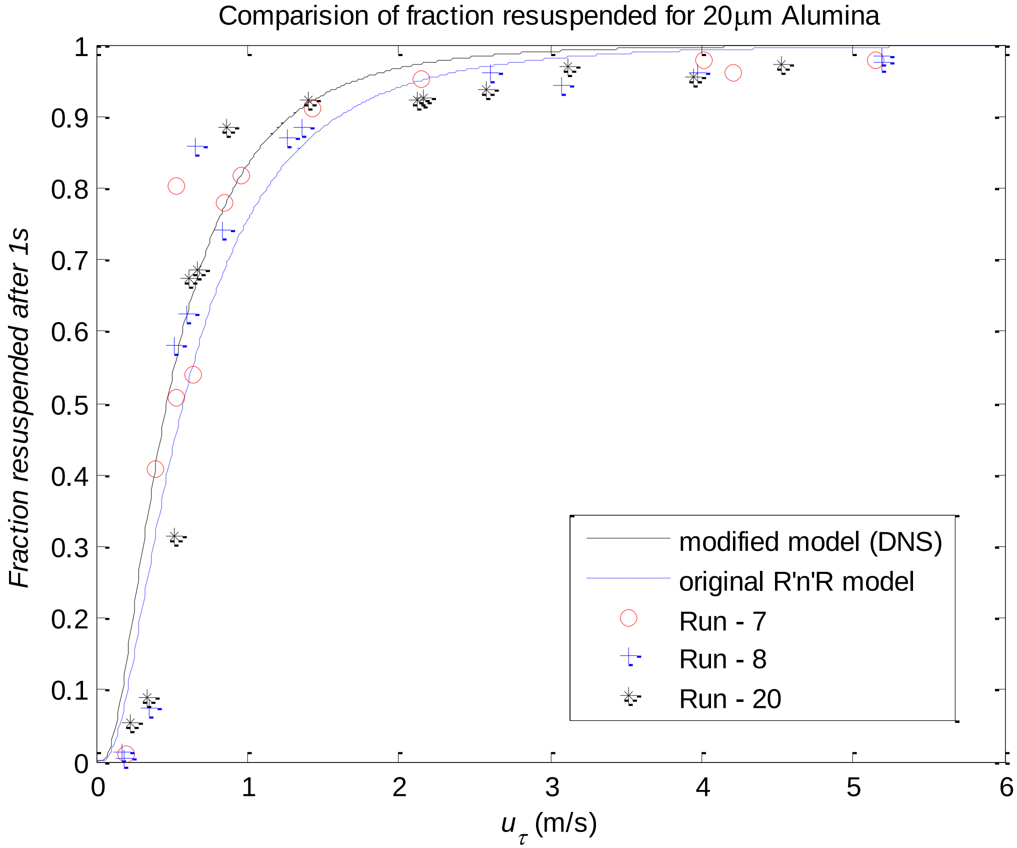
Resuspension Rate Constant



Comparison of Original and Modified R'n'R model

Comparison with Hall's experimental results

	ω^+	$\langle f^2 \rangle^{1/2} / \langle F \rangle$
Modified (DNS)	0.164189	0.366
original	0.0413	0.2



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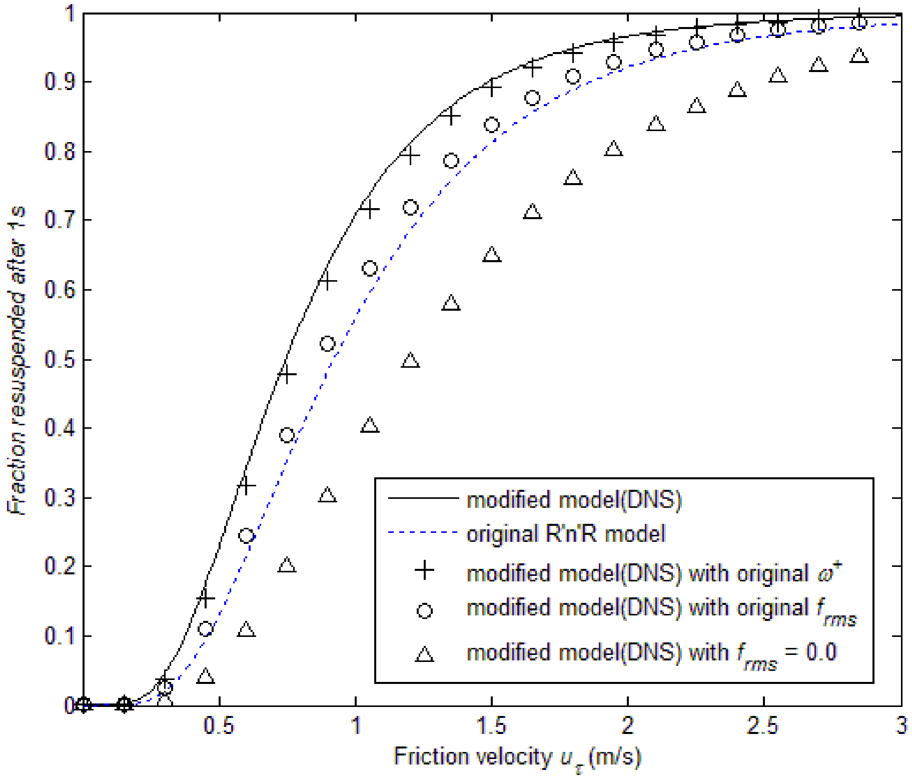
resuspension fraction after 1s modified versus original models



Hall's experimental flow and adhesion properties
for 10 micron alumina particles

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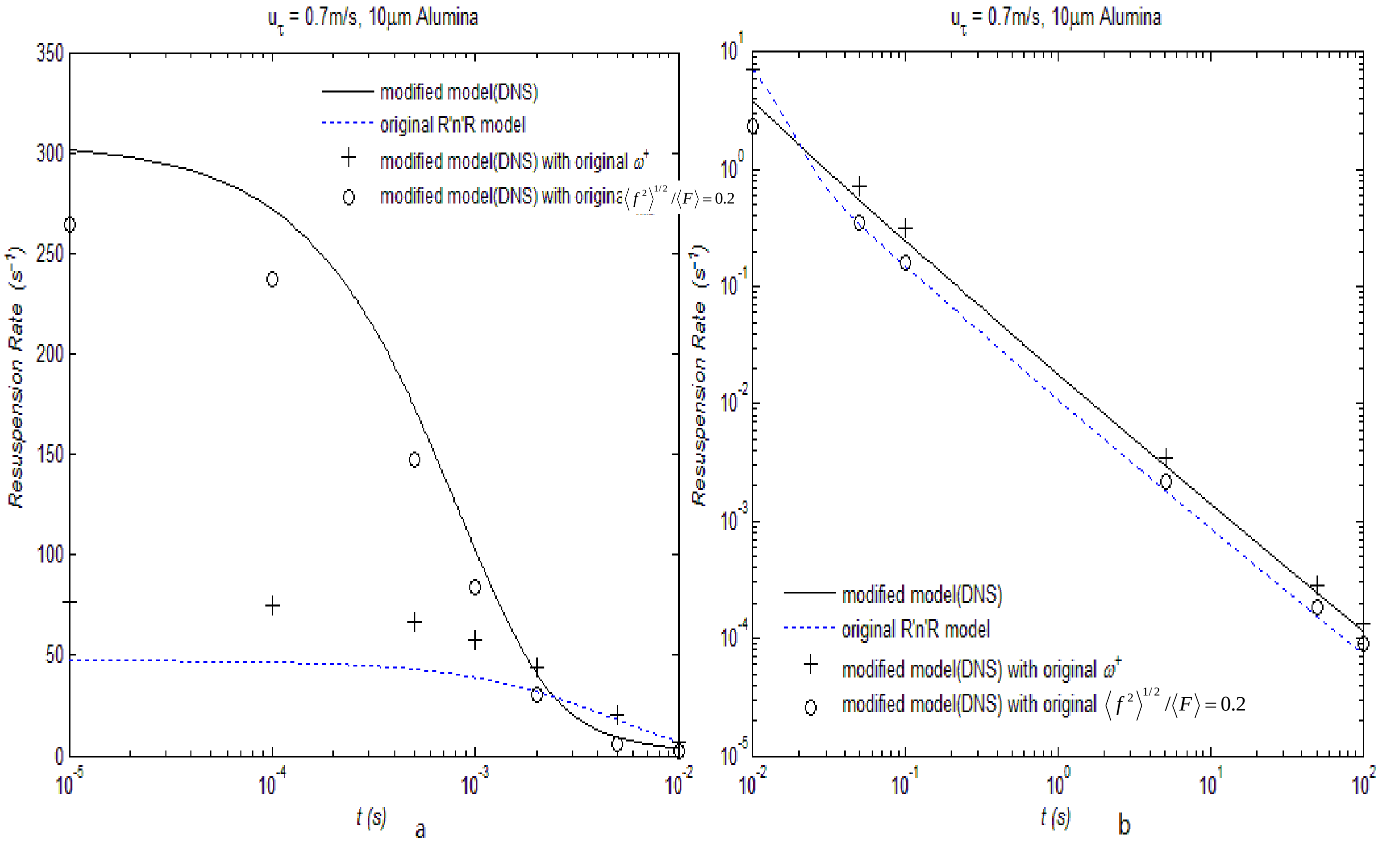
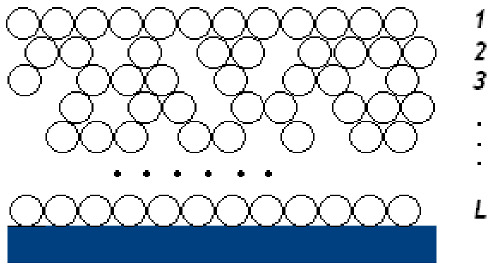
fractional resuspension rates for modified and original models



Multilayer modelling



Friess and Yadigaroglu (FY), 2001

ξ = adhesive force, flow etc.

Suppose we let $n_i(\xi, t)d\xi$ denote the number of particles between $\xi, \xi + d\xi$ in the $i-th$ layer of a deposit composed of L layers, the layers being numbered sequentially from the top layer (totally exposed to the flow) downward as $i = 1, 2..., L$. The set of ODE equations are thus

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

$$\Lambda_i(t) = \sum p n_i(\xi, t)\Delta\xi$$

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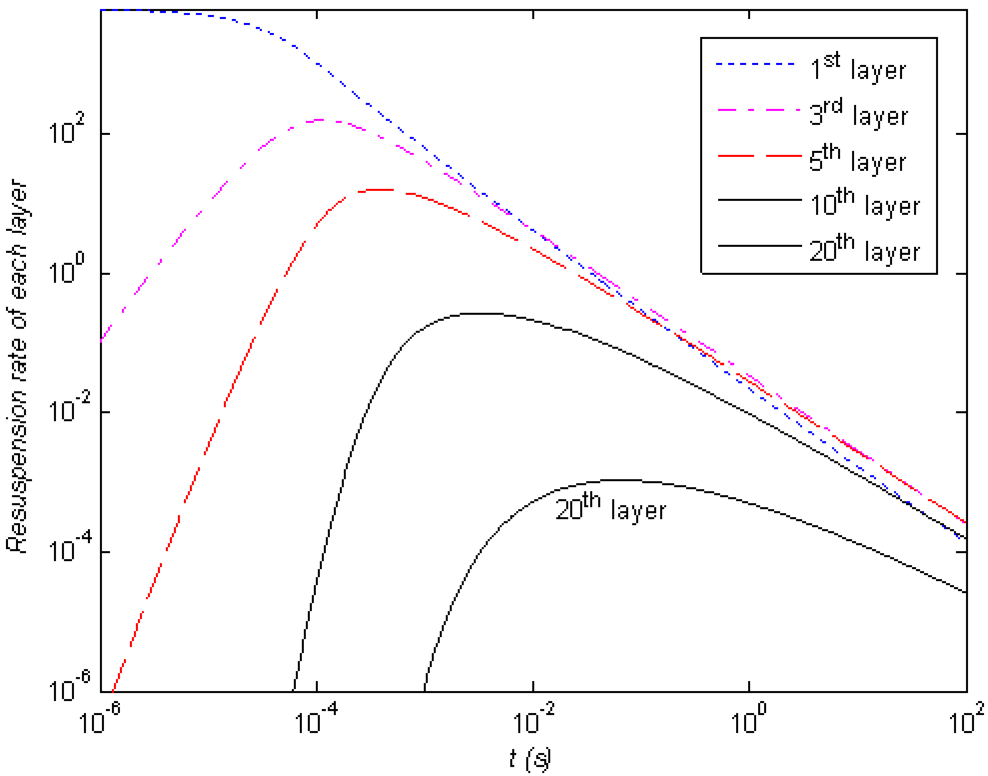
Average radius (μm)	Fluid density ($kg.m^{-3}$)	Fluid kinematic viscosity ($m^2.s^{-1}$)	Wall friction velocity ($m.s^{-1}$)
0.227	0.5730	5.2653 x 10^{-5}	6.25
Surface energy ($J.m^{-2}$)	Adhesion reduction factor (geometric mean)	Adhesion spread factor (geometric standard deviation)	Geometric mean of normalised adhesive force $\overline{z_a} = \frac{3/2\pi\gamma r}{f_{rms}\langle F\rangle}\overline{r'_a}$
0.5	0.015	1.817	5.94

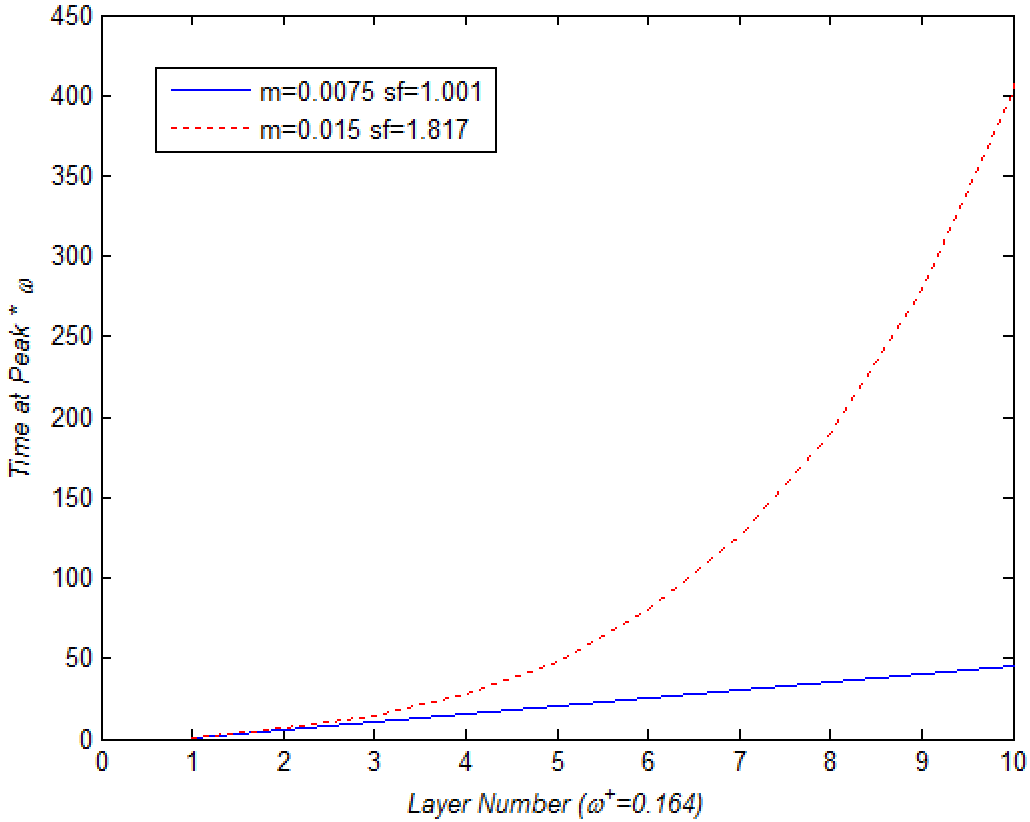
– Values of parameters in STORM SR11 Phase 6. Flow properties correspond to nitrogen gas at 12 bar pressure and temperature of 370 deg C typical of a PWR severe accident

Resuspension rate of each layer for hybrid generic model STORM Test SR11 flow conditions

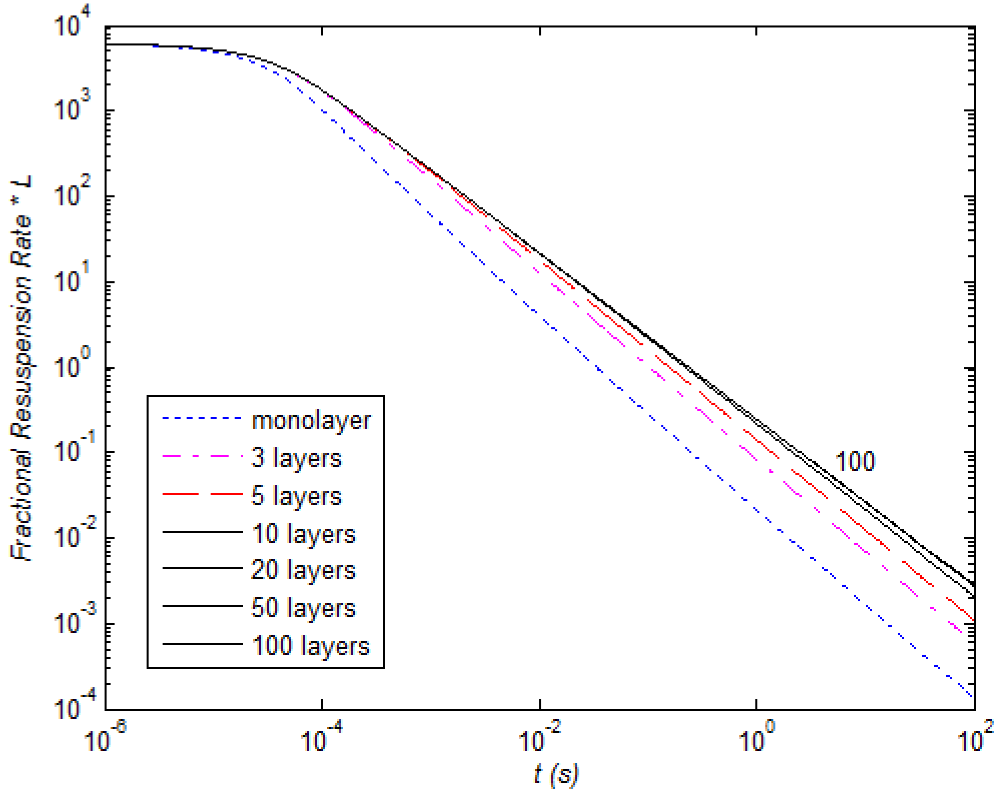


Reduction in adhesion 0.015,spread in adhesion 1.87

Resuspension of each layer vs. time

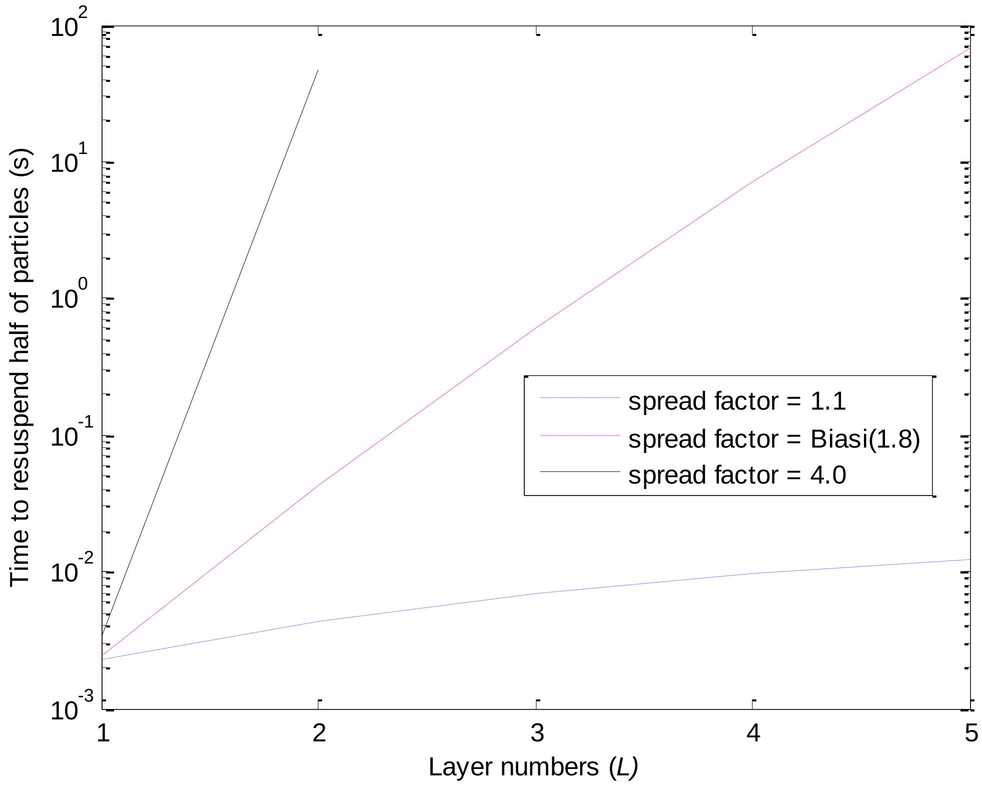


Fractional resuspension rate as a function of number of layers



(particle diameter: 0.45μm) based on STORM test (SR11) Phase 6 conditions

Resuspension half-life vs. layer thickness



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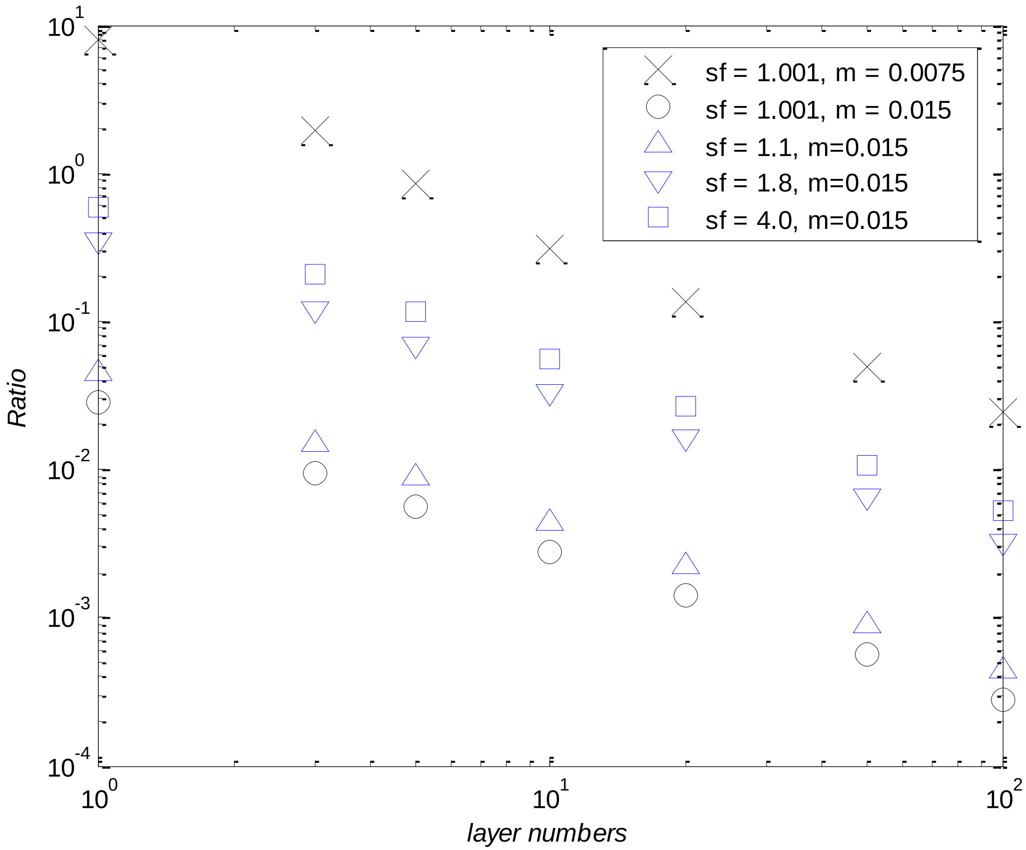
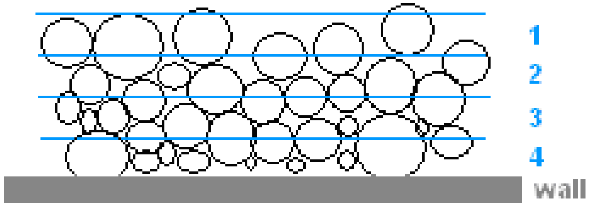
- Ratio of short-term (<10^{-4} s) to long-term resuspension fraction



Influence of size distribution

- Monodisperse model (single particle size)

$$\frac{\partial n_1(r'_a,t)}{\partial t} = -p(r'_a)n_1(r'_a,t)$$



$$\frac{\partial n_i(r'_a,t)}{\partial t} = -p(r'_a)n_i(r'_a,t) + \varphi(r'_a)\int_0^{\infty} p(\tilde{r}'_a)n_{i-1}(\tilde{r}'_a,t)d\tilde{r}'_a \quad (i \geq 2)$$

- Polydisperse model

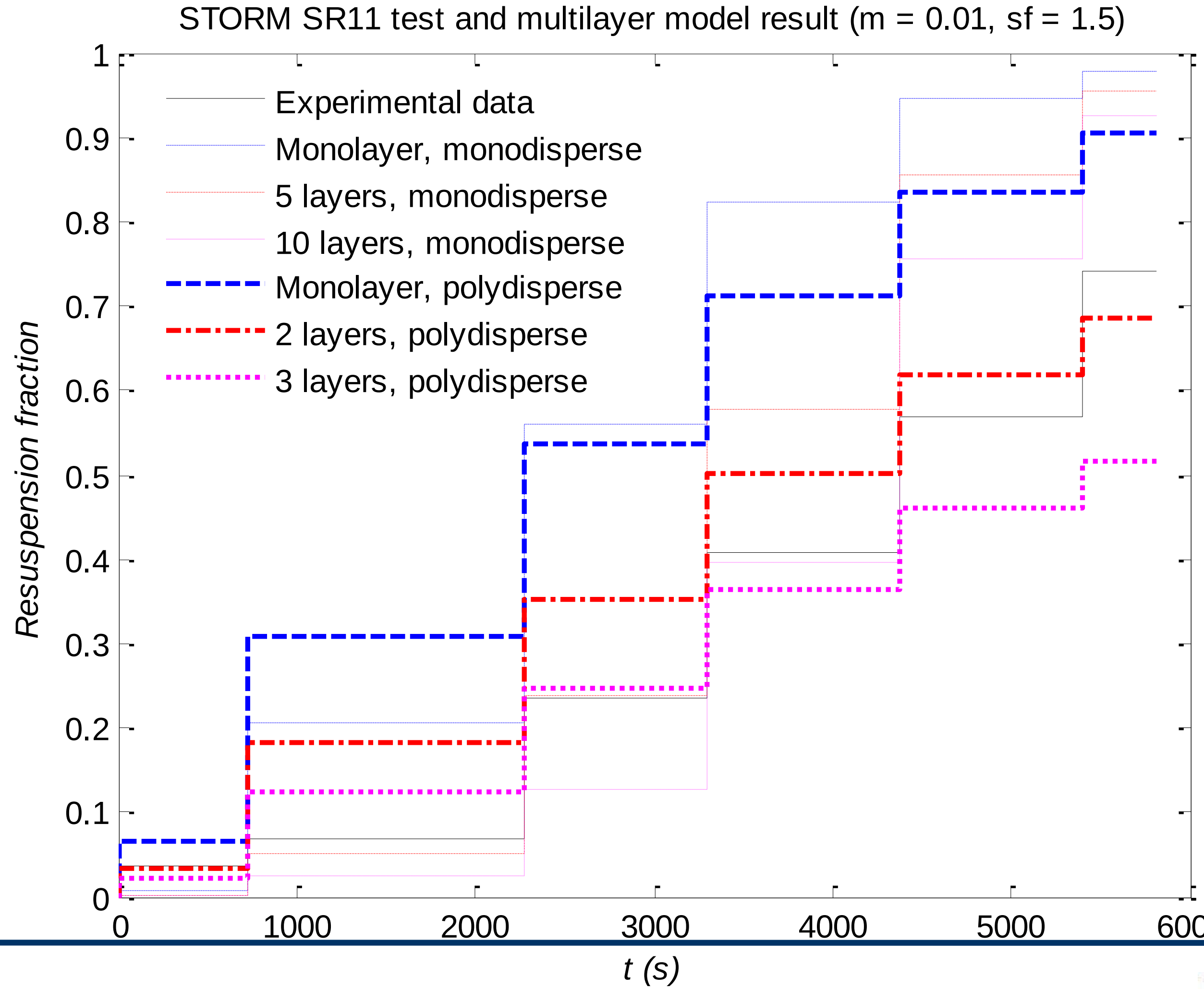
Size distribution

$$\psi(r) = \frac{1}{\sqrt{2\pi}}\frac{1}{r}\frac{1}{\ln\sigma_r}\exp\left(-\frac{[\ln(r/\bar{r})]^2}{2(\ln\sigma_r)^2}\right)$$

$$\frac{\partial n_1(r,r'_a,t)}{\partial t} = -p(r,r'_a)n_1(r,r'_a,t)$$

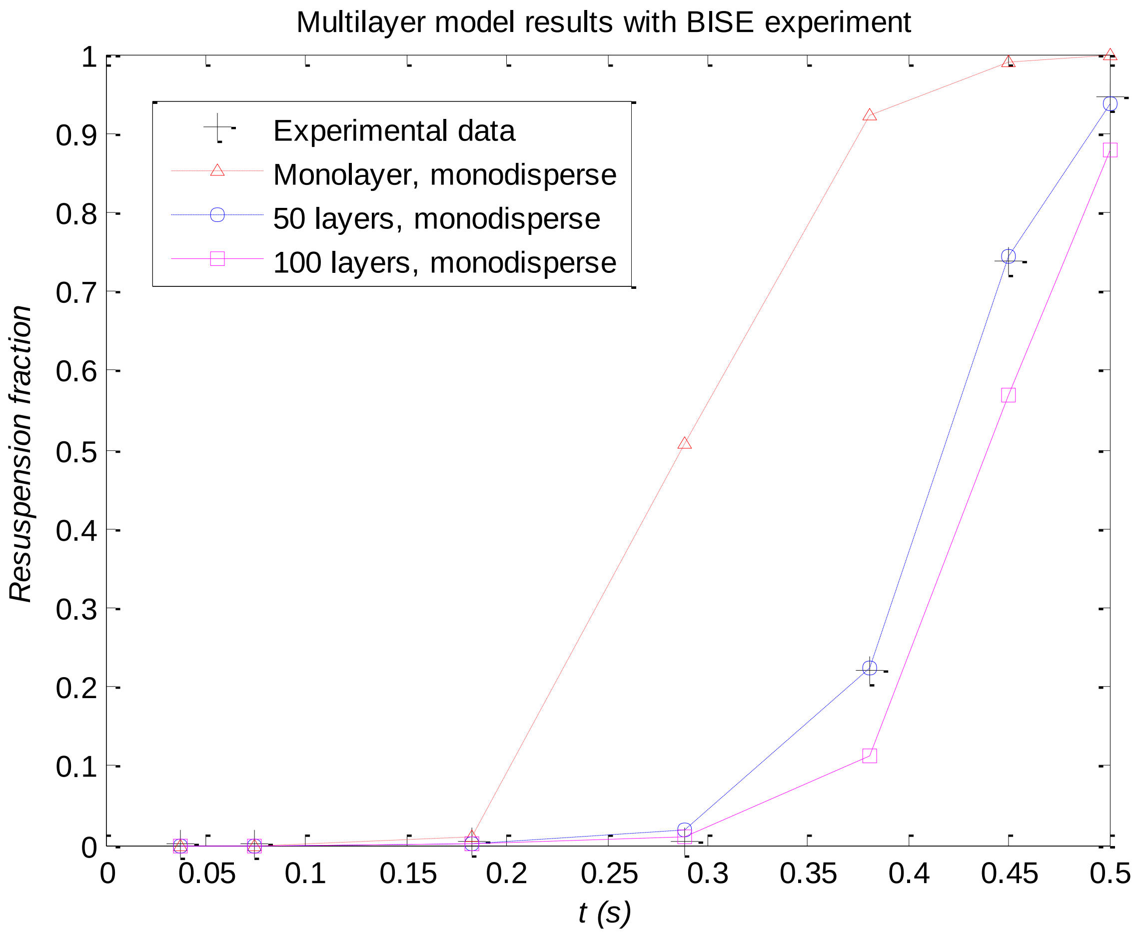
$$\frac{\partial n_i(r,r'_a,t)}{\partial t} = -p(r,r'_a)n_i(r,r'_a,t) + \psi(r)\psi(r'_a)\int_r^{\infty}\int_0^{\infty} p(\tilde{r},\tilde{r}'_a)n_{i-1}(\tilde{r},\tilde{r}'_a,t)\,d\tilde{r}'_a\,d\tilde{r} \quad (i \geq 2)$$

STORM SR11 Test



BISE Experiment

Alloul-Marmor (2002)



Summary & Conclusions

- Kinetic model for resuspension of particles by a turbulent boundary
  - Rate constant for removal for a particle from a surface
  - Analogy with desorption rate of molecules from a surface (Arrhenius)
  - resonant energy transfer/quasi-static removal
  - Originally developed for removal by lift forces $(\langle F \rangle, f, E_f(n))$
  - Broad distribution of surface adhesive forces log normal) geom spread factor
  - Factor of 100 reduction in adhesion compared to perfectly smooth contact
- Short term (e^{-pt}) and long term resuspension $\Lambda(t) \sim \xi t^{-1}$
  - Decay of gas borne concentration in reactor coolant circuit (deposition and resuspension
- Model validation
  - Centrifuge measurements of surface adhesion,
  - Tangential force easier to remove particles than normal force - 'rolling over lift off'
  - Development RnR model using moments of drag forces
    - Much better agreement with R&H resuspension measurerments
- RnR treatment for non Gaussian removal forces
  - Significant increase in the resuspension rate for rough surface $\langle F_R \rangle \ll$ g.mean adhesive force