

Particle Resuspension Simulation Capability to Substantiate DOE-HDBK-3010 Data

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INTRODUCTION

The data provided in the U.S. Department of Energy (DOE) Handbook, DOE-HDBK-3010 [1] provides data such as airborne release fractions and respirable fractions which are widely used in safety analysis and facility design. These fractions are often used as conservative bounds, despite the fact that the original data may have been obtained at a different scale or in a different configuration than the end application. The use of computational techniques to augment these data can be used to extend laboratory-scale data applicability to facility-scale decisions. Our prior report described an approach using Sandia National Laboratories (SNL) computer codes to simulate particle releases from various accident scenarios [2]. The relevant physics controlling the particle resuspension phenomena can be highly problem-dependent. They can include surface tension for particles or surfaces with liquid present, van der Waal forces for small particles, electrostatic forces for charged particles, and mechanical interactions with surface features larger than the particles sizes. The complexity of this phenomenon and recent developments have been described in a recent review by Henry and Minier [3].

MODELING APPROACH

Of particular interest to this work is the scenario where airborne particles settle on a surface then are disturbed by airflow or mechanical agitation. In such a scenario, the resulting airborne particle distribution can depend strongly on the physical configuration and agitation method.

The primary focus of this work is for solid particles. Resuspension considerations for liquid particles would need to include different adhesion models based on surface tension and wetting angle to be appropriate. Such models can be implemented in the given framework, but are not the focus here. In this work we implement and demonstrate model methods using the SNL code SIERRA/Fluid Mechanics (Fuego), which is a low-Mach number fluid mechanics CFD code targeting fire simulations and particle transport [4].

Basic Resuspension Model

The two basic interaction modes between particles and surfaces in SIERRA/Fuego, namely reflection models and adhesion models. Reflection models are primarily applicable to liquid particles, and include particle shattering and Weber number-based adhesion criteria [5]. Resuspension is applied as an adhesion model, where a local force balance is applied

to a particle on a surface to determine whether it can re-enter the flow field or must remain on the surface.

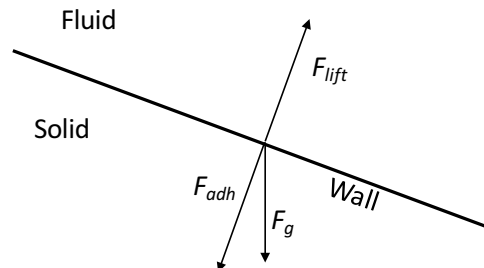


Fig. 1. Particle force balance on a surface

The basic resuspension model is based on equations derived by Wichner and summarized by Young [6], and can be described in this force balance context using the following force models:

$$F_{lift} = \alpha A_p \tau_w \quad (1)$$

$$F_{adh} = 10^{-9} \frac{r}{\epsilon} \quad (2)$$

where α is a lift coefficient (nominally 5.0) and ϵ is the surface roughness. Unlike the original form by Wichner, we also consider gravity forces in our model (Fig. 1).

Because of the empirical nature of the above force terms (being representative for only specific datasets), we have chosen to implement the force terms generally, so the lift and adhesion force can be specified individually at runtime as any arbitrary function of A_p , τ_w , $\overline{\tau_w}$, k , r_p , μ_f , ρ_f , ϵ , t , and $\partial \overline{\tau_w} / \partial t$. The overbar on wall shear stress indicates a time average, while the value of τ_w includes turbulent variations, described in a subsequent section.

Stochastic Resuspension Model

One limitation of the basic resuspension model described above is that it does not have a mechanism to account for variations in particles other than diameter (e.g. shape or aspect ratio) or variations in local surface properties. To account for this, we introduce a resuspension probability function, that can depend on any of the variables the lift and adhesion force depend on. When the resuspension probability function is active, each particle is assigned a random number from a uniform distribution between 0 and 1. The force balance shown in Fig. 1 is still applied first to

see whether a particle could resuspend. If so, the resuspension probability is calculated at the current conditions and if the calculated probability is greater than the particle's random number the particle is removed from the surface, re-inserted into the fluid flow, and assigned a new random number. For example, one could use a force-based version of this probability function, defined as

$$P = 1 - \exp\left(-\frac{F_{\text{lift}}}{F_{\text{adh}}}\right), \quad (3)$$

where the lift and adhesion forces used here are those defined by Wichner [6] (Eqns. 1 and 2).

Wall Shear Stress Calculations

The wall shear stress used in the resuspension calculations described previously is calculated at the walls during the fluid mechanics solve using models which depend on the selected turbulence model. When considering laminar flow, no wall models are used and wall shear is simply

$$\tau_w = \mu \frac{\partial u}{\partial y}. \quad (4)$$

For turbulent simulations, an appropriate wall model is used to determine the wall friction velocity (u_τ), which is used to calculate wall shear stress as

$$\tau_w = u_\tau^2 \rho_f \quad (5)$$

The friction velocity can be calculated either assuming local equilibrium between production and dissipation, as

$$u_\tau = C_\mu^{0.25} \sqrt{k} \quad (6)$$

or using Newton iteration to solve

$$\frac{u_\tau}{u_\tau} = \frac{1}{\kappa} \ln(Ey^+) \quad (7)$$

since y^+ also depends on u_τ .

To model the effects of turbulence in the fluid flow on particle motion, the fluid velocity the particle experiences is perturbed by a normal distribution with zero mean and a standard deviation based on the local turbulent kinetic energy. The standard deviation of this distribution is calculated from the expression for the velocity variation (u') as

$$u' = \sigma_u = \sqrt{\frac{2}{3}k}. \quad (8)$$

In order to apply a similar effect to the wall shear stress, we leverage the experimental data by Keirsbulck et al. [7], who measured the wall shear stress variation as a function of friction velocity ranging from 0.015 to 0.08 m/s in a 1 by 15 cm rectangular duct with centerline velocities ranging from 0.26 to 1.6 m/s. Fitting a logarithmic relationship to their results gives the relative wall shear stress variation as

$$\frac{\tau_w'}{\tau_w} = 0.0375 \ln(u_\tau) + 0.482. \quad (9)$$

RESULTS

To test the particle resuspension capability, we devised a notional scenario that involves a physical domain with a particle spray in a large box and a smaller air jet that enters the box tangentially to the surface accumulating particles (Fig. 2). The box is 30 x 30 x 15 cm and the inflow channel is 4 x 4 x 20 cm, with a uniform 5 mm hex mesh. The spray is positioned opposite the inflow channel with a cone angle of 30 degrees, pointed downward and towards the center of the open box. The injected particle diameters are controlled by a mass-weighted log-normal distribution. The particle spray is active for 1 second, after which time it is deactivated, and the surface roughness is 50 μm .

Results from two resuspension models are shown here; the model by Wichner [6] (Eqns. 1 and 2) using the mean, non-fluctuating wall shear stress, and the same model but including turbulent variations in wall shear stress (Eq. 9). Under the conditions in these simulations, the variation in wall shear stress is expected to be as high as 50%.

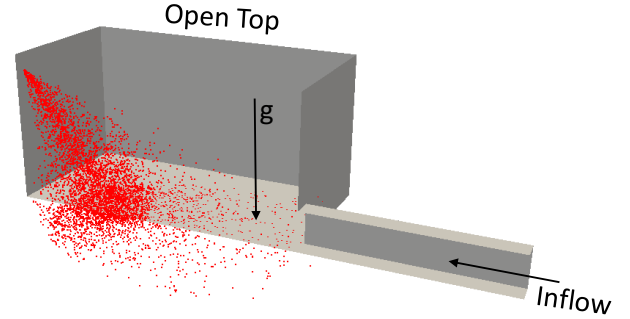


Fig. 2. Resuspension test domain (cut in half), showing spray location.

After the 1 second particle injection is complete, the particles are allowed to settle for 0.5 seconds before the inflow air velocity is increased linearly from 0 to 10 m/s over 1 second, then held constant at 10 m/s for another 1.5 seconds, giving a total simulation time of 4.0 seconds. This results in a maximum friction velocity of around 0.5 m/s through the center of the particle deposition region. To compare the effects of the different resuspension models, we compare the distribution of particles stuck on the bottom surface of the domain (with respect to gravity) at different times, as well as the diameter distribution of the stuck particles before and after the jet (Fig. 3). The distribution of particles just before the jet initiation is shown in Fig. 4.

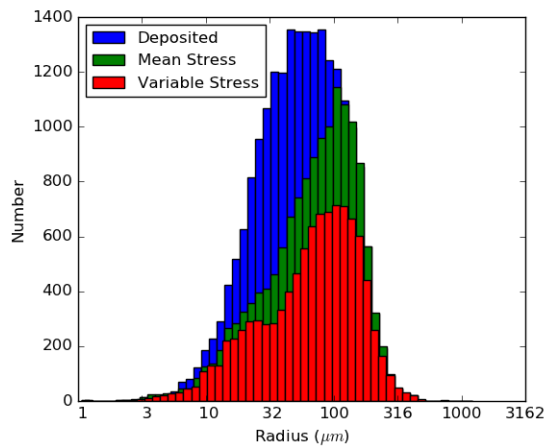


Fig 3. Size distribution of particles stuck on base surface at 1.5 seconds (blue) and 4.0 seconds with both the mean (green) and variable (red) shear stress models.

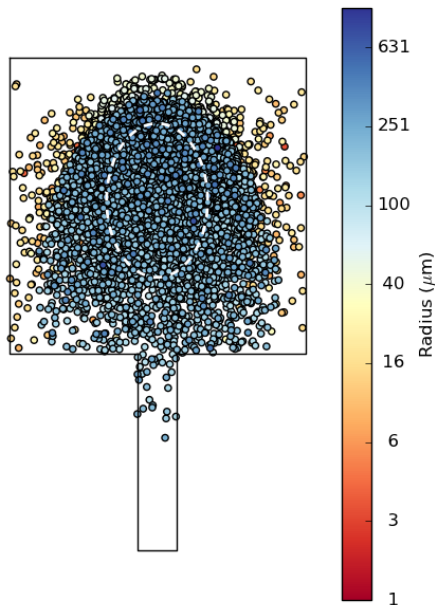


Fig 4. Particle deposition pattern on base surface at 1.5 seconds, just before the jet initiation, with the spray cone intersection ellipse shown by the white dashed line.

After the air jet is activated, the particles on the surface are disturbed and some particles are resuspended. Small particles are not resuspended because the adhesion force is greater than the lift force, while large particles are not resuspended because the gravity force is greater than the lift force. For this particular configuration, most of the resuspended particles have radii between 10 and 100 μm . The change in the distribution before and after the jet is shown in Fig. 3, which illustrates this size dependence.

The spatial distribution of particles at the end of the mean stress simulation is shown in Fig. 5. While it is clear that some particles have been removed from the jet path, the larger particles still remain stuck. Near the top of the domain,

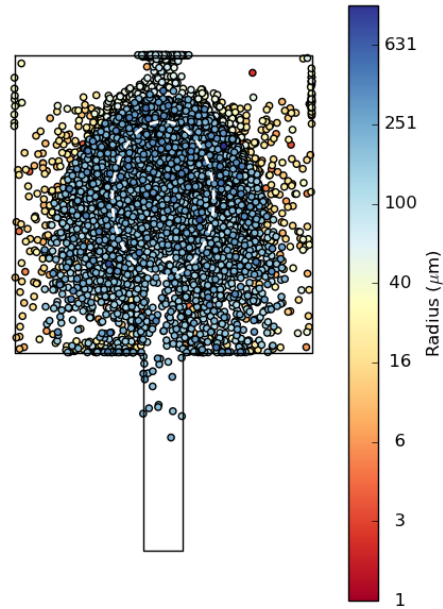


Fig 5. Particle deposition pattern on base surface at 4.0 seconds, after being disturbed by the jet and using the mean shear stress model.

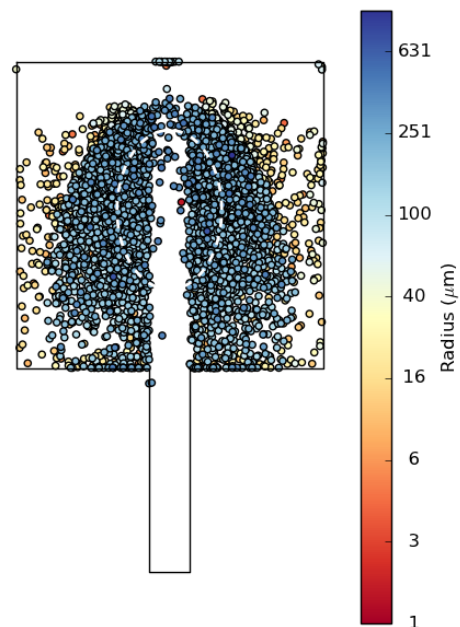


Fig 6. Particle deposition pattern on base surface at 4.0 seconds, after being disturbed by the jet and using the variable shear stress model.

some of the particles have re-adhered to the surface at the jet stagnation point, where the shear stress is lower. By comparison, the spatial distribution at the simulation end with variable shear stress is shown in Fig. 6, where the jet path is almost completely clear of particles.

SUMMARY

In this work we have presented a particle resuspension model implemented in the SNL code SIERRA/Fuego, which can be used to model particle dispersal and resuspension from surfaces. The method demonstrated is applicable to a class of particles, but would require additional parametric fits or physics models for extension to other applications, such as wetted particles or walls. We have demonstrated the importance of turbulent variations in the wall shear stress when considering resuspension, and implemented both shear stress variation models and stochastic resuspension models (not shown in this work). These models can be used in simulations with of physically realistic scenarios to augment lab-scale DOE Handbook data for airborne release fractions and respirable fractions in order to provide confidences for safety analysts and facility designers to apply in their analyses at DOE sites. Future work on this topic will involve validation of the presented model against experimental data and extension of the empirical models to be applicable to different classes of particles and surfaces.

NOMENCLATURE

A_p = Particle cross-sectional area
 C_μ = Turbulence model parameter
 E = Turbulence model law of wall roughness
 F_{adh} = Particle adhesion force
 F_g = Particle gravity/buoyancy force
 F_{lift} = Particle lift force
 P = Resuspension probability
 k = Turbulent kinetic energy
 r = Particle radius
 y^+ = Dimensionless distance to the wall
 u_τ = Friction velocity
 u_\parallel = Velocity parallel to wall
 α = Particle lift coefficient
 ε = Surface roughness
 κ = Turbulence model parameter
 μ = Fluid viscosity
 ρ = Fluid density
 τ_w = Wall shear stress

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