Simulation of windblown dust transport from a mine tailings impoundment using a computational fluid dynamics model

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A B S T R A C T

Mining operations are potential sources of airborne particulate metal and metalloid contaminants through both direct smelter emissions and wind erosion of mine tailings. The warmer, drier conditions predicted for the Southwestern US by climate models may make contaminated atmospheric dust and aerosols increasingly important, due to potential deleterious effects on human health and ecology. Dust emissions and dispersion of dust and aerosol from the Iron King Mine tailings in Dewey-Humboldt, Arizona, a Superfund site, are currently being investigated through in situ field measurements and computational fluid dynamics modeling. These tailings are heavily contaminated with lead and arsenic. Using a computational fluid dynamics model, we model dust transport from the mine tailings to the surrounding region. The model includes gaseous plume dispersion to simulate the transport of the fine aerosols, while individual particle transport is used to track the trajectories of larger particles and to monitor their deposition locations. In order to improve the accuracy of the dust transport simulations, both regional topographical features and local weather patterns have been incorporated into the model simulations. Results show that local topography and wind velocity profiles are the major factors that control deposition.

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1. Introduction

The Iron King mine tailings site located in Dewey-Humboldt, Arizona is a potentially hazardous source of contaminated aerosols. The Iron King Mine tailings and nearby inactive smelter site were officially added to the Environmental Protection Agency (EPA) national priorities list in 2008. The smelter was operational from 1904 till 1969. It was used to extract lead, gold, silver, zinc and copper at different times. The 220,000 m^2 tailings were impounded on property (EPA, 2010). Sediment from these mine tailings has significantly elevated concentrations of both lead (up to 0.20 wt%), and arsenic (up to 0.24 wt%), amongst other toxic species. Additional tests of top soil from nearby sampling sites have shown elevated contaminant concentrations outside the boundaries of the Iron King Mine property. The spread of the contaminants is in part caused by aeolian dust transport from the mine tailings.

Aerosol and dust transport is a potentially dangerous mechanism for spreading contamination because of the high mobility of the smaller suspended particulate, especially for accumulation mode aerosols (<1 μm diameter). This particle size range is potentially hazardous to human health since they have the potential to deeply penetrate in the respiratory system. The relatively large diffusivity of these aerosols causes them to have an increased likelihood to deposit in the smaller airways such as the alveolar regions of the lungs (Hinds, 1999). Long-term exposure to these aerosol and dust particles may cause adverse health effects. Lifetime excess cancer risks for a similar arsenic contaminated copper mine located in Hayden, Arizona, was estimated to be 1 in 5000 by the Arizona Department of Health Services (Public Health Assessment, 2002), and up to 1 in 100, as estimated by EPA (Earth Justice, 2003).

In this work, we apply a Computational Fluids Dynamics (CFD) software tool, ANSYS FLUENT, to investigate aeolian transport and deposition rates of aerosols emitted from the Iron King Mine tailings to the surrounding region. The CFD is based on the turbulent Reynolds Averaged Navier-Stokes (RANS) equations. The complex topography of the terrain in the simulation area is included in the model. In addition, this CFD model can track both mixed gaseous species as well as predict the trajectories of individual...
particles (FLUENT Theory Guide). By utilizing these schemes within the CFD model, realistic simulations of aerosol and dust transport can be achieved.

2. Methodology

2.1. Site description

The Iron King Mine Tailings are located in north central Arizona at 34.500° north latitude and 112.253° west longitude with an average altitude of 1436 m above sea level. The topography of the land directly adjacent to the mine tailing impoundment is characterized by rolling hills with the Chaparral gulch bordering the northern edge of the mine property and the Galena gulch bordering the southern edge. Larger mountains are located slightly further away in the surrounding Prescott and Tonto National Forests. It is a semiarid region that receives an annual average of 480 mm of precipitation (NCDC, 2004).

The tailings impoundment rises vertically from the hillside with a rectangular shape and flat top. The tailings material has regions of reddish brown color and consists of gravelly sands and silty sands (Remedial Investigation Report, 2010). The tailings have a loam texture that consists of 34.7% sand, 44.8% silt, and 20.4% clay (Solís-Dominguez et al., 2012). The tailings are encrusted with white efflorescence deposits after rain storms.

2.2. Observations

Since December 2011, the Iron King Mine tailings have been equipped with two 10-m height towers fitted with meteorological instruments and dust monitors. Each tower has three anemometers located at 10 m, 3 m and 1 m heights. The north tower is equipped with all cup anemometers; while the south tower has a 3-D sonic anemometer located at 1 m above the ground. Additional meteorological instrumentation was used to measure wind direction, temperature, relative humidity, soil moisture and temperature. Three TSI DUSTTRAK II 8530 dust monitors were fitted to each tower at 10 m, 3 m, and 1 m heights. Each dust monitor utilizes an omnidirectional inlet that has a particle size cutoff of 27 μm aerodynamic diameter. Fig. 1 shows 4 days of observations taken during 2012, including the 3-m height wind speed and direction, as well as the 1-m height DUSTTRAK data. As expected, there is a noticeable diurnal pattern in both in wind speed and direction with wind speed increasing during the morning hours and turning to calm conditions in the early evening. The dust monitor data show a similar diurnal pattern with higher dust concentrations as the wind speeds increase during the day. Occasional peaks in dust concentration during the day are due to brief wind gusts or top soil perturbations.

The region’s climate is characterized by two windy and dry seasons during spring and fall. This is ideal for producing aeolian dust. In this study, we focus on the 2012 spring windy season which we define as being from April 1st to June 30th. The end of the spring windy season coincides with the start of the North American Monsoon when convective outbreaks can cause localized heavy rains that increase soil moisture, which inhibits dust emission.

The average wind rose of the 2012 spring windy season can be seen in Fig. 2. The wind rose was produced using the 10 m anemometer daylight observations (800–2000 h local time). The dominant wind direction for all wind speed observations are Southerly, Southwesterly, Southeasterly and Northerly. The northerly winds tend to be very low speed and occur during the overnight hours. When we take into consideration only wind speeds exceeding 4 m/s southerly wind direction dominates with 36% occurrence, while 85.2% of wind speeds that exceed 4 m/s come from one of the four wind directions: southeast, south, southwest or west. These observations were used in conjunction with the EPA AP 42 wind erosion model (EPA, 1988) to physically constrain the emission scheme that was used in the CFD species transport model.

2.3. Emission scheme

The emission model used to estimate wind erosion of the mine tailings comes from the EPA AP 42 report (EPA, 1988). The friction velocity is estimated from the near-surface logarithmic wind profile (Eq. (1)), where is the wind speed (m/s) at height , is the von Karman constant, and is the friction velocity (m/s) and is the roughness height (m). The friction velocity is a measure of the shear stress exerted on the surface, and when this shear stress

![Fig. 1. Time series of observations taken from the eddy flux tower located directly on the tailings from June 13th to June 17th, 2012. The top plot is the 1 m height dust concentrations with a 10 s sample frequency. The middle plot is a time series of the 3 m height wind speed with a 5 min sample frequency. The bottom plot is the corresponding wind direction. The x axis represents time in days with integer values corresponding to midnight.](http://dx.doi.org/10.1016/j.aeolia.2014.02.008)
becomes sufficiently large and exceeds a critical threshold, \( u^* \), erosion of surface particles may occur. Portable wind tunnel experiments conducted on a similar copper mine tailing impoundment also located in Arizona found \( u^* = 0.172 \text{ m/s} \) (Nicking and Gillies, 1986).

\[
U_{(z)} = \frac{u^*}{k} \ln \left( \frac{z}{z_0} \right)
\]  

The emission factor \( E \) (g/m² per event) of a surface is defined in Eq. (2), where \( k \) is the particle size multiplier, \( N \) is the number of disturbances per event and \( P_i \) is the erosion potential for the \( i \)th time period. The particle size multipliers for PM₃₂, PM₁₅, PM₁₀, and PM₂.₅ are 1.0, 0.6, 0.5, and 0.075, respectively (Cowherd, 2006).

\[
E = k \sum_{i=1}^{N} P_i
\]  

The erosion potential for each time interval is calculated using Eq. (3). In the case where \( u^* = u^*_0 \), the erosion potential is zero. The friction velocity for each time interval is calculated from observed “fastest mile” within the time period. Fastest mile is defined as the shortest time required for a single mile’s worth of distance to be advected past the anemometer.

\[
P = \begin{cases} 
58(u^* - u_i^*)^2 + 25(u^* - u_i^*) & \text{for } u^* > u_i^* \\
0 & \text{for } u^* \leq u_i^* 
\end{cases}
\]  

Frictional wind velocities were calculated using the fastest mile observations from the sonic anemometer located 1 m above the tailings because of its relatively high accuracy and since it requires less interpolation to the surface. An analysis of fastest mile friction velocities was conducted for one hour time intervals for the 2012 windy season. The resulting fastest mile friction velocities were used in the calculation of the erosion potential.

2.4. Model description

FLUENT 12.0 (distributed by ANSYS Corporation) has been used in a variety of studies involving aerosol transport, including flow over stockpiles (Diego et al., 2009; Badir and Harion, 2005); quantification of the effect of industrial buildings on the wind erosion of stock piles (Turpin and Harion, 2010a, 2010b); influence of the turbulent kinetic energy in the atmospheric boundary layer (Gorle et al., 2009); and deposition and clearance of particles in human airways (Anthony and Flynn, 2006). Our simulations utilize a turbulent flow field, species transport and discrete phase modeling.

2.4.1. Fluid flow

Fluid flow simulations used the \( k - \varepsilon \) turbulent kinetic model, a two equation method used to solve for the Reynolds stresses term of the Reynolds Average Navier-Stokes (RANS) equations of motion (Eq. (6)). The Reynolds stresses (Eq. (8)) are an apparent force that arises from the time averaging of the instantaneous Navier-Stokes equations and they are represented in terms of a turbulent viscosity (Eq. (6)).

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial}{\partial x_j} (\mu_l \frac{\partial u_i}{\partial x_j}) + \frac{\partial}{\partial x_j} (-\rho u_i' u_j')
\]

\[
-\rho u_i' u_j' = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( \rho k + \mu_t \frac{\partial u_i}{\partial x_i} \right) \delta_{ij}
\]

\[
\mu_t = \rho C_p \frac{k^2}{\varepsilon}
\]

The \( k - \varepsilon \) turbulence model introduces two transport equations to solve for the Reynolds stresses, one describes the transport of turbulent kinetic energy \( k \), and the other the turbulent energy dissipation rate \( \varepsilon \). Using an iterative process, the turbulent kinetic energy and turbulent dissipation rate of the eddies is constrained.

The fluid flow boundary conditions used for the outer walls of the domain include velocity inlets, pressure outlets, zero-shear boundaries, and no-slip boundaries. The ground around the tailings was initialized as a no-slip boundary with a surface roughness of 0.1 m and roughness constant of 0.5 m. The tailing walls were also defined as no-slip boundaries; however, they were assigned a significantly small surface roughness of 0.0014 m because of the lack of vegetation. The top of the domain was chosen as the limit of the atmospheric boundary layer (ABL) and was set as a zero-shear boundary, and walls parallel to the mean flow were setup as zero-shear boundaries as well. The velocity inlet boundaries where initialized with a user defined logarithmic wind profile, with a 7 m/s wind speed at 10 m height, and surface roughness of 0.1 m was used in the logarithmic wind profile. The velocity inlet’s magnitude and direction can be controlled, allowing for non-orthogonal flows relative to the velocity inlet boundary. The lateral boundaries are modified from zero-shear boundary to periodic boundaries for these non-orthogonal simulations. Pressure outlets oppose velocity inlets and are initialized with a constant static pressure of 0 Pa. The backflow direction is also appropriately specified for all pressure outlets. The inlet profile utilizes an isothermal temperature profile of 300 K. This will produce a stably stratified boundary layer and not include the effects of convective mixing.

For all the simulations, we specified uniform \( k \) and \( \varepsilon \) on inlet surfaces with values of 0.5 m²/s² and 0.1 m²/s³, respectively. This was done following a recommendation by the FLUENT user guide, which states that for “flows where accurate profiles of turbulent quantities are unknown, uniform specification of turbulent quantities at a boundary are reasonable” (FLUENT User Guide). In addition, we also explicitly created a very large model domain with a significant run-up distance which allows the \( k \) and \( \varepsilon \) to fully develop from the specified inlet boundary values.

2.4.2. Species transport (Eulerian approach)

The species transport model within FLUENT uses the convective-dispersion mass transport equation (Eq. (12)), where \( Y_i \) is the local species mass fraction, \( v \) is the velocity vector, \( J_i \) is the dispersive flux, \( R_i \) is the net rate of production via a chemical...
reaction ($R_i = 0$ in this case), and $S_i$ is the rate of creation from user defined sources (FLUENT Theory Guide). For the regional simulations, the mine tailings act as the source of the aerosols, $S$, utilizing a mass flow boundary condition. Considering that we are in a turbulent flow, the dispersive flux is obtained using Eq. (8), where $T$ is the temperature and $D_m$, $D_t$, $S_c$ are the mass diffusivity, thermal diffusivity and turbulent Schmidt number, respectively. The default turbulent Schmidt number used is 0.7, and the thermal diffusivity is calculated from the tracer species thermal conductivity (FLUENT User Guide).

$$
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{v} Y_i) = -\nabla \cdot (J_i + R_i) + S_i
$$

(7)

$$
J_i = -\left( \rho D_{\text{mm}} + \frac{\rho}{S_c} \right) \nabla Y_i - D_{\text{tr}} \nabla T
$$

(8)

In this work, properties of the species were used to represent 1 μm diameter aerosol particles, so that particle advection and dispersion is representative of an accumulation mode dust plume. It is reasonable to assume that 1 μm aerosols are likely to remain airborne after suspension because of their high mobility and relatively long gravitational settling time (settling velocity = $7.5 \times 10^{-5}$ m/s for particle density of 2.5 g/cm$^3$) relative to the simulated time period of 900 s.

For the species transport simulations, a user defined inert species was created to act as a tracer for accumulation mode aerosols. The mass diffusivity of the tracer species was set equal to the diffusivity calculated for a 1 μm particle, $2.77 \times 10^{-11}$ m$^2$/s, its viscosity was set as $1.72 \times 10^{-5}$ Pa s and its thermal conductivity at 0.0454 W/m K. The density is not defined for either the tracer species or the air because it is assumed they are homogenously mixed within each model element and that the fluid behaves as an incompressible ideal gas.

Species transport boundary conditions include inlet mass fraction, inlet mass flux, inlet direction specification and boundary species fraction specifications. A user defined function was used to define the inlet mass fraction and mass flux for the top of the tailings. Each simulation had an emission mass flux of $6.316 \times 10^{-3}$ g/m$^2$ s and the emission lasted for 30 s for total emission of 0.1895 g/m$^2$. The mass fraction boundary condition was set so 100% of the mass emitted was the tracer species and the emission occurred normal to the upper tailings boundary. A fixed zero mass fraction for the species tracer was used as the surrounding ground boundary condition, which implies complete capture of particles by the ground surface.

2.4.3. Discrete Phase Modeling (Lagrangian approach)

FLUENT’s Discrete Phase Modeling (DPM) tracks the trajectory of individual particles as they are injected into the flow. This Lagrangian approach requires that the tracked particles have a very small volume number fraction relative to the fluid volume mesh cells. However, the volume mass fraction of the tracked particles relative to the fluid can be quite large without significant consequences (FLUENT Theory Guide). The DPM particles were released into the same steady flow field with the identical wind profile and processing. Following the Matlab processing, the regional grey scale image was converted to a Non-Uniform Rational B-Spline (NURBS) surface utilizing Rhinoceros, a 3-D NURBS based modeling software (Rhinoceros 4.0, 2008). The tailings were added by hand to the topographic surface using both satellite imagery and GPS coordinates that were collected on the tailings. Once the tailings were added, the ground surface was enclosed by a bounding box. The 5 km regional domain, with the buffer region included, had a total horizontal and vertical extent of 6750 m × 6300 m × 3780 m. The fully formed model domain was then imported into the ANSYS Design Modeler (2013) that was used to mesh the domain. Utilizing the ANSYS Mesher, the model domain was meshed using a tetrahedral meshing method. The most refined mesh used in the simulations had 450,899 nodes, and 2,463,913 tetrahedral finite elements. The meshes were then exported for use in the FLUENT CFD model.

2.4.4. Mesh generation

Prior to running simulations with FLUENT, a model domain was created that was representative of the Dewey-Humboldt region, adjacent to the Iron King Mine tailings. To accurately represent the area of around the tailings, topographic data was gathered from the United States Geological Survey Seamless Data Server (USGS, 2012). Topographic data for a 25 km$^2$ area centered on the Iron King mine tailings that included portions of the adjacent town of Dewey-Humboldt was downloaded with a horizontal resolution of 1/3 arc second or about 10.3 m. The topographic data underwent processing in Matlab to create a grey scale image representative of the regional elevation. The image had a buffer round the outer boundary that adds a 514.5 m run-up that slopes the edge of the topographic region down to a fixed elevation for the entire edge. The reason for adding this buffer region is to create a fixed flat edge that represented a base surface for mesh generation and processing. Following the Matlab processing, the regional grey scale image was converted to a Non-Uniform Rational B-Spline (NURBS) surface utilizing Rhinoceros, a 3-D NURBS based modeling software (Rhinoceros 4.0, 2008). The tailings were added by hand to the topographic surface using both satellite imagery and GPS coordinates that were collected on the tailings. Once the tailings were added, the ground surface was enclosed by a bounding box. The 5 km regional domain, with the buffer region included, had a total horizontal and vertical extent of 6750 m × 6300 m × 3780 m. The fully formed model domain was then imported into the ANSYS Design Modeler (2013) that was used to mesh the domain. Utilizing the ANSYS Mesher, the model domain was meshed using a tetrahedral meshing method. The most refined mesh used in the simulations had 450,899 nodes, and 2,463,913 tetrahedral finite elements. The meshes were then exported for use in the FLUENT CFD model.

2.4.5. Mesh verification

Mesh verification is vitally important to maintain realism and repeatability of simulations. Two common techniques are used to
verify the mesh accuracy, which include iterative convergence and mesh independence. In order to verify mesh independence three different meshes were created. The grid refinement ratio is defined as the ratio of cell spacing for two separately sized meshes; for example, for meshes termed “fine” and “medium”, \( R_c = \Delta x_{fine} / \Delta x_{med} \). A grid refinement ratio of \((2)^{0.5}\) is recommended (Stern et al., 2001). However, due to computational limitations, a more reasonable refinement ratio of \((1.5)^{0.5}\) was used. The total number of nodes for the three meshes, coarse, medium and fine are 330,462, 390,778 and 450,899, respectively. The total number of tetrahedral finite elements for the three meshes are 1,796,275, 2,124,416 and 2,463,913.

The \( R_b \) value (Eq. (12)) was used to determine if there is mesh independence. It was calculated by first estimating error quantities from three different sized mesh simulations for each degree of freedom. There are six degrees of freedom needed to fully describe the turbulent fluid motion, turbulent kinetic energy \( (k) \), turbulent dissipation rate \( (\epsilon) \), static pressure, and the three components of the wind velocity vector. The error was calculated from Eq. (11), where \( e_{ij} \) is the difference in value for a single degree of freedom simulated on two differently sized meshes, \( j \) and \( k \) (Roache, 1998).

If the \( R_b \) values are less than one, the simulation is considered to be mesh-independent, indicating that an appropriate approximate solution has been found.

\[
|e| = \sqrt{\sum e_{ij}^2} \quad (11)
\]

\[
R_b = \frac{\|e_{med, fine}\|}{\|e_{course, mid}\|} \quad (12)
\]

Convergence of the iterative procedure employed in the solution of the differential equations is calculated using the \( L_2 \) error norm value, which is calculated by differencing a degree of freedom for two simulations using the same mesh but different global simulation error (GSE) tolerances. Eq. (13) shows how the \( L_2 \) error norm is calculated, where \( x_i \) and \( x_{i-1} \) are degrees of freedom, \( i \) represents the more strict GSE tolerance and \( i - 1 \) represents the less strict GSE simulation tolerance. A strict limit of 5 percent or better was used to verify iterative convergence (Roache, 1998).

\[
L_2 = \frac{\sum (x_i - x_{i-1})^{0.5}}{\sum (x_i)^{0.5}} \quad (13)
\]

3. Results and discussion

3.1. Simulation verification

Twenty locations within the model domain were randomly selected to verify mesh independence and iterative convergence. The locations were selected by dividing the model domain into 100 equal sized horizontal areas of which twenty were randomly selected for analysis. A vertical rake was used to sample the 6 degrees of freedom at 5 m intervals from the ground surface to a height of 3000 m. Fig. 3 shows the locations of the 20 random rakes within the model domain.

The finest mesh was used to determine iterative convergence. Three simulations were run using a GSE tolerance of \( 10^{-3} \), \( 10^{-4} \), and \( 10^{-5} \) for the six degrees of freedom. The \( L_2 \) iterative convergence parameter was then calculated for all six degrees of freedom using the three differently sized meshes (Table 1). Only the vertical component of the flow field did not meet the 5% criterion to show iterative convergence for the \((10^{-4} \text{ to } 10^{-5}) \) \( L_2 \) error norm test. An additional simulation was conducted using a GSE of \( 10^{-4} \) which resulted in a \( L_2 \) value of less than 1%, which meets the 5% criterion to show iterative convergence. The \( R_b \) values were calculated for the six degrees of freedom to show mesh independence and can also be seen in Table 1. The \( R_b \) values for all six degrees of freedom were less than 1, which confirms mesh independence. These verification tests indicate that the finest mesh used represents accurately the solution of the problem within the tolerance limits selected.

3.2. Species transport simulations

Four simulations where conducted using the principal wind directions measured on the tailings during the 2012 spring windy season: northwestward, northward, northeastward and eastward wind directions. First, wind velocity profiles were generated using a logarithmic wind profile that was initialized with a 7 m/s wind speed at 10 m height. This wind profile speed was selected from hourly fastest mile observations that had friction velocities large enough to produce wind erosion. The logarithmic profile was used as a boundary condition on the inlet surface, depending on wind direction. Fig. 4a shows wind velocity vectors calculated from the CFD simulation at the centroid value of the elements directly adjacent to the tailings and ground boundaries for an eastward wind direction. The color mapping of the vectors represents the velocity magnitude (m/s). Eddies and sudden changes in the velocity vectors can be identified downwind of significant surface elevation variations, including an adjacent open pit mine, located northwest of the tailings, and the tailing walls. Fig. 4b shows wind speed contours along an eastward orientated vertical plane. The western edge of tailings creates oscillations in the vertical wind speed profile that propagate downwind. The tailings also generate a sheltered region of low wind velocities downwind of the eastern edge where elevation significantly drops compared to the top of
the tailings. These results confirm the expected sensitivity of the CFD simulations to the local topography.

The species emission rate was calculated with the EPA AP42 wind erosion model using threshold friction velocities and sonic anemometer observations taken on the mine tailings from March 25, 2012 through June 26, 2012. The AP42 wind erosion model estimates that windy season average hourly emission for periods that generated soil erosion were 2.527, 1.516, 1.263, 0.190 g/m$^2$ for PM$_{30}$, PM$_{15}$, PM$_{10}$ and PM$_{2.5}$, respectively. PM$_{2.5}$ is the smallest particle size regime estimated by the AP 42 wind erosion model and has the largest mobility of all the classifications. PM$_{2.5}$ particles have long gravitational settling time and low rate of Brownian diffusion and can be transported long distances. For this reason the PM$_{2.5}$ erosion rate was used in the species transport simulations. A 30 s emission event is used in the simulations. The transient species transport simulations were conducted for 900 s with 4 s time steps. The four second time step was selected to minimize the computational cost of the simulations while maintaining temporal resolution that allows us to observe the development of the species tracer plumes.

**Fig. 4a.** Sample results from the FLUENT CFD computations: Wind velocity vectors at the centroid of the elements directly adjacent to the tailings and ground boundaries for an eastward (X direction) simulated wind direction. This wind simulation was initialized with a 7 m/s at 10 m height logarithmic wind profile along the eastern boundary. The color mapping of the vectors represents the wind magnitude (m/s). Eddies can be identified downwind of the tailings where changes in elevation occur, and near the open pit mine, located northwest of the tailings. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

**Fig. 4b.** Sample results from the FLUENT CFD computations: Wind speed contours along an eastward orientated vertical plane for an eastward (X direction) simulated wind direction. This wind simulation was initialized with a 7 m/s at 10 m height logarithmic wind profile along the eastern boundary. The color mapping represents the wind magnitude (m/s). The tailings effects on the wind field can be seen along western edge of tailings where the increase in elevation creates oscillations downwind. The tailings also generate a sheltered region of low wind velocities downwind of the eastern edge. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
a distance of 2500 m. For each vertical rake the deposition rate was calculated using Fick’s law. Fig. 6 shows the peak tracer species mass fraction profiles for the northward simulation at 500 m, 1000 m, 1500 m, 2000 m and 2500 m downstream from the center of the tailings. Peak mass fraction time step is defined as being the time step with the highest cumulative mass fractions within the profile for the respective location. Deposition rates were calculated at each rake location for each time step. Fig. 7 shows the time series of deposition rates calculated for the northward simulation at the 500, 1000, 1500, 2000, 2500 m sample locations. Deposition rates were calculated for each 4 s time step using Fick’s first law of diffusion.

Further investigation of the topographic effects on species tracer deposition was conducted by looking at the elevation and upslope information for the rake sample locations. Table 3 shows the elevation at the rake sample points and Table 4 presents the topographic upslope of the rake sample points. The topography of the terrain along the investigated directions is shown in Fig. 8. The elevation information from Table 3 allows us to see if there is a correlation between the elevation and deposition totals from the simulations. The rake locations that observed increasing total depositions as the distance from the tailings increased included: the northwestward 1000 m and 1500 m rakes, northward 500 m and 1000 m rakes, northeastward 1500 m and 2000 m rakes and eastward 2000 m rake.

This is caused by the topography. In general, ground elevation increases with distance from the tailings in the northwestward direction, causing increased species concentrations near to the ground as the species is forced up the topographic slope. The elevation tends to decrease away from the tailings for the other three wind directions, which would suggest the total deposition to be smaller than the northwestward wind direction. There are also seeming anomalies within each individual simulation; for example, the 1000 m rake for northward simulation, has a larger total deposition than the 500 m rake. This increased deposition at 1000 m is caused by the vertical rake being located on the upslope side of a hill, which serves as an enhanced interception surface, thus increasing deposition. The opposite argument can be made for the downslope side of the regional topography.

Integration of the time series of deposition rates at each rake location gives the total deposition for each simulation. The cumulative deposition results for the four simulated wind directions are presented in Table 2. It is noticeable that that the total deposition values for the rakes do not necessarily decrease with distance from the tailings. The northwestward wind simulation has the largest total deposition of the tracer species for all five of the downwind rake locations when compared to the other directional simulations.
eastward 1000 m and 1500 m rakes. There appears to be little correlation between the rakes elevation and total deposition because the northwestward 1000 m and 1500 m rakes have about a 29 m decrease in elevation between them and the northward 500 m and 1000 m rakes have an increase of about 26 m between the sample rakes locations. The last two seemingly anomalous rake pairs, northeastward 1500 m and 2000 m rakes and eastward 1000 m and 1500 m rakes, have small elevation differences between the rake locations on the order of 5.5–7 m. For these simulations, there appears to be no correlation between higher deposition rates and elevation for the species transport method. Nevertheless, it topographic upslope of the landscape may shed light on the observed trends. The upslope of the ground at the rake sample locations is given in Table 4. The northwestward 1500–2000 m, northward 500–1000 m, and eastward 1000 m and 1500 m rakes, have small elevation differences between the rake locations on the order of 5.5–7 m. For these simulations, there appears to be no correlation between higher deposition rates and elevation for the species transport method. Nevertheless, it topographic upslope of the landscape may shed light on the observed trends. The upslope of the ground at the rake sample locations is given in Table 4. The northwestward 1000–1500 m, northward 500–1000 m, and eastward 1000–1500 m seemingly anomalous sample locations have significant increases in upslope values, which are associated with the increase in total deposition. Topography, specifically the upslope degree of the ground surface, seems to play a major role in the spatial variability of species tracer deposition.

3.3. Seasonal deposition estimation

Seasonal deposition rates were estimated utilizing the species simulations and the observed seasonal wind data. The analysis of the windy season data found that 40.2% of the hourly fastest mile friction velocities, from the spring windy season, were sufficient to produce wind erosion according to the EPA AP42 wind erosion model. By scaling the single simulation results by the number of events predicted by the AP 42 wind erosion model for that specific wind direction, we can estimate of the total seasonal PM$_{2.5}$ deposition for all the sample rake locations and for each wind direction simulation. Table 5 shows the 2012 windy season PM$_{2.5}$ deposition as estimated by using the AP42 wind erosion model and the FLU-ENT species transport model. Although these deposition values may seem quite small, they represent only the smallest size fraction aerosols, <2.5 μm diameter.

3.4. DPM simulations

To further investigate the spatial variations observed in the species transport simulations, we conducted a series of DPM simulations. Each DPM simulation emits 4080 particles (2.5 μm in diameter) from the tailings into the mean flow and one simulation is performed for each principal wind direction. Most of the injected particles tended to deposit very near to the tailings because of swirling winds that arise from the tailings having an elevated position relative to the surrounding ground. However, some particles managed to be transported further downwind and some, less than 5%, escaped the whole simulation domain; that is, were

<table>
<thead>
<tr>
<th>Distance from tailings (m)</th>
<th>500</th>
<th>1000</th>
<th>1500</th>
<th>2000</th>
<th>2500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Northwestward deposition (pg/m$^2$)</td>
<td>73.7</td>
<td>19.3</td>
<td>20.0</td>
<td>18.6</td>
<td>9.13</td>
</tr>
<tr>
<td>Northward deposition (pg/m$^2$)</td>
<td>17.7</td>
<td>17.1</td>
<td>8.06</td>
<td>6.69</td>
<td>6.20</td>
</tr>
<tr>
<td>Northeastward deposition (pg/m$^2$)</td>
<td>7.39</td>
<td>4.84</td>
<td>3.77</td>
<td>4.13</td>
<td>3.91</td>
</tr>
<tr>
<td>Eastward deposition (pg/m$^2$)</td>
<td>12.6</td>
<td>5.15</td>
<td>6.98</td>
<td>3.61</td>
<td>2.82</td>
</tr>
</tbody>
</table>

Fig. 8. Topographic elevation (in m) of the terrain following the indicated directions from the tailings. Specific values for the sampled locations (marked with asterisks) are shown in Table 3.

Table 4
Topographic upslope of the 20 sampling locations used in tracer species simulations. Positive values indicate increase in elevation along the specified direction.

<table>
<thead>
<tr>
<th>Distance from tailings (m)</th>
<th>500</th>
<th>1000</th>
<th>1500</th>
<th>2000</th>
<th>2500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Northwestward upslope (m/m)</td>
<td>−0.0246</td>
<td>−0.1472</td>
<td>−0.0141</td>
<td>0.0025</td>
<td>0.0345</td>
</tr>
<tr>
<td>Northward upslope (m/m)</td>
<td>−0.1553</td>
<td>0.2023</td>
<td>0.2707</td>
<td>0.0839</td>
<td>0.2131</td>
</tr>
<tr>
<td>Northeastward upslope (m/m)</td>
<td>−0.0445</td>
<td>0.1377</td>
<td>−0.1011</td>
<td>−0.1187</td>
<td>0.1694</td>
</tr>
<tr>
<td>Eastward upslope (m/m)</td>
<td>−0.1568</td>
<td>−0.0225</td>
<td>0.0199</td>
<td>−0.0381</td>
<td>−0.0485</td>
</tr>
</tbody>
</table>

Table 5
Estimates of total PM$_{2.5}$ deposition for the 2012 spring windy season.
transported a distance of more than 3 km. The 5% escaped particle fraction is an underestimate because the thermodynamically stable boundary layer does not allow for vertical mixing that would be associated with a convective boundary layer typical of a clear day.

To study the effect of upslope on particle deposition, Fig. 9 shows a distributed plot of the upslope value at the point where each particle deposits vs. the distance from the tailings where the particle deposited. From this plot it can be seen that once a particle gets far enough away from the tailings (>500 m), it tends to deposit on positive upslope regions. Even though the mean value of the upslope is positive for all particle deposition locations, which would be consistent with an upslope bias for deposition, the standard deviation is so large that a general quantitative conclusion is not possible. However, the average and standard deviations of the upslope value for particles that settled more than 500 m away from the tailings show that particles that escape the swirling eddies created by the tailings topography preferentially deposit in areas of topographic upslope. Additional sensitivity tests occurred that looked at the effect that injection location and injection velocities have on deposition location. Results showed that variations of injection locations and injection velocity produced minimal effects on the deposition location. These DPM results reinforce the results gathered from the species transport simulations, which showed that topography plays a major role in the deposition of fugitive aerosols from the Iron King Mine tailings.

4. Concluding remarks

Utilizing in situ observations and the EPA AP 42 wind erosion model, we were able to estimate wind erosion and local deposition of dust and aerosol from a chemically contaminated mine tailings site. The model coupled three-dimensional velocity fields obtained from CFD calculations employing the $k - \varepsilon$ turbulence model with either the species transport equation (for particles of size less than 1 μm diameter) or the equations of motion for individual particles (for 2.5 μm diameter particles). The simulations showed significant heterogeneity in deposition patterns in the regions surrounding the tailings, with topographic upslope and wind velocity fields playing a major role in the deposition variability. These results show that future predictions of deposition from this and similar sites must rely on accurate descriptions of wind velocity and surrounding terrain.

The calculations presented in this work are preliminary in nature. Further work will be done towards validating the accuracy of the emissions model, which relies on empiricisms that may not be applicable to a specific location. In addition, processes such as salitation and particle creep have not been considered in detail, and they may play an important role in total emissions. Despite the limitations, the results give an estimate of the relative strength of deposition patterns in the region surrounding the tailings which, in turn, can be translated into deposition patterns of contaminants such as lead and arsenic, present at relatively high concentrations in the top soil of the tailings.

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References


Rhinoceros Release 4.0, Robert McNeel & Associates.


