**Analysis: Dioguardi Model**

**Method of running model**

1. Read in Van Melkebeke dataset.
2. Calculate additional required variables:
   1. Surface area of equivalent sphere
   2. mP surface area
   3. Equivalent spherical volume
   4. mP mass
   5. Corey Shape factor
   6. Relative density
   7. Projected area of volume equivalent sphere
3. Set initial velocity at time t=0.
4. For each particle:
   1. Calculate the Aschenbrenner shape factor .
   2. For each time step:
      1. Calculate the Reynolds number
      2. Calculate the drag coefficient using Dioguardi’s model:
      3. Calculate the drag force
         1. Note that two cases are used. In the first, S is taken as the mP surface area, as calculated above. In the second case, S is taken as the Zhang’s projected area above.
      4. Calculate the gravitational force
      5. Calculate the buoyant force
      6. Calculate the net force acting on the mP:
      7. Calculate the settling velocity at the next time step
      8. Calculate the distance travelled during the timestep
      9. Add the distance travelled to the total distance travelled
      10. Calculate the acceleration
          1. If acceleration>0.01m/s2, step forward one timestep and restart the loop at point b above.
          2. If acceleration<0.01m/s2, terminal settling velocity has been obtained. Stop the calculation and save the final values of time, timestep, settling velocity, distance, total distance, Re and Cd.
5. For each output file:
   1. Calculate the average error:
   2. Calculate the root mean squared error:

Chart, scatter chart

Description automatically generated**Results and discussion**

Considering all the datapoints, the model is better at predicting the particle settling velocity when the projection area of the equivalent sphere is used as the effective area rather than the particle surface area.

Chart, scatter chart

Description automatically generatedWhen the particle surface area is used, the model tends to underestimate the terminal settling velocity. In contrast, when the projection area is used the model provides a close estimate of the terminal settling velocity, with a gradient of 1.0.649. This straight-line equation also explains the variance in the data well, with an r2 value of 0.9425.

Considering only the mPs with fragment morphology, the model performs better when using the projection area of the volume equivalent sphere as the effective area, rather than the surface area.

Chart, scatter chart

Description automatically generatedWhen the particle surface area is used, the model underestimates the terminal settling velocity of all the fragments. When the projection area of the volume equivalent sphere is used, the model provides a close estimate of the terminal settling velocity of the fragments, with a slight overestimation.

Considering only the fibres, the model performs better when projected area of the volume equivalent sphere than when the particle surface area is used.

Chart, scatter chart

Description automatically generatedWhen the particle surface area is used the model underestimates the terminal settling velocity of all the fibres. The model also tends to underestimate the terminal settling velocity of fibres when the projection area of the volume equivalent sphere is used.

Considering only the films, the model performance is vastly improved by using the projection area of the volume equivalent sphere as the effective area, rather than the particle surface area.

When the particle surface area is used as the effective area, the model underestimates the terminal settling velocity of all the film particles. The model very closely predicts the terminal settling velocity of the film particles when the projection area of the volume equivalent sphere is used, with a gradient of 0.9678.

Chart, scatter chart

Description automatically generated

The calculated Cd is similar to the measured Cd in both cases. The calculated Cd and Re overlaps most with the measured Cd and Re when the projected area of the equivalent sphere is used.

Chart, scatter chart

Description automatically generated

In both set-ups it appears that the model overestimates the drag coefficient of the fibres.

Chart, scatter chart

Description automatically generated

The particle terminal settling velocity increases as particle size increases. The model appears to predict the terminal settling velocity of the particles more accurately when the projection area of the volume equivalent sphere is used. When the particle surface area is used the model underestimates the terminal settling velocity.

Chart, scatter chart

Description automatically generated

The fragments have the largest equivalent spherical diameter. It appears that when the projection area of the volume equivalent sphere is used the model closely estimates the settling velocity of film particles and fibre particles but is slightly less accurate in predicting the settling velocity of fragments.

Chart, scatter chart

Description automatically generated

The fragment mPs have the highest CSF.

Summary table:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Effective Area** | **Shape** | **m** | **R2** | **AE (%)** | **RMSE (%)** |
| SA | All | 0.3634 | 0.8604 | 75.46 | 7.64 |
| SA | Fragment | 0.3810 | 0.8610 | 67.63 | 6.83 |
| SA | Fibre | 0.1738 | 0.3931 | 83.86 | 8.42 |
| SA | Film | 0.1496 | 0.7727 | 86.90 | 8.70 |
| Projected area | All | 1.0649 | 0.9425 | 15.82 | 2.13 |
| Projected area | Fragment | 1.0918 | 0.9485 | 13.87 | 1.67 |
| Projected area | Fibre | 0.6598 | 0.3995 | 36.45 | 4.26 |
| Projected area | Film | 0.9678 | 0.9373 | 9.41 | 1.11 |

Based on the values of m, the model performs vastly better when the projection area of the volume equivalent sphere is used. In this case, it is also most accurate at predicting the settling velocity of films, which is unexpected since the model is formulated for ash particles and films are unnatural shapes. The smallest average error occurs for films when the particle surface area is used.

**Conclusion**

* Model performs best when projected area of volume equivalent sphere is used.
* Model performs better for films, followed by fragments. Performance is lowest for fibres.