**Analysis: Stokes 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 the timestep value.
4. Set initial velocity at time t=0.
5. For each particle:
   1. For each time step:
      1. Calculate the Reynolds number
      2. Calculate the drag coefficient using Stokes 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.
6. For each output file:
   1. Calculate the average error:
   2. Calculate the root mean squared error:

**Results and discussion**

Chart, line chart

Description automatically generated

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

In both cases, the model overestimates the terminal settling velocity. This occurs since Stokes model assumes that the particles are spherical and therefore in reality the particles will experience a larger drag force, leading to a lower settling velocity.

Chart, line chart

Description automatically generated

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

In both cases the model overestimates the terminal settling velocity of the fragments.

Chart, line chart

Description automatically generated

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

When the particle surface area is used the model tends to overestimate the terminal settling velocity of the fibres. The model overestimates the terminal settling velocity of all the fibres when the projection area of the volume equivalent sphere is used.

Chart, scatter chart

Description automatically generated

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

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 closely overestimates the terminal settling velocity of the film particles when the projection area of the volume equivalent sphere is used.

Chart, scatter chart

Description automatically generated

The calculated Cd and Re is most similar to the measured Cd and Re when the particle surface area is used.

Chart, scatter chart

Description automatically generated

When the projected area is used, the Reynolds number is higher since the terminal settling velocity is vastly overestimated.

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 surface area is used. When the projection area is used there is a regular relationship between the particle size and terminal settling velocity.

Chart, scatter chart

Description automatically generated

The fragments have the largest equivalent spherical diameter.

Chart, scatter chart

Description automatically generated

The fragment mPs have the highest CSF.

Summary table:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Effective Area** | **Shape** | **m** | **R2** | **AE (%)** | **RMSE (%)** |
| SA | All | 2.0199 | 0.8120 | 59.88 | 7.34 |
| SA | Fragment | 2.1014 | 0.8006 | 61.24 | 7.99 |
| SA | Fibre | 1.4162 | 0.5120 | 46.01 | 5.87 |
| SA | Film | 0.4880 | 0.6390 | 64.08 | 6.62 |
| Projected area | All | 13.7993 | 0.8054 | 1171.19 | 128.09 |
| Projected area | Fragment | 13.5730 | 0.7841 | 1054.98 | 115.22 |
| Projected area | Fibre | 18.0044 | 0.3663 | 1709.76 | 177.83 |
| Projected area | Film | 13.0216 | 0.5950 | 1134.33 | 122.72 |

Based on the values of m, the model performs better when the particle surface area is used. In this case, it is also most accurate at predicting the settling velocity of fibres, followed by films. The average error and RMSE is lowest for Fibres when the surface area is used.

**Conclusion**

* Model performs better when surface area is used.
* When surface area is used, the model performs best for fibres followed by films and fragments.