**Analysis: Zhang 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
   8. Zhang’s estimated volume
   9. Zhang’s volume equivalent spherical diameter
   10. Zhang’s equivalent diameter based on ProjAESD
   11. Zhang’s projected area
   12. Zhang’s estimated mass
3. Set initial velocity at 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 Zhang’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 particle surface area is used as the effective area rather than the projection area estimated from the maximum cross-sectional 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 tends to overestimate the terminal settling velocity

Considering only the mPs with fragment morphology, the model performs better when using the particle surface area as the effective area, rather than the projection area estimated using the maximum cross-sectional area.

When the particle surface area is used, the model tends to slightly underestimate the terminal settling velocity. When the projection area estimated from the maximum cross-sectional area is used, the model tends to overestimate the terminal settling velocity of fragments.

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Considering only the fibres, the model performs better when using the particle surface area as the effective area, rather than the projection area estimated using the maximum cross-sectional area.

When the particle surface area is used the model tends to slightly underestimate the terminal settling velocity. However, the linear model cannot describe the variance in the data very well, with the points lying far from the line. When projection area estimated from the maximum cross-sectional area is used the model tends to overestimate the terminal settling velocity of the fibres.

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Considering only the films, the model performs better when using the particle surface area as the effective area, rather than the projection area estimated using the maximum cross-sectional area.

When the particle surface area is used as the effective area, the model tends to slightly underestimate the terminal settling velocity of the film particles. When the projection area is estimated as the maximum cross-sectional area the model tends to overestimate the terminal settling velocity of the particles.

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The calculated Cd tends to be lower than the measured Cd but follows the same general trend whereby Cd decreases as Re increases.

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The film particles have the lowest drag coefficient at the same Re whilst the fibres have the highest drag coefficient.

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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 particle surface area is used compared to the maximum cross-sectional area.

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The fragments have the largest equivalent spherical diameter.

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The fragment mPs have the highest CSF.

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The ASF appears to be an appropriate shape factor to distinguish between the mP morphologies, with films having the lowest ASF and fibers having the highest ASF.

Summary table:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Effective Area** | **Shape** | **m** | **R2** | **AE (%)** | **RMSE (%)** |
| SA | All | 0.8613 | 0.8905 | 23.48 | 2.78 |
| SA | Fragment | 0.8603 | 0.8572 | 26.11 | 3.02 |
| SA | Fibre | 0.8674 | 0.6044 | 19.14 | 2.39 |
| SA | Film | 0.8837 | 0.7890 | 20.40 | 2.42 |
| Projected area | All | 1.5461 | 0.9004 | 33.80 | 4.38 |
| Projected area | Fragment | 1.5635 | 0.8787 | 35.00 | 4.65 |
| Projected area | Fibre | 1.3692 | 0.6413 | 39.26 | 4.51 |
| Projected area | Film | 1.3139 | 0.7919 | 28.66 | 3.72 |

Based on the values of m, the model performs best when the particle surface area is used. It also is most accurate at predicting the settling velocity of films, which is unexpected since it is formulated primarily for fibres. The smallest average error occurs for fibres when the particle surface area is used.

**Conclusion**

* Model performs best for films.
* Model performs better when the particle surface area is used.
* ASF is an appropriate shape factor to differentiate between fragments, films and fibres.