**Overall table of results:**

**Key:** \_4\_ = Best, \_3\_ = Second best, \_2\_= Third best, \_1\_ = Fourth best.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Model** | | **Implicit Models** | | | | | | | | **Explicit Models** | | |
| **Stokes (1851) Proj** | **Stokes (1851) SA** | **Dioguardi et al. (2018) Proj** | **Dioguardi et al. (2018) SA** | **Bagheri and Bonadonna (2016) Proj** | **Bagheri and Bonadonna (2016) SA** | **Zhang and Choi (2021) Proj** | **Zhang and Choi (2021) SA** | **Dietrich (1982)** | **Francalanci et al. (2021)** | **Yu et al. (2022)** |
| **Overall** | **m** | 13.80 | 2.02 | 1.06 | 0.36 | 1.08 | 0.35 | 1.55 | 0.86 | 0.92 | 1.88 | 1.08 |
| **|1-m|** | **12.80** | **1.02** | **0.06** | **0.64** | **0.08** | **0.65** | **0.55** | **0.14** | **0.08** | **0.88** | **0.08** |
| **r2** | 0.81 | 0.81 | 0.94 | 0.86 | 0.96 | 0.87 | 0.90 | 0.89 | 0.80 | 0.89 | 0.96 |
| **AE** | 1171.19 | 11.18 | -1.47 | -75.46 | 8.97 | -77.68 | 28.44 | -18.60 | -14.70 | 128.31 | 6.21 |
| **|AE|** | 1171.19 | 59.88 | 15.82 | 75.46 | 13.95 | 77.68 | 33.80 | 23.48 | 19.43 | 128.31 | 14.81 |
| **RMSE** | 1280.87 | 73.43 | 21.28 | 76.41 | 20.56 | 78.53 | 43.81 | 27.75 | 28.46 | 151.07 | 22.67 |
| **Fragment** | **m** | 13.57 | 2.10 | 1.09 | 0.38 | 1.07 | 0.36 | 1.56 | 0.86 | N/A | 1.83 | 1.08 |
| **|1-m|** | **12.57** | **1.10** | **0.09** | **0.62** | **0.07** | **0.64** | **0.56** | **0.14** | **N/A** | **0.83** | **0.08** |
| **r2** | 0.78 | 0.80 | 0.95 | 0.86 | 0.97 | 0.87 | 0.88 | 0.86 | N/A | 0.93 | 0.96 |
| **AE** | 1054.98 | 43.78 | 7.27 | -67.63 | 3.21 | -71.66 | 28.42 | -21.13 | N/A | 95.48 | 3.54 |
| **|AE|** | 1054.98 | 61.24 | 13.87 | 67.63 | 10.51 | 71.66 | 35.00 | 26.11 | N/A | 95.48 | 11.55 |
| **RMSE** | 1152.18 | 79.87 | 16.69 | 68.30 | 13.27 | 72.20 | 46.49 | 30.20 | N/A | 102.56 | 14.95 |
| **Fibres** | **m** | 18.00 | 1.42 | 0.66 | 0.17 | 1.30 | 0.26 | 1.37 | 0.87 | N/A | 2.58 | 1.27 |
| **|1-m|** | **17.00** | **0.42** | **0.34** | **0.83** | **0.30** | **0.74** | **0.37** | **0.13** | **N/A** | **1.58** | **0.27** |
| **r2** | 0.37 | 0.51 | 0.40 | 0.39 | 0.58 | 0.46 | 0.64 | 0.60 | N/A | -0.02 | 0.47 |
| **AE** | 1709.76 | 31.30 | -35.23 | -83.86 | 32.75 | -75.31 | 34.90 | -14.33 | N/A | 176.13 | 30.63 |
| **|AE|** | 1783.46 | 31.36 | 36.45 | 83.86 | 34.59 | 75.31 | 39.26 | 19.14 | N/A | 176.13 | 33.18 |
| **RMSE** | 1778.34 | 58.75 | 42.56 | 84.17 | 42.47 | 75.93 | 45.06 | 23.89 | N/A | 193.36 | 43.23 |
| **Films** | **m** | 13.02 | 0.49 | 0.97 | 0.15 | 1.05 | 0.11 | 1.31 | 0.88 | N/A | 2.38 | 0.95 |
| **|1-m|** | **12.02** | **0.51** | **0.03** | **0.85** | **0.05** | **0.89** | **0.31** | **0.12** | **N/A** | **1.38** | **0.05** |
| **r2** | 0.60 | 0.64 | 0.94 | 0.77 | 0.90 | 0.72 | 0.79 | 0.79 | N/A | -0.06 | 0.71 |
| **AE** | 1134.33 | -64.08 | -2.07 | -86.90 | 8.60 | -90.92 | 25.24 | -15.68 | N/A | 170.05 | -0.68 |
| **|AE|** | 1134.33 | 64.08 | 9.41 | 86.90 | 10.51 | 90.92 | 28.66 | 20.40 | N/A | 170.05 | 12.14 |
| **RMSE** | 1227.18 | 66.25 | 11.05 | 86.97 | 15.02 | 90.98 | 37.16 | 24.22 | N/A | 200.36 | 20.42 |
|  | **Sum of |1-m|** | 54.40 | 3.05 | 0.53 | 2.93 | 0.50 | 2.92 | 1.79 | 0.53 | N/A | 4.67 | **0.49** |

Best performing model overall: Dioguardi Proj, Best performing model for fragments: Bagheri Proj

Zhang and Choi specify that their model should be used with the projection area, not surface area.

Dietrich model not considered further as it is not valid for all particles in the dataset considered.

Best performing model for fibres: Yu et al, Best performing model for films: Dioguardi Proj

The implicit models were tested using both the particle surface area, calculated from the properties given in the dataset in Van Melkebeke et al. (2020), and the projected area of the volume equivalent sphere as the effective area during the drag force calculation. The models by Dioguardi and Bagheri were formulated using the projected area and as a result performed poorly when the surface area was used. Therefore, only the output obtained using the estimated projection area is presented in this paper. Stokes’ model produced very inaccurate results when the estimated projection area was used as the effective area, with an overall average error of 1171%, compared to an overall average error of 11.18% when the surface area was used. This may have occurred due to the order of magnitude difference between the projected area and the surface area. According to (Gregory, 2005) the simplest procedure is to use the projected area.

**Results:** Gradient of fitted line:

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Model** | **Overall** | | **Fragments only** | | **Films only** | | **Fibres only** | |
| **m** | **r2** | **m** | **r2** | **m** | **r2** | **m** | **r2** |
| Stokes (1851) Proj | 13.80 | 0.81 | 13.57 | 0.78 | 13.02 | 0.60 | 18.00 | 0.37 |
| Stokes (1851) SA | 2.02 | 0.81 | 2.10 | 0.80 | 0.49 | 0.64 | 1.42 | 0.51 |
| Dioguardi et al. (2018) Proj | **1.06** | 0.94 | 1.09 | 0.95 | **0.97** | 0.94 | 0.66 | 0.40 |
| Dioguardi et al. (2018) SA | 0.36 | 0.86 | 0.38 | 0.86 | 0.15 | 0.77 | 0.17 | 0.39 |
| Bagheri and Bonadonna (2016) Proj | 1.08 | 0.96 | **1.07** | 0.97 | 1.05 | 0.90 | 1.30 | 0.58 |
| Bagheri and Bonadonna (2016) SA | 0.35 | 0.87 | 0.36 | 0.87 | 0.11 | 0.72 | 0.26 | 0.46 |
| Zhang and Choi (2021) Proj | 1.55 | 0.90 | 1.56 | 0.88 | 1.31 | 0.79 | 1.37 | 0.64 |
| Zhang and Choi (2021) SA | 0.86 | 0.89 | 0.86 | 0.86 | 0.88 | 0.79 | **0.87** | 0.60 |
| Dietrich (1982) | 0.92 | 0.80 | N/A | N/A | N/A | N/A | N/A | N/A |
| Francalanci et al. (2021) | 1.88 | 0.89 | 1.83 | 0.93 | 2.38 | -0.06 | 2.58 | -0.02 |
| Yu et al. (2022) | 1.08 | 0.96 | 1.08 | 0.96 | 0.95 | 0.71 | 1.27 | 0.47 |

Chart, scatter chart

Description automatically generated

* Considering all the shapes together, the model by Dioguardi et al (2018) using the projected area is most accurate at predicting the measured terminal settling velocity, with m=1.06. This is very closely followed by Bagheri and Bonadonna (2016) and Yu et al (2022) which both similarly over-predict the measured values with m=1.08 and Dietrich (1982) which underestimates the data to the same degree with m=0.92.
* Considering only the particles with a fragment morphology, the model by Bagheri and Bonnadonna (2016) using the projected area is most accurate at predicting the measured terminal settling velocity, with m=1.07. The model by Yu et al (2022) provides a very similar level of accuracy, with m=1.08. The model by Dioguardi et al (2018) using the projected area provides m=1.09.
* Considering only the particles with film morphology, Dioguardi et al (2018) using the projected area provides the most accurate prediction of the terminal settling velocity, with m=0.97, followed by Yu et al (2022) with m=0.95 and Bagheri and Bonnadonna (2016) using the projected area with m=1.05.
* Considering only the particles with fibrous morphology, the model by Zhang and Choi (2021) is most accurate at replicating the measured terminal settling velocity of fibres, with m=0.87. Whilst Yu et al (2022), Bagheri and Bonnadonna (2016) and Dioguardi et al (2018) performed well for the other morphologies they were noticeably less accurate at predicting the terminal settling velocity of fibrous fibres, with values of m=1.27, m=1.30 and m=0.66 respectively.
  + It should be noted that the performance of Zhang and Choi (2021) model when using the particle surface area as the effective area in the calculation of the drag force was better than when using the surface projected area that was suggested in the paper whereby they estimated the particle volume by approximating to a cuboid, used this volume to find the equivalent spherical diameter and used the ESD to find the projected area of the equivalent sphere. Also note that the performance of the model by Zhang and Choi (2021) is consistent in predicting the terminal settling velocity for all of the shapes, with m ranging from 0.86 to 0.88.
* Yu overestimates fragments and fibres, underestimates films.
* Bagheri overestimates all shapes.
* Dioguardi overestimates fragments and underestimates films and fibres.
* **Overall, Dioguardi et al (2018) using projected area, Bagheri and Bonadonna (2016) using the projected area and Yu et al (2022) are the best performing models, with very similar high performance for fragments and films and reduced performance for fibres. The model by Yu et al (2022) has a slightly better performance for fibres than the other models and as an implicit model is more computationally efficient than the explicit models which require many iterations before the terminal settling velocity can be obtained. Therefore, this model would be most appropriate for use in the transport modelling context.**

**Results:** Error

|  |  |  |  |
| --- | --- | --- | --- |
| **Model** | **Overall** | | |
| **AE** | **|AE|** | **RMSE** |
| Bagheri and Bonadonna (2016) Proj | 8.97 | **13.95** | **20.56** |
| Yu et al. (2022) | 6.21 | 14.81 | 22.67 |
| Dioguardi et al. (2018) Proj | **-1.47** | 15.82 | 21.28 |
| Dietrich (1982) | -14.70 | 19.43 | 28.46 |
| Zhang and Choi (2021) SA | -18.60 | 23.48 | 27.75 |
| Zhang and Choi (2021) Proj | 28.44 | 33.80 | 43.81 |
| Stokes (1851) SA | 11.18 | 59.88 | 73.43 |
| Dioguardi et al. (2018) SA | -75.46 | 75.46 | 76.41 |
| Bagheri and Bonadonna (2016) SA | -77.68 | 77.68 | 78.53 |
| Francalanci et al. (2021) | 128.31 | 128.31 | 151.07 |
| Stokes (1851) Proj | 1171.19 | 1171.19 | 1280.87 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Model** | **Fragments only** | | | **Films only** | | | **Fibres only** | | |
| **AE** | **|AE|** | **RMSE** | **AE** | **|AE|** | **RMSE** | **AE** | **|AE|** | **RMSE** |
| Bagheri and Bonadonna (2016) Proj | **3.21** | **10.51** | **13.27** | 8.60 | 10.51 | 15.02 | 32.75 | 34.59 | 42.47 |
| Yu et al. (2022) | 3.54 | 11.55 | 14.95 | **-0.68** | 12.14 | 20.42 | 30.63 | 33.18 | 43.23 |
| Dioguardi et al. (2018) Proj | 7.27 | 13.87 | 16.69 | -2.07 | **9.41** | **11.05** | -35.23 | 36.45 | 42.56 |
| Dietrich (1982) | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A |
| Zhang and Choi (2021) SA | -21.13 | 26.11 | 30.20 | -15.68 | 20.40 | 24.22 | **-14.33** | **19.14** | **23.89** |
| Zhang and Choi (2021) Proj | 28.42 | 35.00 | 46.49 | 25.24 | 28.66 | 37.16 | 34.90 | 39.26 | 45.06 |
| Stokes (1851) SA | 43.78 | 61.24 | 79.87 | -64.08 | 64.08 | 66.25 | 31.30 | 31.36 | 58.75 |
| Dioguardi et al. (2018) SA | -67.63 | 67.63 | 68.30 | -86.90 | 86.90 | 86.97 | -83.86 | 83.86 | 84.17 |
| Bagheri and Bonadonna (2016) SA | -71.66 | 71.66 | 72.20 | -90.92 | 90.92 | 90.98 | -75.31 | 75.31 | 75.93 |
| Francalanci et al. (2021) | 95.48 | 95.48 | 102.56 | 170.05 | 170.05 | 20.04 | 176.13 | 176.13 | 193.36 |
| Stokes (1851) Proj | 1054.98 | 1054.98 | 1152.18 | 1134.33 | 1134.33 | 1227.18 | 1709.76 | 1783.46 | 1778.34 |

**Average error:**

Diagram

Description automatically generated

* Dioguardi has the lowest overall average error and closely predicts the terminal settling velocity of the particles with a slight tendency to underestimate the settling velocity. Considering each of the morphologies separately, Dioguardi’s model overestimates the settling velocity of fragments on average by 7.27%, underestimates the settling velocity of films on average by 2.07% and underestimates the settling velocity of fibres by 35.23%.
* Yu et al has the second lowest overall average error at 6.21%, showing a tendency to overestimate the terminal settling velocity. Considering each of the morphologies separately, Yu’s model performs better for fragments, films and fibres than Dioguardi’s model, with average errors of 3.54%, -0.68% and 30.63% respectively.
* Bagheri and Bonadonna has the third lowest overall average error at 8.97%. When only fragment particles are considered it has the lowest average error at 3.21% but it performs less well than both Dioguardi and Yu for fibres and films, with average error of 8.60% and 32.75% respectively.
* When considering all the morphologies together, Stokes’ model has a relatively low average error of 11.18%. The average error for individual morphologies is high at 43.78% for fragments and -64.08% for films and 31.30% for fibres. The average error for fibres is similar to that of Bagheri, Dioguardi and Yu, highlighting their poor performance for fibres.
* Instead, the model by Zhang and Choi is most accurate at predicting the terminal settling velocity of fibrous particles, with an average error of -14.33%. This is expected since the model is derived primarily for fibrous particles. However it is consistent in predicting the terminal settling velocity of the other morphologies considered, with an average error of -21.13% for fragments and -15.68% for films. Interestingly, these results were obtained when using the particle surface area as the effective area in the drag force calculation. When the particle projection area was estimated using the method outlined in the paper the model was less accurate in predicting the terminal settling velocity . This may be because ??
* The model by Dietrich has an average error of -14.70%. Due to the requirement that CSF>0.2, the model was not applicable to any film particles and all but one of the fibrous particles and therefore will not be useful for use in a modelling context for irregularly shaped mPs.
* Francalanci’s model overestimated the terminal settling velocity of all morphologies considered, with an overall average error of 128.31% and an average error of 95.48%, 170.05% and 176.13% for fragments, films and fibres respectively. Similar results were found during the validation of Francalanci’s model by the authors using Van Melkebeke’s dataset, when the output showed that all points were overestimated.

**Results:** Absolute Average Error

Chart, waterfall chart

Description automatically generated

* Unlike the average error, Bagheri and Bonnadonna has the lowest absolute average error overall at 13.95%, closely followed by Yu et al at 14.81% and Dioguardi at 15.82%.
* Bagheri and Bonnadonna is also has the lowest absolute average error for fragments at 10.51%, closely followed by Yu at 11.55% and Dioguardi at 13.87%.
* The lowest absolute average error for films is achieved when Dioguardi et al is used at 9.41%, followed by Bagheri and Bonnadonna at 10.51% and Yu at 12.14%.
* However, these models don’t perform as well for fibrous particles and their absolute average error is more than doubled to 33.18%, 34.59% and 36.45% for Yu, Bagheri and Dioguardi respectively. Instead, the best performing model for fibrous particles is Zhang using the surface area, producing an absolute average error of 19.14%. The model by Stokes also performs better than Yu, bagheri and Dioguardi with an average error of 31.36%.

**Results:** RMSE

Chart, waterfall chart

Description automatically generated

* The model by BB has the lowest RMSE overall, at 2.06%. It also has the lowest RMSE for fragments, at 1.33%.
* The model by Dioguardi has the lowest RMSE for films, at 1.11% but is closely followed by BB at 1.50%.
* The model by Zhang has the lowest RMSE for fibres at 2.39%, which is expected since this model has been developed with a focus on fibrous particles. The model by BB also has the second lowest RMSE for fibres at 4.25%.
* The model by Yu has the lowest RMSE of all the explicit models tested, with 2.27% overall. It performs slightly less well than BB for fragments with RMSE 1.49% and performs less well than both BB and Dioguardi for films and fibres, at 2.04% and 4.32% respectively.
* The results of Zhang using SA were most consistent across all shapes, at 3.02%, 2.42% and 2.39% for fragments, films and fibres respectively. Unlike the models by Dioguardi, BB and Yu, its performance doesn’t drop significantly for fibres.

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