

A. Appendix

A.1 Surrogate models

The surrogate models developed for predicting particle residence time, velocity and mass fraction in the spray zone demonstrated satisfying predictive accuracy across a range of operational conditions in fluidized beds. This section provides an overview of the velocity and mass fraction model performance, highlighting the capability of CFD-DEM in capturing the complex interactions between particles and fluid dynamics in fluidized beds. All properties residence time, velocity and mass fraction are influenced by many factors such as the bed mass, particles size and inlet air velocity. The surrogate models capture the most important factors as outlined in the following chapters.

A.1.1 Velocity model analysis

The overall trend of the velocity magnitude is well captured with the Reynolds number, as shown in Figure 1.

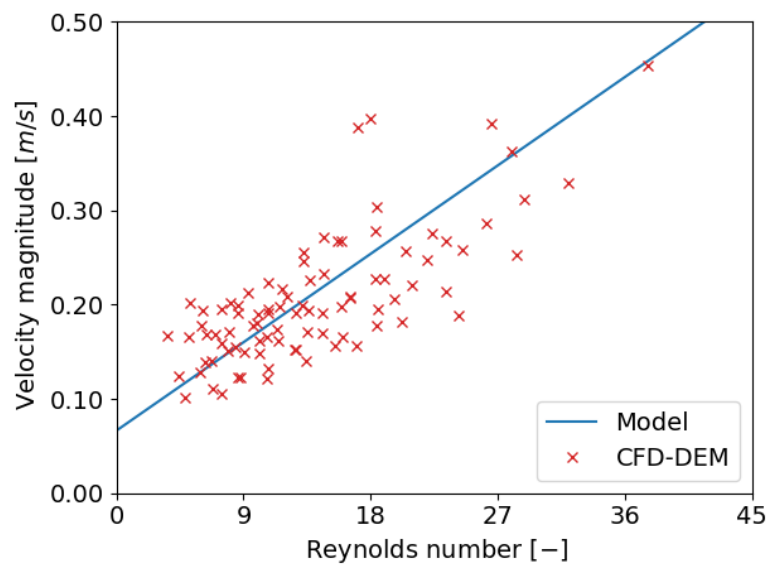


Figure 1: Predicted velocity magnitude over Reynolds number.

The velocity model fits with an R^2 of 45%. Figure 2 shows the parity plot for the velocity model prediction.

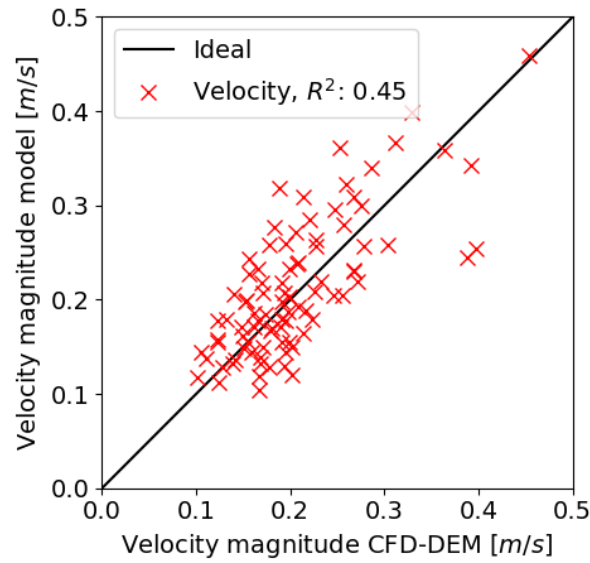


Figure 2: Parity plot showing the predicted velocity magnitude compared to the velocity magnitude from CFD-DEM simulations.

A.1.2 Mass fraction model analysis

The overall trend of the mass fraction in the spray zone can be well captured with a polynomial of second degree of the Reynolds number, as shown in Figure 3.

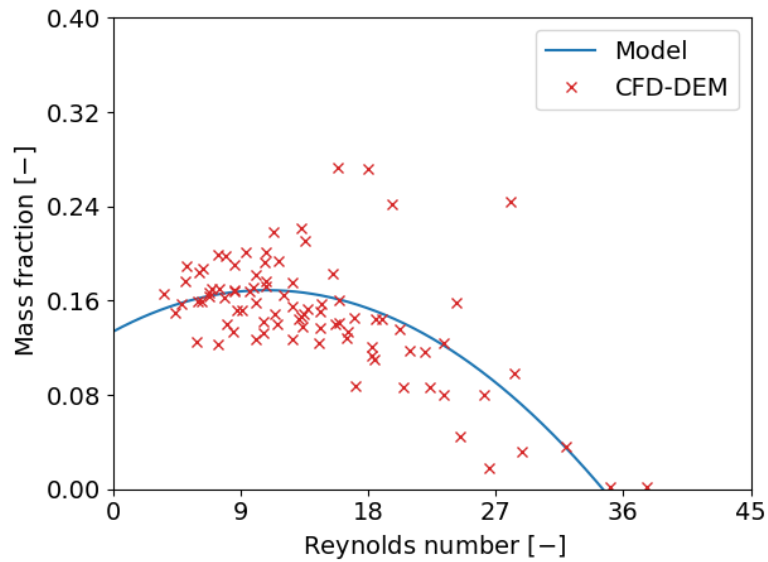


Figure 3: Predicted mass fraction of particles in the spray zone over Reynolds number.