Improving aerosol and spray process computational fluid dynamics models with machine learning approaches

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Background

Spray drying is a technique for transforming atomized slurries or solutions into powders. This process is behind commonly used products such as: **pharmaceuticals, milk powder, detergent powder, …**

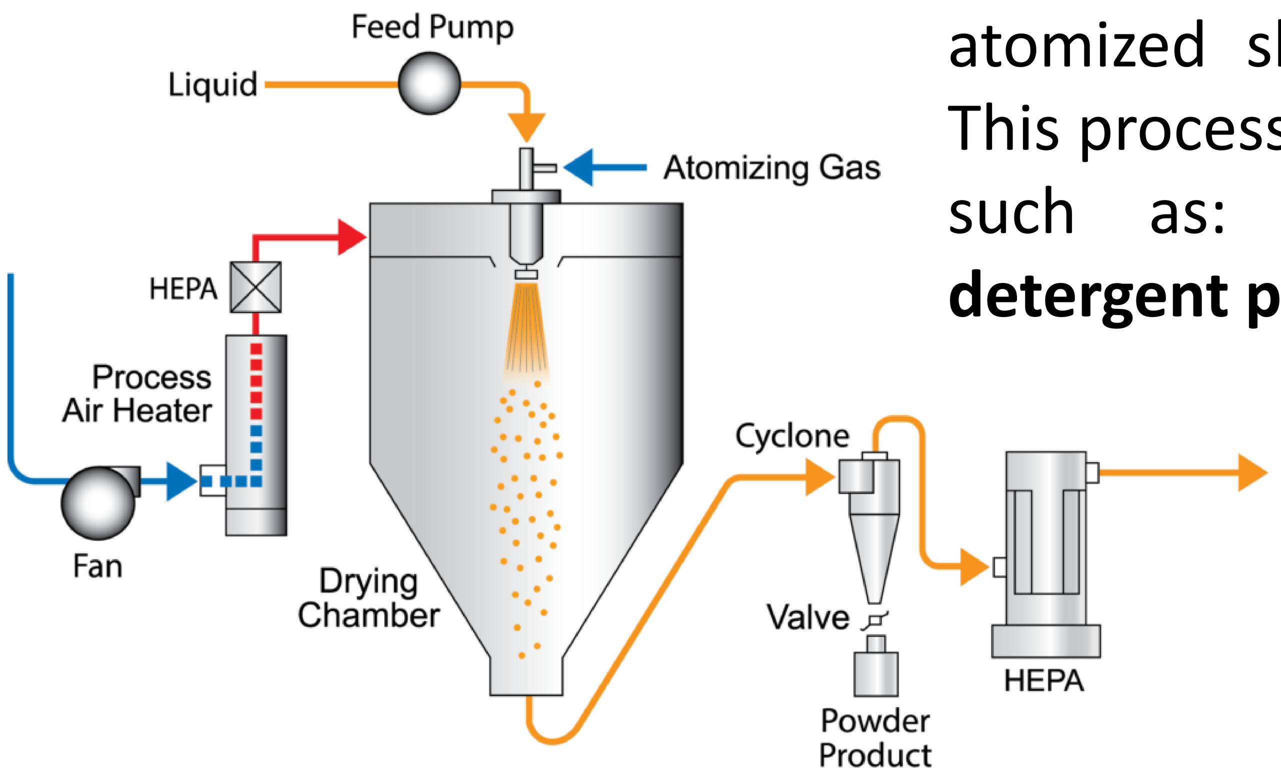


Figure 1: A schematic diagram of the spray dryer [1]

The drying process is complex

The characteristics of the powders produced, for example, density and porosity, **are significantly influenced by a range of factors**, including the diameter of the spray drying chamber, air temperature, air mass flow rate, and feed temperature.

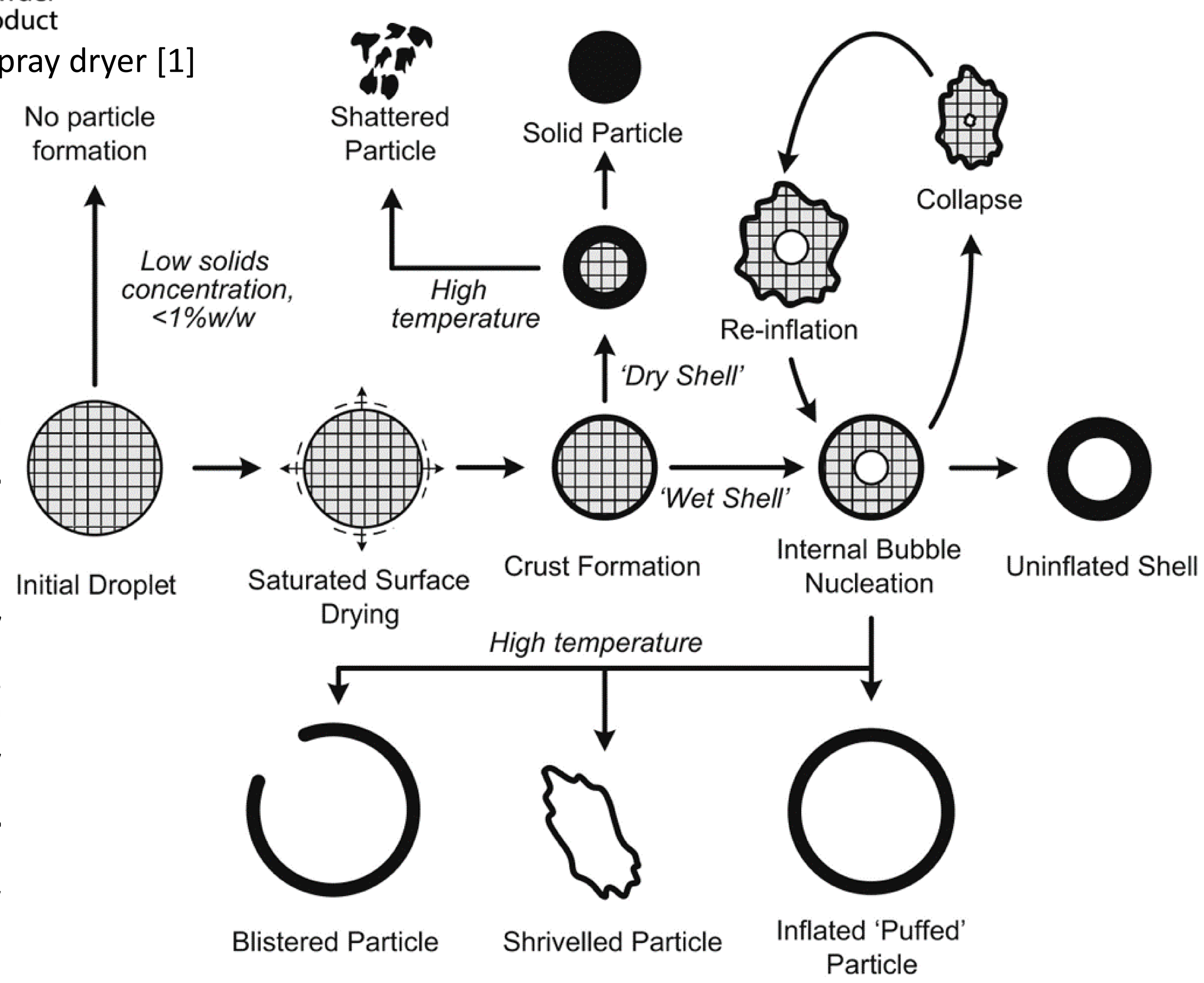


Figure 2: Different particle morphology determined by its drying history [2]

Statement of Problem

Computational fluid dynamics (CFD) models provides detailed information for identifying the optimal operating variables.

However, the drying models used in the CFD models are semi-empirical. This means they fall short of capturing the actual behaviours of droplets and the impact of drying history on particle characteristics.

Objectives

Speed-up of single droplet drying models

Inclusion of more complex phase change physics

Coupling of more complex single-particle drying models into spray dryer CFD models

Methodology

Physics-Informed Neural Networks

The learning process is to **minimize loss function** L

$$L = MSE_u + MSE_f \begin{cases} MSE_u = \dfrac{1}{N_u}\sum_{i=1}^{N_u}\left|\hat{u}^i - u(x_u^i, t_u^i)\right|^2 \\ MSE_f = \dfrac{1}{N_f}\sum_{i=1}^{N_f}\left|f(x_f^i, t_f^i)\right|^2 \end{cases}$$

PDE

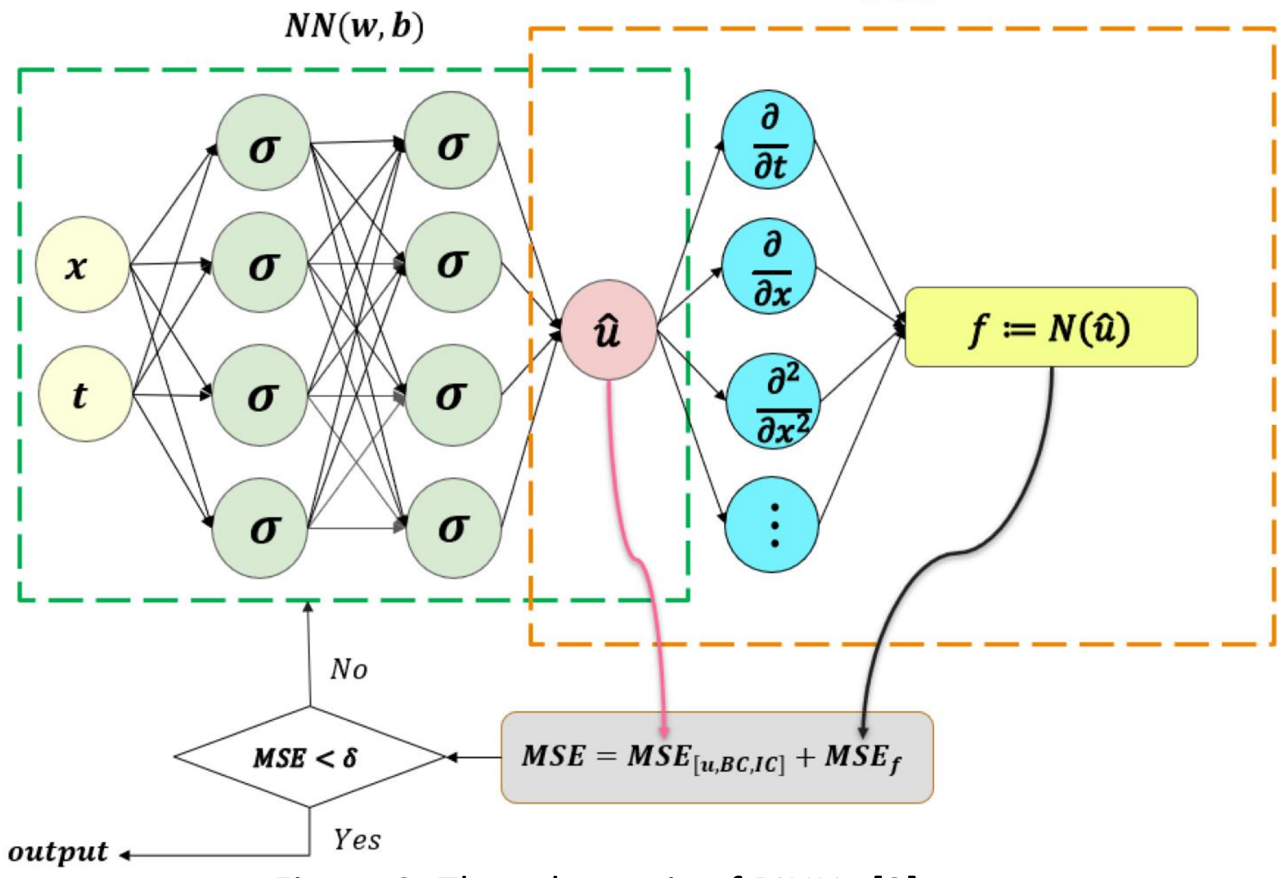
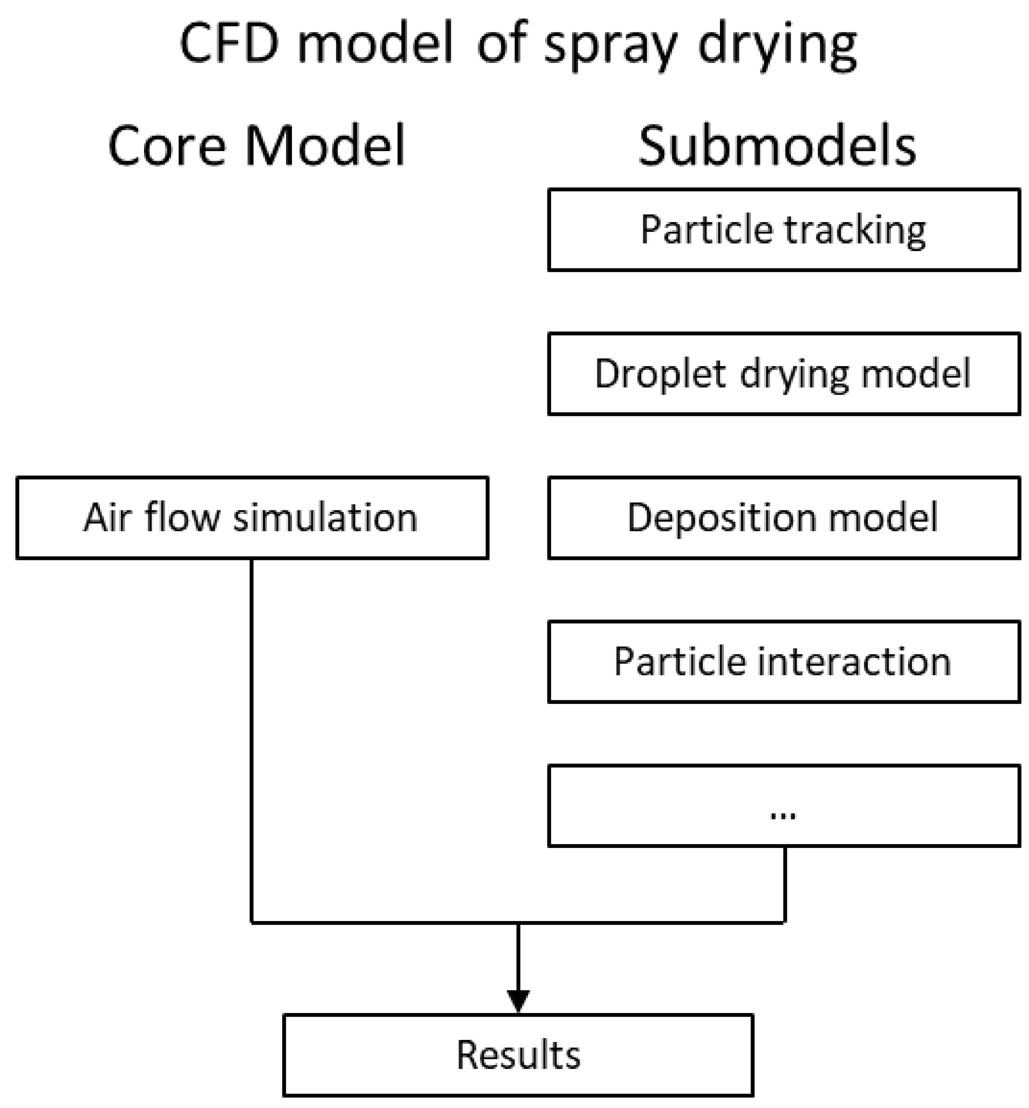


Figure 3: The schematic of PINNs [3]

Computational Fluid Dynamics



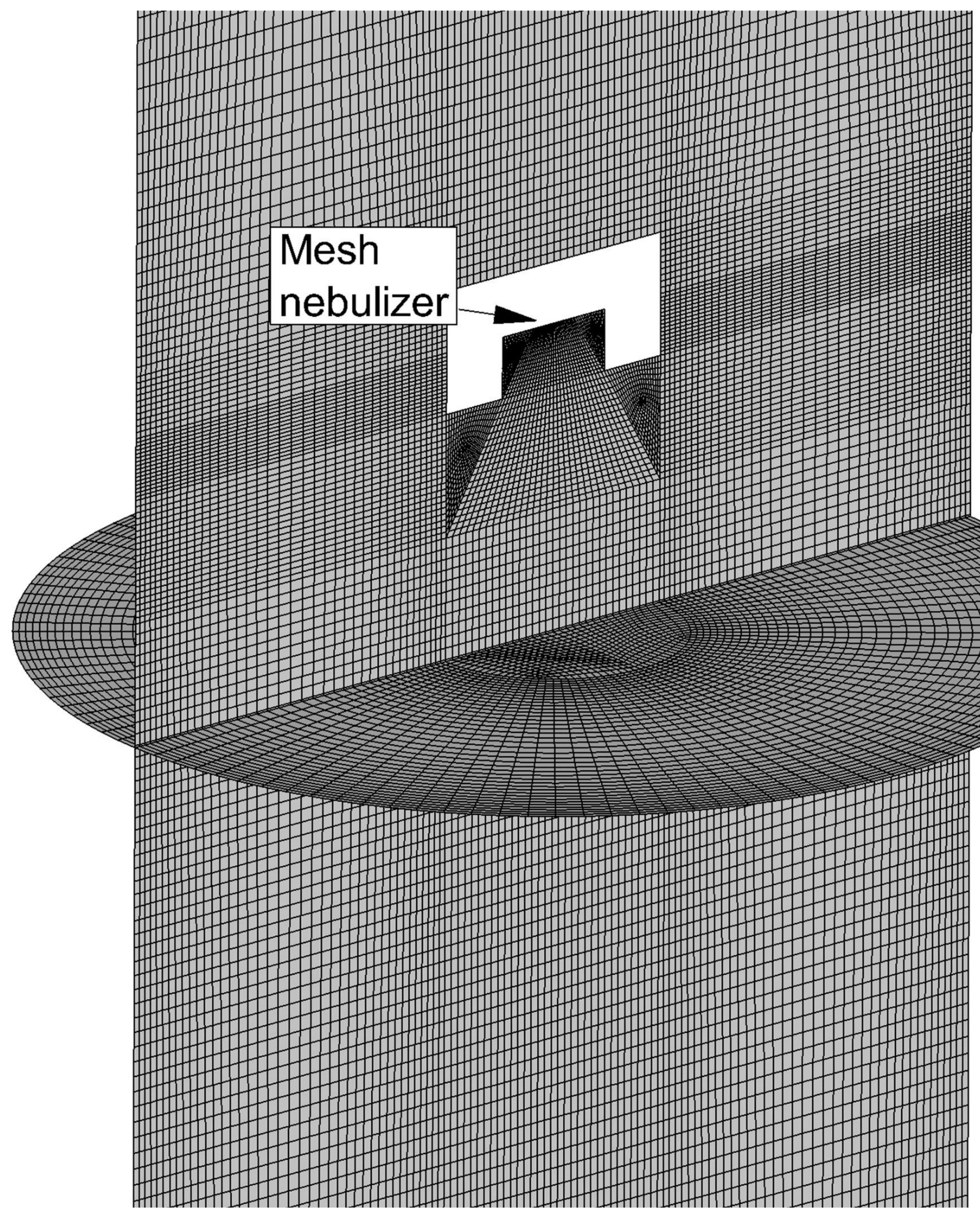


Figure 4: Hexahedral mesh of a spray dryer [4]

Eulerian-Lagrangian framework is employed in air flow simulations.

Eulerian approach calculates the continuous phase utilizing the Reynolds-averaged continuity equation and Navier Stokes equations.

Lagrangian approach applies Newton's Law to determine particles trajectories and velocity profiles

Responsible Innovation

- Integration of advanced models into Computational Fluid Dynamics (CFD) models for spray drying, addressing prolonged computational times due to complex model integration.
- Enabling quicker access to detailed information for scientists and engineers, facilitating the design of superior spray dryers.
- Enhancement of the capability to produce specially engineered particles and troubleshoot operational problems.

[1] M. Winkler, 'Spray Drying'. Accessed: Apr. 03, 2024. [Online]. Available: https://www.freund-vector.com/technology/spray-drying/
[2] C. S. Handscomb, M. Kraft, and A. E. Bayly, 'A new model for the drying of droplets containing suspended solids', Chemical Engineering Science, vol. 64, no. 4, pp. 628–637, Feb. 2009, doi: 10.1016/j.ces.2008.04.051.
[3] Y. Guo, X. Cao, B. Liu, and M. Gao, 'Solving Partial Differential Equations Using Deep Learning and Physical Constraints', Applied Sciences, vol. 10, no. 17, Art. no. 17, Jan. 2020, doi: 10.3390/app10175917.
[4] P. W. Longest, D. Farkas, A. Hassan, and M. Hindle, 'Computational Fluid Dynamics (CFD) Simulations of Spray Drying: Linking Drying Parameters with Experimental Aerosolization Performance', Pharm Res, vol. 37, no. 6, p. 101, May 2020, doi: 10.1007/s11095-020-02806-y.