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AI-Driven Surrogate Modelling of Wet Stirred Media Mills

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Abstract. Modelling of wet-operated stirred media mills (WSMMs) using coupled CFD-DEM simulations provides detailed insights into stress energy distributions and particle breakage mechanisms. However, the high computational cost of these simulations limits their applicability for dynamic process modelling and integration with population balance models (PBMs), which require continuous stress energy distribution inputs to capture evolving process conditions. In this work, an AI-based surrogate model is proposed to replace CFD-DEM simulations by predicting stress energy distributions, stress frequency, and power consumption as functions of key operating and material parameters, including grinding media size and filling degree, stirrer tip speed, as well as contact properties. The surrogate is trained on systematically generated CFD-DEM data using an active learning strategy to efficiently explore the high-dimensional parameter space. New simulation conditions are iteratively selected based on model uncertainty to maximize information gain while minimizing computational cost. The resulting framework enables rapid and physically consistent prediction of process behaviour, providing a pathway toward dynamic modelling, process optimization, and scale-up of WSMM systems.

1. Introduction

Wet-operated stirred media mills (WSMMs) are widely used for fine grinding applications, where process performance is governed by stress energy distributions and stress frequency [1,2]. High-fidelity modelling using coupled CFD-DEM simulations enables detailed resolution of bead-fluid and bead-bead interactions, providing valuable insight into breakage-relevant quantities [3-5]. However, the computational cost associated with such simulations limits their applicability for large-scale parametric studies and dynamic process modelling. In particular, population balance models (PBMs) require continuous inputs of stress energy distributions to capture evolving process conditions, which cannot be efficiently obtained through direct coupling with CFD-DEM simulations. Changes in process conditions, such as slurry viscosity, directly influence stress energy distributions and consequently affect breakage behaviour, requiring continuous updates of model inputs. To address this limitation, the present work proposes an AI-based surrogate modelling framework to replace CFD-DEM simulations and enable rapid prediction of key process descriptors across a wide operating space.

2. Methodology

2.1. CFD-DEM Simulations and Data Generation

A high-fidelity unresolved CFD-DEM framework [3,4] is employed to generate the dataset required for training the surrogate model [6-8]. The simulations are performed on a laboratory-scale wet stirred media mill (PML-1), where bead-fluid and bead-bead interactions are resolved through volume-averaged fluid coupling (CFD) and soft-sphere contact mechanics (DEM). A representative simulation snapshot is shown in Figure 1, illustrating bead motion and velocity distribution within the mill.

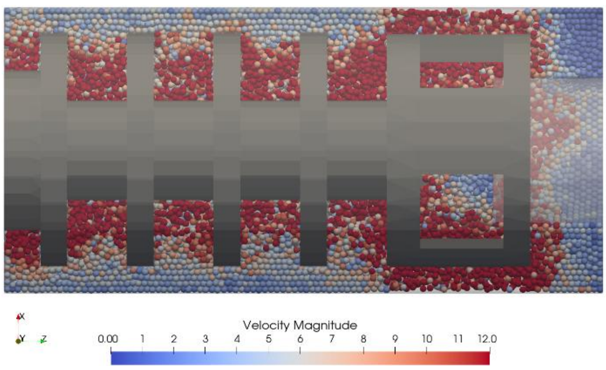

Figure 1. Instantaneous bead velocity distribution of PML-1. Case: stirrer tip speed $(v_t) \sim 12$ m/s, bead diameter $(d_{gb}) = 2$ mm, filling degree $(\phi) = 80\%$

To systematically explore the operating space, key process and material parameters are varied over a representative range of operating conditions. These include stirrer tip speed, grinding media (bead) diameter, bead filling degree, bead density, slurry viscosity, and contact parameters.

For each simulation case, stress-based descriptors relevant for breakage (stress energy distributions, stress

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frequency, and power consumption) are extracted using customized post-processing routines. In particular, the stress energy per collision is evaluated based on relative bead velocities and effective mass considerations (as described in [4]):

$$SE = \frac{1}{2} m_{eff} v_{rel}^2 \quad (1)$$

where m_{eff} is the effective mass of interacting beads and v_{rel} is the relative collision velocity. From this, stress energy distributions (SEDs) and stress frequency are computed, along with mill power consumption.

The resulting dataset establishes a mapping between operating conditions and breakage-relevant quantities, forming the basis for surrogate model development.

2.2 AI-Based Surrogate Model and Active Learning

An AI-based surrogate model [6-8] is developed to approximate the nonlinear relationship between process parameters and stress-based descriptors obtained from unresolved CFD-DEM simulations. The model takes operating and material (DEM) parameters as inputs and predicts outputs including stress energy distributions, stress frequency, and mill power consumption. Particular emphasis is placed on accurately capturing stress energy distributions over multiple orders of magnitude, as these directly govern breakage behaviour in WSMMs [1,2].

To efficiently explore the high-dimensional parameter space, the surrogate model is trained using an active learning strategy, as illustrated in Figure 2. Initially, a limited number of CFD-DEM simulations (Generation 0) is performed to construct a baseline training dataset. Based on the trained surrogate, regions of high prediction uncertainty are identified, and additional simulation points are selectively sampled in these regions.

This iterative loop, comprising simulation, training, uncertainty estimation, and resampling, continues until convergence criteria are met, such as stabilization of prediction accuracy or diminishing information gain. The approach enables targeted data generation, significantly reducing the number of required CFD-DEM simulations compared to exhaustive sampling.

The resulting framework is expected to deliver accurate predictions across the operating space while maintaining computational efficiency, thereby enabling rapid evaluation of process conditions.

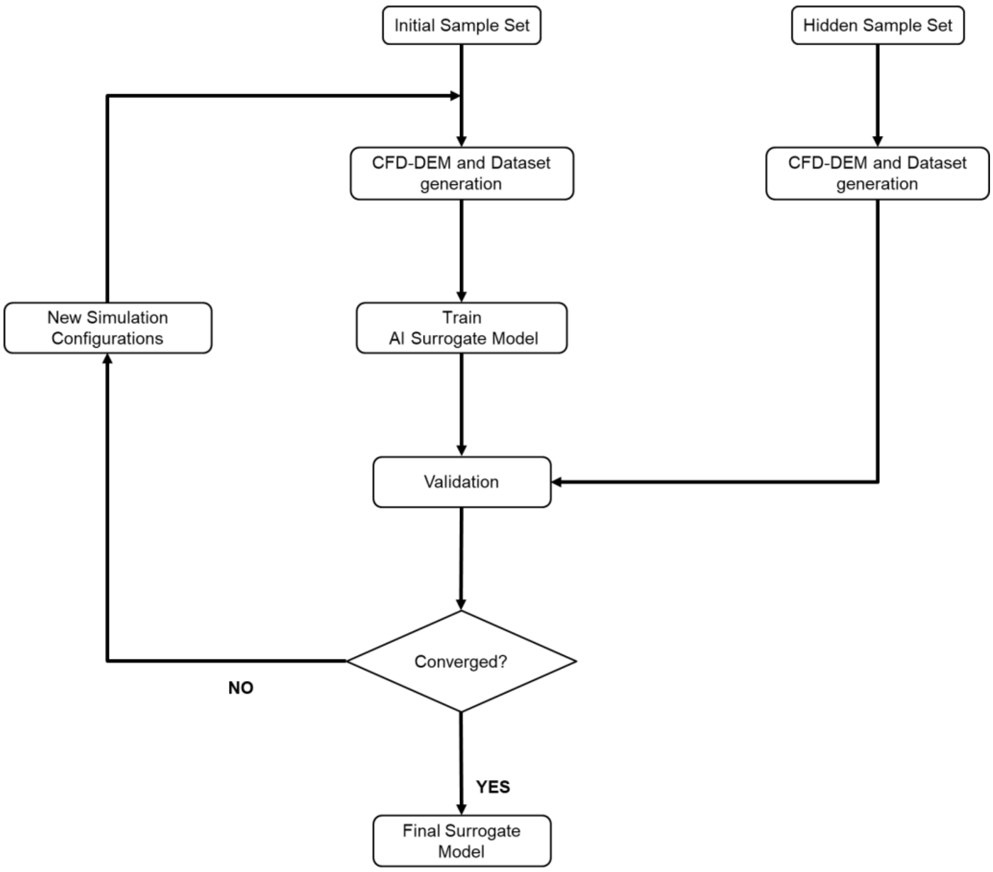

Figure 2. Active learning framework for AI-based surrogate modelling of wet stirred media mills. An initial set of CFD-DEM simulations is used to train the surrogate model. New simulation conditions are iteratively selected based on prediction uncertainty, while model performance is evaluated using a hidden validation set until convergence is achieved.

3. Conclusions

This work presents a framework for AI-driven surrogate modelling of wet stirred media mills, aimed at replacing computationally expensive CFD-DEM simulations. The proposed approach integrates high-fidelity simulation data with machine learning techniques to predict stress energy distributions, stress frequency, and power consumption across a wide range of operating conditions.

By incorporating an active learning strategy, the framework enables efficient exploration of the parameter space while minimizing simulation effort. The developed surrogate model is expected to facilitate rapid and physically consistent process modelling, enabling future integration with dynamic process models and population balance approaches.

Ongoing work focuses on generating the CFD-DEM dataset and validating the predictive capability of the surrogate model, with particular emphasis on generalization and robustness across operating conditions.

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