# Modelling wet-operated stirred media mills with population balances based on mechanistic models

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**Abstract.** A fully mechanistic population balance model for wet-operated stirred media mills is presented and implemented into the Dyssol simulation environment. The framework consistently links material-specific breakage behaviour with machine-specific stressing and transport phenomena. Breakage functions are determined experimentally using a modified counter-rotating three-roller mill and combined with stress energy distributions obtained from CFD–DEM simulations to calculate physically based breakage rates. In addition, mechanistic sub-models for grinding media and particle transport are developed to account for back-mixing effects and the influence of internal classification devices. The model integrates four interacting components: breakage function, breakage rate, grinding media transport, and particle transport. Validation against experimental grinding results shows good agreement for batch, continuous, and circulation operation modes. The developed framework provides a robust basis for predictive simulation and future extension towards scale-up and alternative mill geometries.

## 1. Introduction

Stirred media mills are extensively used for fine and ultrafine wet grinding due to their high energy efficiency and capability to produce narrow particle size distributions. Nevertheless, comminution remains one of the most energy-intensive unit operations, motivating continuous efforts to improve process understanding and model-based optimization [1].

Previous studies have demonstrated that particle breakage in stirred media mills is governed by both the magnitude and frequency of stressing events, which are strongly influenced by mill geometry, operating parameters, and suspension properties [2–5]. Population balance modelling (PBM) provides a rigorous framework to describe comminution processes by tracking the evolution of particle size distributions [6]. However, many PBM approaches rely on phenomenological parameters and simplified descriptions of stressing conditions, limiting their predictive capability for stirred media mills [7–9].

To overcome these limitations, recent work has increasingly combined PBM with numerical methods such as the discrete element method (DEM) and computational fluid dynamics (CFD) [10–17]. Multiscale approaches linking CFD–DEM-derived stress energy distributions to PBM formulations have improved breakage rate prediction [18–20], but the consistent integration of material-specific breakage behaviour and transport phenomena remains challenging.

The objective of this work is therefore to develop a fully mechanistic population balance model for wet-operated stirred media mills, integrating experimentally determined breakage behaviour, CFD–DEM-based stressing conditions, and mechanistic descriptions of grinding media and particle transport. The model is implemented into the dynamic flowsheet simulation framework Dyssol [21,22].

## 2. Modelling Approach

### 2.1. Population Balance Framework

The model is based on the general population balance equation describing particle mass transfer between size classes due to breakage and transport. A key concept is the separation of material-specific properties from machine-specific stressing conditions. Material behaviour is described by breakage energies and breakage functions, while stressing conditions depend on operating parameters and internal mill dynamics. This modular structure facilitates parameter transfer between operating conditions and mill geometries.

The stirred media mill model is implemented into the dynamic simulation environment Dyssol, enabling both steady-state and transient simulations. This allows the investigation of start-up behaviour, parameter changes, and interactions between grinding, transport, and classification phenomena at flowsheet level.

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## 2.2. Breakage Behaviour of Particles

Particle breakage is characterised by the specific breakage energy and the breakage function. The specific breakage energy defines the probability of fracture under a given stressing condition, while the breakage function describes the resulting fragment size distribution. Figure 1 shows experimentally determined median breakage energies as a function of particle size.

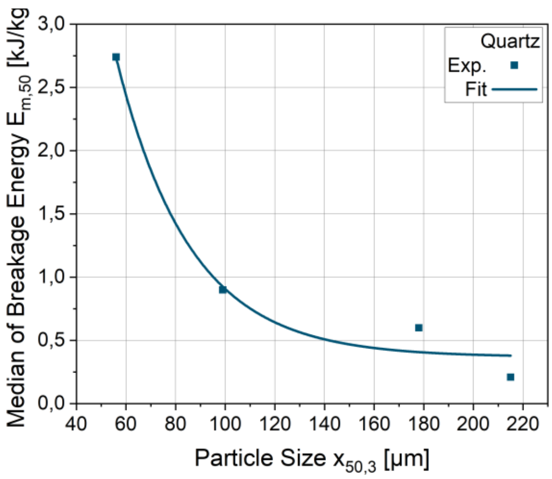


**Figure 1.** Breakage energies determined with single-particle breakage in nanoindentation experiments

Material-specific breakage functions are obtained using a modified counter-rotating three-roller mill, which enables controlled single-particle stressing under defined energy input. Experimental results are evaluated over multiple stressing events to capture cumulative breakage behaviour relevant for stirred media milling. The derived breakage functions are compared with established literature models (Figures 2 and 3) and serve as central input parameters for the population balance model.

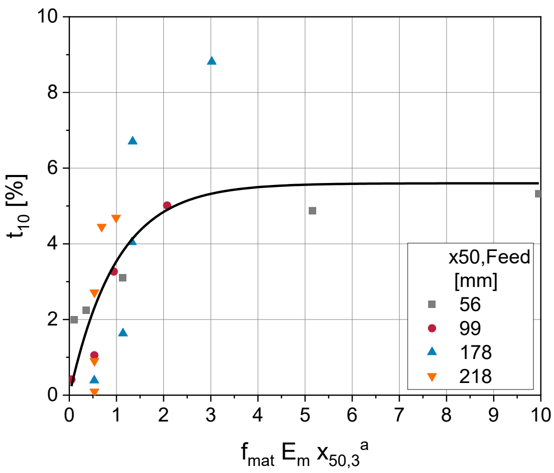


**Figure 2.** Prediction of $t_{10}$ based on Shi et al. [9]

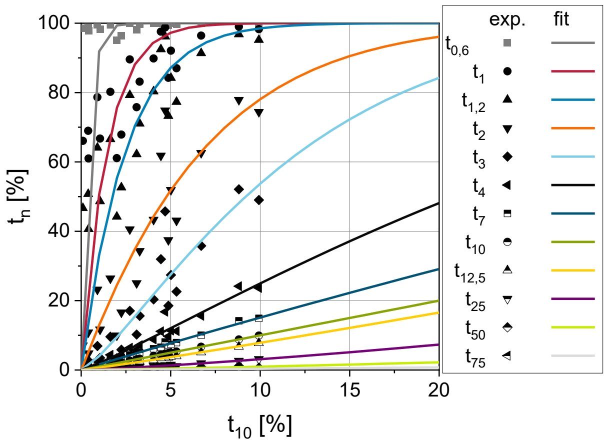


**Figure 3.** Modelling of breakage function based on $t_{10}t_n$-Model

## 2.3. Stress Energy Distribution and Breakage Rate

While breakage functions describe the fragmentation behaviour, the breakage rate quantifies the frequency of breakage events. Breakage rates are calculated by coupling the material-specific breakage behaviour with stress energy distributions obtained from CFD–DEM simulations (Figure 4).

CFD–DEM simulations provide spatial and temporal distributions of grinding media collision energies and stressing frequencies. To account for the fact that not all stressing events contribute equally to breakage, effective stress energies are introduced. The breakage rate is then formulated as the fraction of particles breaking per unit time and size class, resulting in a physically consistent description linking numerical simulations with experimental material data.

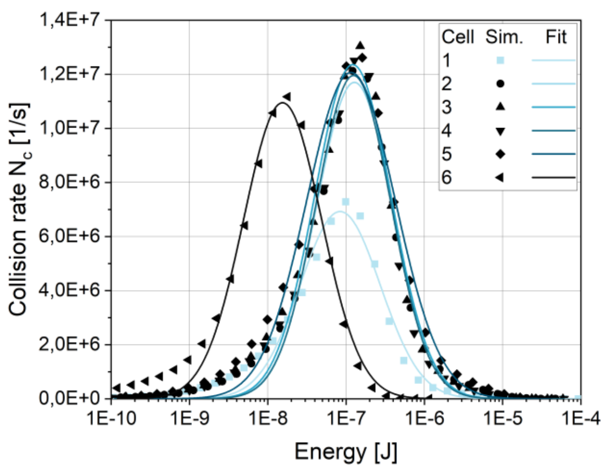


**Figure 4.** CFD–DEM-based stress energy distribution inside a stirred media mill.

## 2.4. Grinding Media Transport

Grinding media motion strongly influences stressing conditions in stirred media mills. A mechanistic model for grinding media transport is developed based on force balances acting on individual beads, including centrifugal, drag, and contact forces. This approach enables the description of bead motion as a function of operating parameters and mill geometry.

The model is validated using CFD–DEM simulations and captures the influence of parameters such as tip speed, bead filling degree, and suspension viscosity. The presence of a deflector wheel is explicitly considered, as it induces reverse flow zones and significantly alters grinding media distribution and stressing conditions (Figure 5).

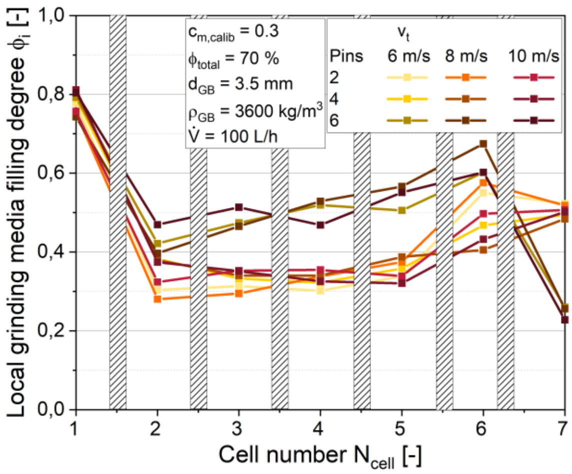


**Figure 5.** Simulated grinding media axial grinding media filling degree with deflector wheel.

### 2.5. Particle Transport and Residence Time Behaviour

Particle transport is described by axial and radial flow combined with back-mixing effects. Residence time distributions are measured experimentally using tracer methods and reveal pronounced material retention when a deflector wheel is installed.

To represent this behaviour within the population balance framework, a separation function is introduced (Figure 6). This function enables a mechanistic description of internal classification effects and their influence on particle transport and size distribution evolution.

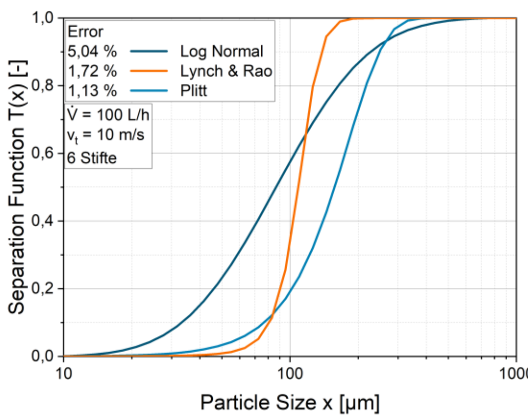


**Figure 6.** Modelled separation function and resulting error based on grinding results

## 4. Model Implementation and Validation

### 4.1. Implementation in Dyssol

Within Dyssol, the stirred media mill is represented using a cell-based population balance model, dividing the mill into ideally mixed compartments. Each cell is characterised by its local grinding media distribution, stress energy distribution, and transport behaviour. The breakage matrix is updated dynamically based on CFD–DEM results and experimentally determined breakage functions.

This formulation allows simulation of batch, continuous, and circulation operation modes, including transient effects and the influence of internal classification devices.

### 4.2 Model Validation

Model predictions are validated against experimental grinding results for glass and quartz in laboratory-scale stirred media mills. For batch operation, the model reproduces the overall shape of measured particle size distributions, with deviations for particles below approximately 10 µm attributed to experimental limitations in breakage characterization (Figure 7).

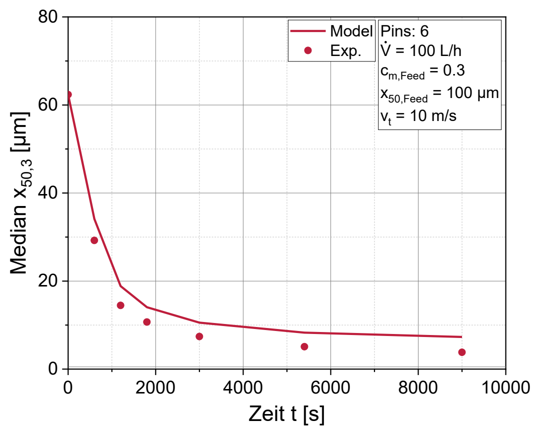


**Figure 7.** Validation of model for a mill geometry without internal classification

In continuous and circulation operation, the model captures the temporal evolution and final product size distributions with good agreement in the coarse and intermediate size ranges (Figure 8). The transferability of model parameters between different mill geometries demonstrates the benefit of separating material-specific and machine-specific model components.

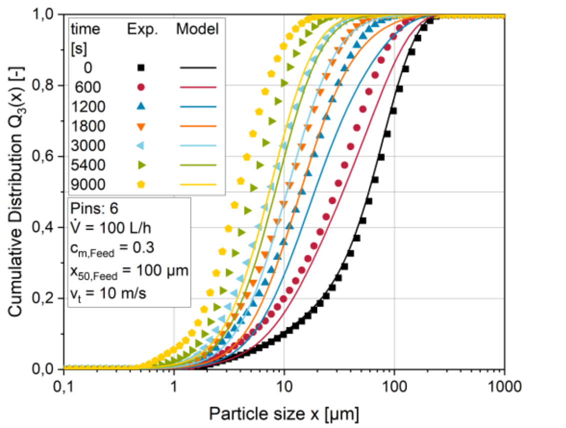


**Figure 8.** Validation of model for a mill geometry with internal classification

### 4.3 Conclusion

A fully mechanistic population balance model for wet-operated stirred media mills has been developed and implemented into the Dyssol simulation framework. By consistently integrating experimental breakage functions, CFD–DEM-derived stress energy distributions, and mechanistic transport models, the approach enables predictive simulation without reliance on purely empirical fitting parameters. The framework provides a solid basis for future extensions towards scale-up, alternative mill geometries, and enhanced internal classification modelling.

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