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Intelligent Decision Support and Control Technologies
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(ICT-CMAC): WP4 Plant-wide Modelling and Control

University of Strathclyde Science Engineering

A Population Balance-based Dynamic Impact Milling Model with an Enhanced Single Particle Breakage Kernel

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Introduction

Process models of solids handling operations, based on rigorous and dynamic population balance model are challenging to implement [1]. In this work, Process Systems Engineering (PSE) tools have been applied to the design and control of a milling operation within a continuous pharmaceutical manufacturing process. Vogel and Peukert (2005) identified a steady-state milling model with two material properties: (i) the particle resistance against fracture, f_{Mat}, and (ii) the mass specific energy a particle can absorb without fracture, $W_{m,min}$; thus, particle breakage probability and breakage function can be independently obtained from a single particle impact experiment [2]. The coupling of these properties with dynamics operating conditions in a rigorous population balance model has rarely been reported [3].

Single Particle Breakage Model

Breakage probability P_B
Denotes the fraction of particles of size w which is broken after k stressing events.

$$P_B = 1 - exp\left(-f_{Mat.}wk\left(W_{m,kin} - W_{m,min}\right)\right)$$

- $f_{Mat.}$: mass-based material strength parameter, kg/Jm
- w : particle size, m
- k : number of successive impacts, dimensionless
- $W_{m,kin}$: mass specific impact energy, J/kg
- $W_{m,min}$: mass specific threshold energy, J/kg

Breakage function B
The size distribution of the fragments, not taking into account the amount of undestroyed particles, is given by

$$B_{M,p}(w,v) = \left(\frac{w}{v}\right)^q \frac{1}{2}\left(1 + tanh\left(\frac{w - w'}{w'}\right)\right)$$

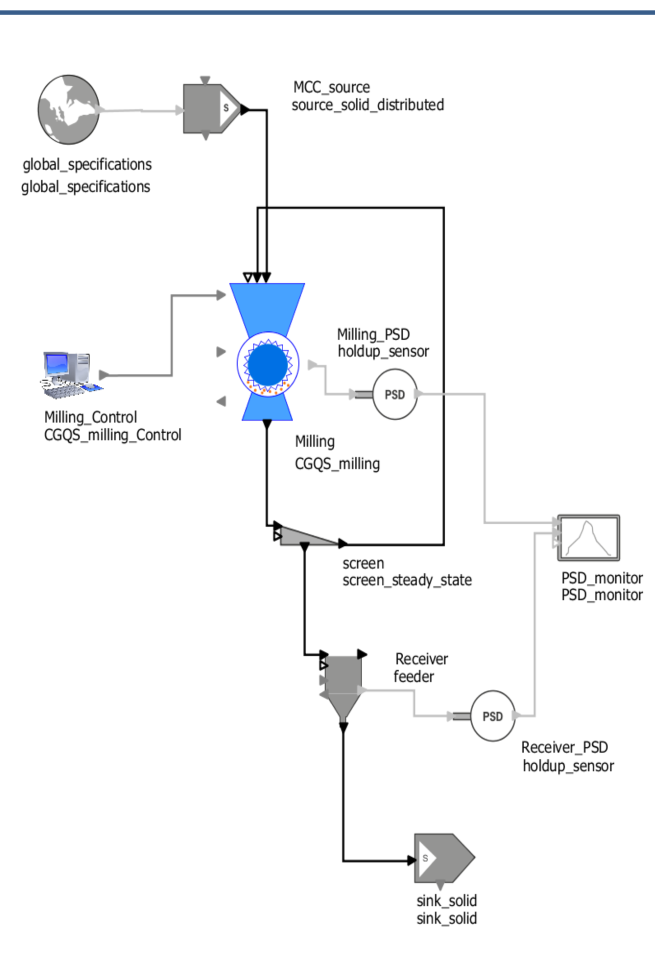
- w : fragmental particle size, m
- v : the size of the mother particle, m
- w' : fragment size for additional fading, m
- q : power law exponent, dimensionless

Conclusions and future work

- An improved approach of incorporating the single particle breakage model of Vogel and Peukert (2005) into a rigorous population balance model has been developed.
- By considering the distributed impact events and their effect on fragment particle size distributions, the bimodal particle size distribution of final particles can be obtained without the use of complex breakage functions [5].
- Flowsheet models of batch and continuous impact milling processes have been developed in the gSOLIDS software and will be further explored in with regard to process design and control.

- The dependence of the impact rate constants $F_{k,w}$ on the milling rotation speed needs more investigation effort from both experimental and modelling work.
- An integrated model for screen milling in the model library is expected for convenient drag & drop flowsheeting in gSOLIDS platform.
- Pilot plant data for pharmaceutical continuous secondary manufacturing process are important to validate the flowsheet model and to propose efficient and robust process control strategies for industrial scale processes.

Batch milling



Population balance model with Vogel and Peukert (2005) breakage kernel

$$\underbrace{\frac{\partial M_p(w,t)}{\partial t}}_{\text{Accumulation}} = \underbrace{\int_w^{w_{max}} S_M(v,t) b_{M,p}(w,v) M_p(v,t)dv}_{\text{Birth term}} - \underbrace{S_M(w,t)M_p(w,t)}_{\text{Death term}} + \underbrace{\sum_{i=1}^{N} M_i(w,t)}_{\text{Flow term}}$$

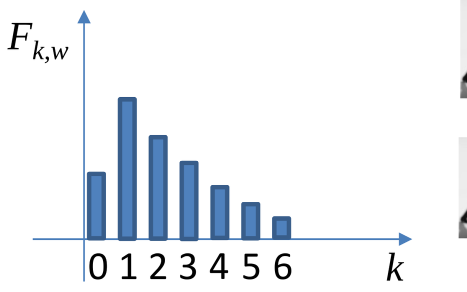
Particle breakage rate

$$S_M(w,t) = \sum_{k=0}^{k=\infty} F_{k,w} P_B(k,w)$$

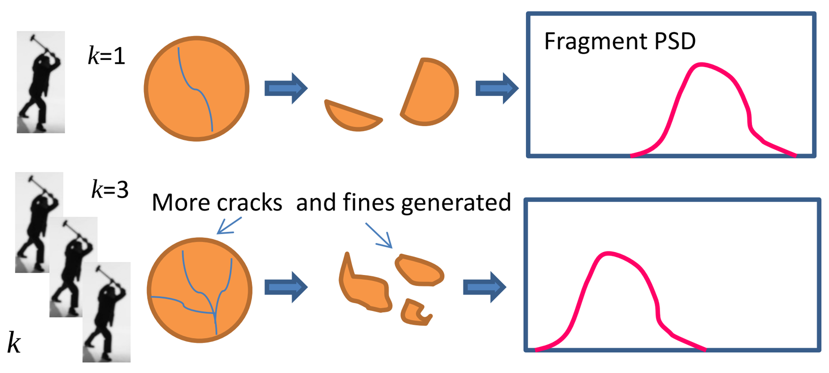
Fragment size density distribution

$$b_{M,p}(w,v) = \frac{\partial B_{M,p}(w,v)}{\partial v}$$

$F_{k,w}$: impact rate constant for particles of size w receiving the k^{th} successive impacts, or physically the fraction of particles of size w receiving the k^{th} successive impacts per unit of time, s^{-1}.

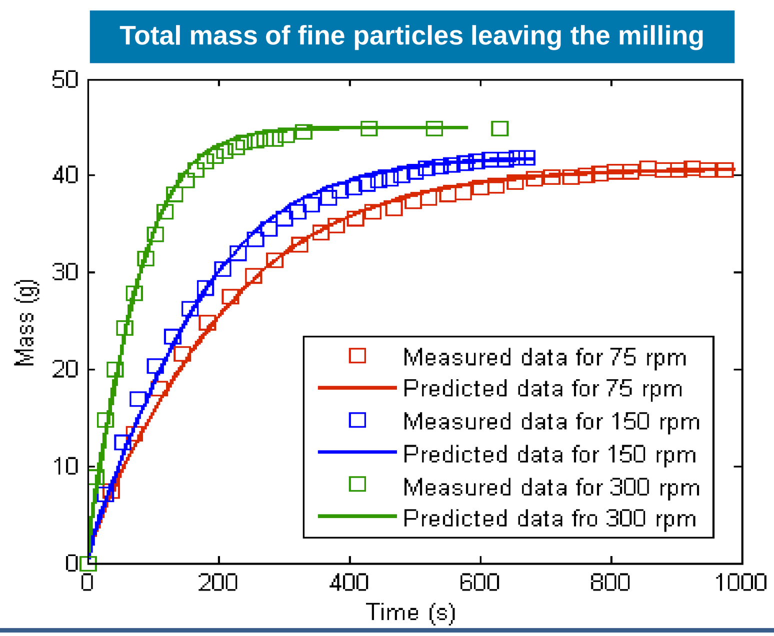


Histogram distribution of $F_{k,w}$ vs. k

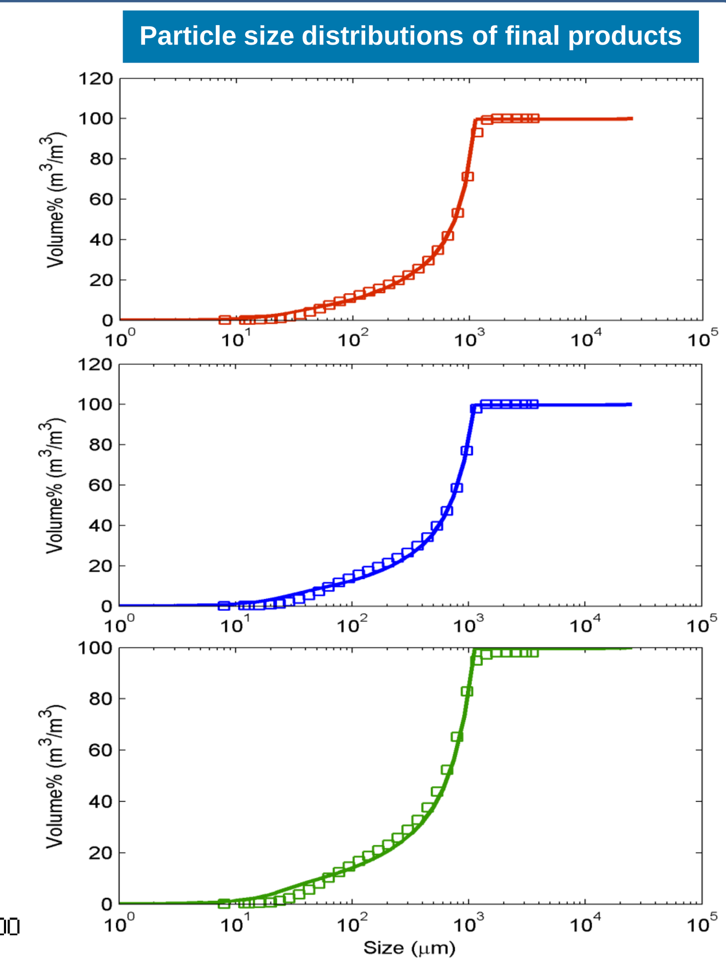


- Experimental data from batch milling under three rotation speeds were used to estimate the model parameters and to validate the model [3].
- Notably good matches between the measured and predicted data were observed.

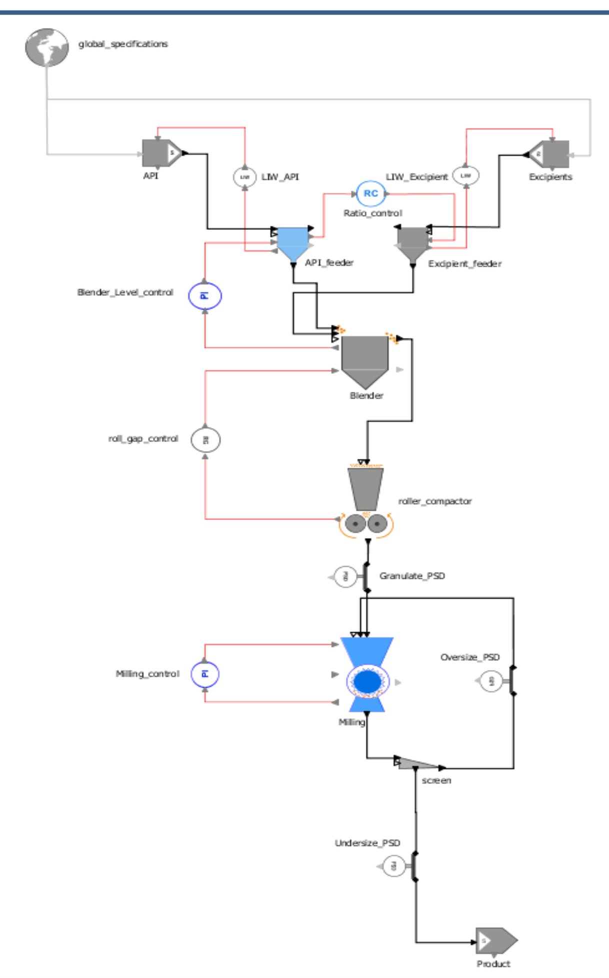
Total mass of fine particles leaving the milling



Particle size distributions of final products

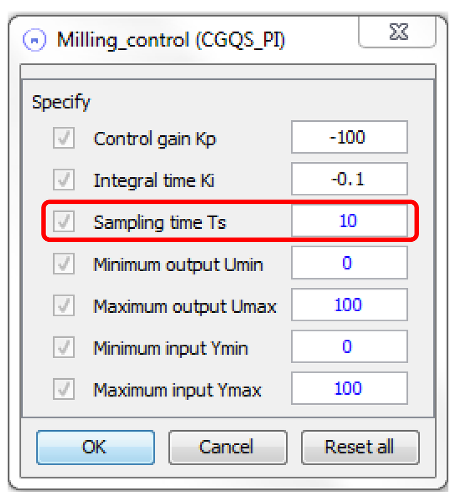


Continuous milling



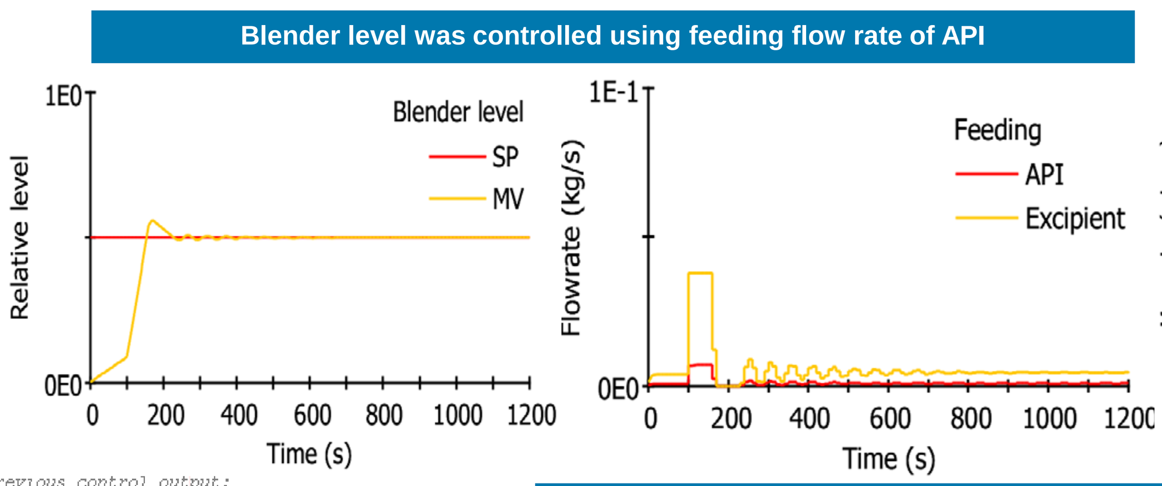
- A flowsheet model for a continuous dry granulation process, considering feeder, blender, roller compaction and dry milling, was developed in gSOLIDS 3.1 according to Gavi and Reynolds (2014) [4].
- A series of customised *digital* Ratio and Proportional and Integral (PI) controllers have been implemented to control the process from start-up to the steady-state operation.

PI controller within the "*Processes*" file in gSOLIDS.

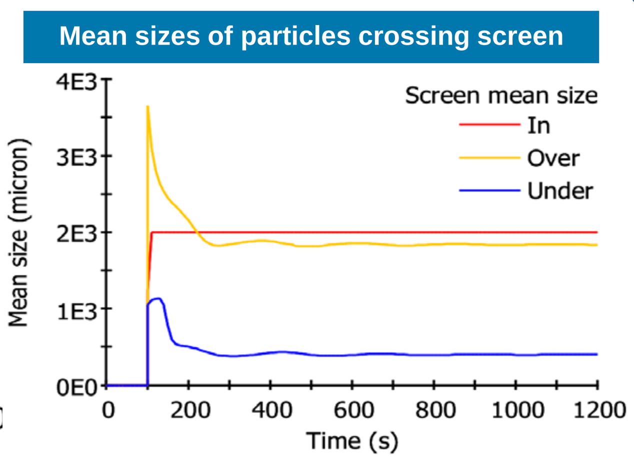



```
REASSIGN
   WITHIN Flowsheet DO

       WITHIN Blender_Level_control DO
          U_k := OLD(Control_Output.signal); # Previous control output;

       Y_mv_k := OLD(Control_Input.signal);  # Previous control input;

          E_k := OLD(Y_sp_k) - OLD(Control_Input.signal); # Current control error
         dE_k := OLD(Y_sp_k) - OLD(Control_Input.signal) - OLD(E_k); # difference in the co
      END # Blender_Level_control

      WITHIN Milling_control DO
          U_k := OLD(Control_Output.signal); # Previous control output;

       Y_mv_k := OLD(Control_Input.signal);  # Previous control input;

          E_k := OLD(Y_sp_k) - OLD(Control_Input.signal); # Current control error
         dE_k := OLD(Y_sp_k) - OLD(Control_Input.signal) - OLD(E_k); # difference in the co
      END

  END # Flowsheet
END # REASSIGN
```

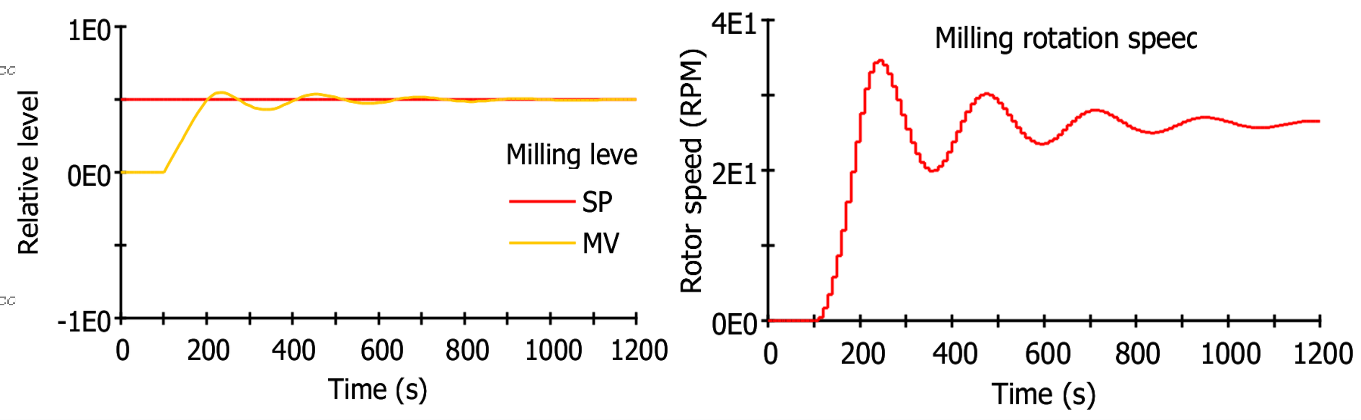
Blender level was controlled using feeding flow rate of API



Mean sizes of particles crossing screen



Milling level was controlled using rotor ration speed



References

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