# HYBRID PHYSICS/DATA-BASED MODEL OF TWIN SCREW FEEDERS FOR CONTINUOUS PHARMACEUTICAL TABLET MANUFACTURING PROCESS

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## Abstract

In this work, the dynamics of a screw feeder system for a continuous drug product manufacturing process has been investigated with the goal to predict the behavior of the system based on different bulk solids, feeder geometries and operating conditions. A mathematical model of twin screw feeders has been developed in MATLAB (MathWorks). A process data- and model-driven approach has been used for model validation in order to minimize the uncertainty of prediction and thus to improve the robustness of process simulation. The resulting model can be used to establish the mass flow – screw feed relationships and the optimal range of operating conditions. The model can also be exploited to identify alternative control strategies with the ultimate goal to improve product homogeneity in an inherently complex process.

## Keywords

Dynamic modelling, Screw feeders, Pharmaceutical.

### Introduction

Screw feeders are popular equipment for the handling and metering of bulk solids in the pharmaceutical industry, particularly in continuous tablet manufacturing.

Despite the increasing research in the last decade in the manufacturing of powder-based products, there is still a lack of knowledge of how input variables, in particular material properties, affect process operation and product quality. Predictive models are crucial to meet quality requirements, however a limited number of predictive process models have been developed so far in the scientific literature. The first-principles models for systems such as powder feeding operations have not been properly validated in both open and closed loop operations. Yu (1997), from a study of the particulate mechanics, developed a physics-based model to estimate the "steady" mass flow rate (i.e. no dynamics investigated). Engisch and Muzzio (2012) described the performance of screw feeders by an experimental and statistical approach. A surrogate model-based approach has often been used for process design and control (Boukouvala et al., 2010). Boukouvala et al. (2012) suggested a first order delay differential equation to model the dynamic mass flow rate provided by the feeder. Wang et al. (2017) proposed a semi-empirical model to predict the mass flow rate delivered. They incorporated the variation of volumetric efficiency and powder density in a single time-dependent material property, the effective density, as function of the amount of materials in the feeder hopper.

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The aim of this work is to investigate the dynamics of a twin screw feeder for a continuous drug product manufacturing. A hybrid physics/data-based model model, suitable for on-line control and significantly different bulk solids, is suggested.

#### Mathematical model

Self-cleaning concave screws were used in the experiments (twin concave screws, feeder Coperion KT20 and KT35, www.ktron.com), minimizing the possibility that cohesive material adhered on the screw surface. Therefore, no parameters to take into account the reduction of the mass flow rate due to a reduction of the cross sectional area (Yu, 1997) have been included in the model. Furthermore, both agitator and vibrating mechanism (flow aid systems) should preclude arching or ratholing effects in the hopper, hence they are not considered by the model.

Following the aforementioned assumptions, the mass flow rate delivered by the screw feeder can be calculated as:

$$\dot{m}(t) = AnPN\rho_b\eta(t) \tag{1}$$

where A is the overall sectional area, n is the number of starts of the screw thread, P is the pitch,  $\eta$  is the volumetric efficiency, N is the screw speed,  $\rho_b$  the bulk density. The overall sectional area A can be calculated if the following geometrical parameters are known: outside diameter of screw flights  $R_o$ , shaft diameter  $R_c$ , clearance between flight and casing c, distance between the two screw centers  $l_i$ . (see Figure 1).

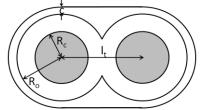


Figure 1. Sketch of cross sectional area.

The volumetric efficiency is described by a 1<sup>st</sup> order differential equation:

$$\tau \frac{d\eta(t)}{dt} + \eta(t) = \alpha W(t)^{\beta}$$
<sup>(2)</sup>

where W(t) is the amount of solid in the hopper, whilst  $\tau$ ,  $\alpha$  and  $\beta$  are parameters achieved from experimental data. Any small variation in the powder density is included in Eq. (2).

#### Results

The model parameters have been estimated for several powders, fitting the experimental data by the *fminsearch* 

function in the MATLAB environment. Excellent agreement between predicted and experimental mass flow rates has been observed (see Figure 2, the mean absolute percentage error is 1.1%). The model satisfactorily predicts the mass output until *W* reaches a lower thresold, different for each powder, below which the mass flow rate abruptly drops. No pulsating output is predicted by the model, as no characteristic frequencies have been identified by Wavelets and Fourier Transforms.

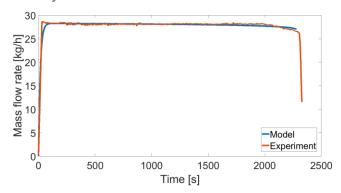


Figure 2. Predicted mass flow using microcrystalline cellulose PH 102, 38.4 rpm, fine twin concave screw, feeder KT35.

Model parameters have been analyzed by PCA (Jackson, 1991) and a negative correlation between  $\tau$  and the screw speed has been observed.

## Conclusions

A semi-empirical model to predict the mass flow rate provided by a twin screw feeder has been proposed. The model has been validated against operational data.

As the model does not require high computational efforts, future works will include the exploration of the model on-line and the identification of alternative control strategies to improve product homogeneity.

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