Modelling and nonlinear model predictive control of a twin screw feeder ⋆

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Abstract: In this work, a dynamic model of a twin screw feeder, for continuous tablet manufacturing, has been developed. In particular, a First Order Plus Dead Time (FOPDT) model has been suggested. The delayed dynamics depends on operating conditions, equipment design and physical properties of the bulk solid. Model parameters are estimated by fitting the model to experimental data. Due to the nonlinear input-output relationships and the time delays involved, a Nonlinear Model Predictive Control (NMPC) is investigated to maintain an accurate mass flow rate, with the ultimate goal to improve product homogeneity in an inherently complex process. The performance of the designed control system is found to be satisfactory in a wide operating range and its potential use in a continuous manufacturing process is worth being investigated in the future.

Keywords: Dynamic modelling; Nonlinear model predictive control; Time-delay systems; Screw feeder; Pharmaceutical.

1. INTRODUCTION

Screw feeders are used to handle and meter bulk solids in continuous tablet manufacturing. They consist of three main elements: i) a hopper, as receptacle of the bulk solids, ii) an agitator at the bottom of the hopper, which acts as a flow-aid system, and iii) a screw which acts as a conveying mechanism, two screws in the case of twin screw feeders. Feed rate accuracy is crucial, as a proper ratio between the mass flow rates of all ingredients is required to obtain the targeted tablet formulation. However, in particular for cohesive materials, the powder flowability may be poor and very noisy feed rates can be achieved. The key parameter is the screw speed, which is constantly adjusted by a built-in feedback control system to continuously correct the mass flow rate.

Despite the increasing research in the last decade in the manufacturing of powder-based products, the development of first-principles models of screw feeders is still limited and a data-driven approach has often been used to address process design, optimisation and control. Boukouvala et al. (2012) suggested a first order delay differential equation to predict the time-dependant mass flow rate $\dot{m}(t)$:

$$\tau \frac{d\dot{m}(t)}{dt} + \dot{m}(t) = kN(t) \tag{1}$$

$$\theta \frac{\partial \dot{m}_{actual}(t,z)}{\partial t} = - \frac{\partial \dot{m}_{actual}(t,z)}{\partial t} \tag{2}$$

In equation (1) τ is the time constant, k is the process gain and $N(t)$ is the screw speed, whilst in equation (2) θ is the time delay factor, $\dot{m}_{actual}(t,z)$ is the actual, delayed, mass flow rate and z refers to the time delay domain. The initial condition on mass flow rate is $\dot{m}_{actual}(t, z = 0) = \dot{m}(t)$.

Escotet-Espinoza et al. (2015) proposed a semi-empirical model, expressing the mass flow rate as a function of the so-called feed factor *ff(t)*:

$$\dot{m}(t) = ff(t)N(t) \tag{3}$$

The feed factor, which is an indicator of the degree of fill of the screws, is assumed to be related to the mass of solid in the hopper $m(t)$ according to the following pseudo-first order relationship:

$$\frac{1}{\beta} \frac{d[ff(t)]}{d[m(t)]} + ff(t) = ff(t)^{level}_{sat} \tag{4}$$

where β and $ff(t)^{sat}_{level}$ are model parameters.

Engisch and Muzzio (2012) described the performance of screw feeders using an experimental and statistical approach.

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Yu and Arnold (1996) and Roberts (1999) proposed mechanistic models to estimate the output flow rate in screw conveyors. However, they did not consider the effect of the hopper fill level on the flow rate, which was in fact assumed time-independent.

Several control systems for continuous pharmaceutical processes have been proposed (Ramachandran et al., 2011; Singh et al., 2012, 2013, 2014). Singh et al. (2012) suggested a combined single loop feedback-cascade strategy for continuous tablet manufacturing. They also investigated a hydrid PID–Model Predictive Control (MPC) system (Singh et al., 2013). MPC is a popular optimisation-based control strategy, where a cost function is minimised over a future time horizon and an optimal control input sequence is generated.

Processes involving time delays and complex input-output couplings may benefit from a Nonlinear Model Predictive Control (NMPC) (Grimard et al., 2017). To the best of our knowledge, there is no study on the application of NMPC to powder feeding processes.

The aim of this work is to develop a semi-empirical mathematical model of twin screw feeders. Due to the presence of nonlinearities and a time delay, the potential use of a nonlinear model-based control of the feed rate is investigated.

2. MATHEMATICAL MODELLING

The mathematical model of a twin screw feeder is presented in section 2.1. The methodology used for parameter identification and the estimated model parameters are discussed in section 2.2, whilst the simulated mass flow rates are compared with experimental data in section 2.3.

2.1 Dynamic model

A First Order Plus Dead Time (FOPDT) model has been developed to predict the powder mass flow rate out of a twin screw feeder:

$$\tau \frac{d\dot{m}(t)}{dt} + \dot{m}(t) = \dot{m}_{level}(t) \tag{5}$$

$$\dot{m}_{actual}(t) = \dot{m}(t-\theta) \tag{6}$$

where τ is the time constant, $\dot{m}_{actual}(t)$ is the actual, delayed, mass flow rate, θ is the dead time. The mass flow rate $\dot{m}_{level}(t)$, in equation (5), represents the maximum, noise-free, mass flow rate that can be reached after $t \approx 4\tau + \theta$. This mass flow rate is calculated via a physics-based approach from the bulk density of the powder ρ_b, the screw speed $N(t)$, the volumetric efficiency $\eta(t)$ and the twin screws geometry according to the following equation:

$$\dot{m}_{level}(t) = \rho_b n P N(t) A \eta(t) \tag{7}$$

where n is the number of starts of the screw thread, P is the screw pitch and A is the cross-sectional area, calculated as follows:

$$A = 2\pi(R_o^2 - R_c^2) + \pi(2cR_o + c^2) + 2cl_t + 2R_o l_t - \pi R_o^2 \tag{8}$$

The parameters R_o, R_c, c and l_t in equation (8) are geometrical details of the twin screws, as depicted in Fig. 1. The volumetric efficiency $\eta(t)$, assumed time-dependant, is estimated from the following empirical correlation:

$$\eta(t) = \alpha m(t)^{\beta} \tag{9}$$

where α and β are model parameters and $m(t)$ is the mass of solid in the hopper, continuously adjusted by a mass balance in the system (the mass of powder in the twin screws is negligible):

$$m(t) = m_{initial} - \dot{m}_{actual}(t)t \tag{10}$$

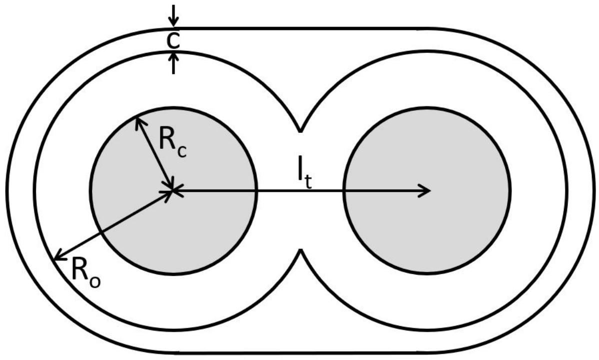

Fig. 1. Sketch of the cross-sectional area of twin screw feeders.

2.2 Parameter estimation

The model described in section 2.1 involves four parameters:

i. τ, the time constant in equation (5);
ii. θ, the dead time in equation (6);
iii. α and β, relating the mass of powder in the feeder hopper and the volumetric efficiency in equation (9).

The parameters above have been identified by fitting the model to experimental data, kindly provided by Eli Lilly and Company. The experimental investigations were carried out using two different twin screw feeders, Coperion K-Tron 20 and Coperion K-Tron 35, several operating conditions and six bulk solids: mannitol SD-100, lactose monohydrate, microcrystalline cellulose PH Avicel 101, microcrystalline cellulose PH Avicel 102, crosscarmellose sodium and sodium stearyl fumarate. A total of 16 experiments were carried out. The main physical properties of the powders used are listed in Table 1.

The model parameters have been estimated formulating an unconstrained optimisation problem where the objective function, to minimise, is the Mean Square Error MSE:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_{exp} - y_{model})^2 \tag{11}$$

The experimental measurements are calculated as $\dot{m}_{exp} = \Delta m_{exp}/\Delta t$. The resulting data were considered excessively noisy and, hence, were smoothed by a thirty-point centred moving average. Furthermore, any negative flow rates, when present, were removed from the data set.

The *fminsearch* optimiser in the MATLAB environment has been used. Equation (5) has been solved using the

Table 1. Physical properties of the bulk solids investigated. Symbols: HR Hausner ratio, FFc flow function coefficient, d_{32} mean diameter over surface, d_{43} mean diameter over volume, ρ_b bulk density.

Bulk solid	HR [-]	FFc [-]	d_{32} [µm]	d_{43} [µm]	ρ_b [kg m^{-3}]
Mannitol SD-100	1.19	19.7	83.8	116.5	470
Lactose monohyd.	1.22	9.7	74.5	127.5	600
Microcryst. cell. PH 101	1.41[1]	4.8	25.8	74.7	340[2]
Microcryst. cell. PH 102	1.35[1]	6.7	40.5	129.4	360[2]
Crosscarm. sodium	1.38	7.0	18.3	58.0	520
Sodium stear. fumarate	1.59	3.5	8.2	24.3	260

[1] from Sun (2010)
[2] from Zhang et al. (2003)

solver *ode45*, based on an explicit Runge–Kutta (4,5) formula. The estimated parameters are listed in Table 2.

The dead times identified are strongly affected by the physical properties of the bulk solids, which affect the withdrawal of the powder from the hopper outlet, and the screw speed. For some powders the dead time decreases as the screw speed increases: this can be explained by the reduced residence time of the powder within the twin screws. In three cases, the dead time θ identified by the optimiser is zero. This is due to the conduction of the experimental investigations in question: the motor had been initially turned on for a short time and then turned off, before the actual experiment started. This was due to overcome some initial reluctance of the material in the feeder hopper to flow downwards. In those three cases, when the actual experiment started a certain amount of material was already present on the surface of the screws and, hence, a mass flow rate was immediately recorded.

2.3 Simulation results

The mass flow rates predicted by the FOPDT model, for a variety of materials and operating conditions, are compared with the experimental measurements in Figures 2–9. In all simulations, the screw speed is constant (open loop system). The feeding operations are simulated until the hopper fill level reaches a minimum value, different for each material, which corresponds to an abrupt drop in the experimental mass flow rate.

In general, the predicted feed rates are in good agreement with the experimental data. In all the illustrated cases, it can be observed how the mass flow rate decreases during time, accordingly to the decreasing hopper fill level and, hence, the decreasing pressure exerted on the powder accessing the twin screws. The FOPDT model captures well the dynamic response of the system for all cases investigated, despite the significant difference in physical properties, feeder geometries and operating conditions.

Figures 2 and 3 show the simulated mass flow rate when feeding mannitol SD-50 with, respectively, feeder K-Tron 20 and feeder K-Tron 35. In both cases, a low screw

Table 2. Estimated model parameters.

Bulk solid	Screw speed [rpm]	α [kg^{-1}]	β [-]	τ [s]	θ [s]	MSE
Mannitol SD-100[1]	7.71	0.39	0.097	119.4	55.2	0.340
Mannitol SD-100[1]	77.10	0.73	0.055	14.6	5.6	0.432
Mannitol SD-100[2]	6.40	0.95	0.013	18.0	47.3	0.013
Mannitol SD-100[2]	19.20	1.00	0.003	15.0	5.4	0.210
Lactose monohydr.[1]	7.71	0.07	0.888	68.8	210.1	0.003
Lactose monohydr.[1]	77.10	0.66	0.077	15.5	0.0	0.375
Microcryst. cellulose PH 101[1]	7.71	0.37	0.084	0.2	0.0	0.003
Microcryst. cellulose PH 101[1]	38.50	0.20	0.005	14.0	33.5	0.002
Microcryst. cellulose PH 102[1]	7.71	0.46	-0.017	13.5	91.8	0.002
Microcryst. cellulose PH 102[1]	77.10	0.74	0.058	15.7	0.0	0.246
Microcryst. cellulose PH 102[2]	6.40	0.78	0.010	16.5	103.3	0.009
Microcryst. cellulose PH 102[2]	38.40	0.82	0.016	11.8	4.4	0.150
Crosscarm. sodium[1]	7.71	0.41	0.061	41.9	64.5	0.341
Crosscarm. sodium[1]	61.70	0.44	0.091	12.6	28.2	0.069
Sodium stearyl fumarate[1]	7.71	0.38	0.113	8.6	106.0	0.002
Sodium stearyl fumarate[1]	61.70	0.38	0.091	19.0	7.7	0.003

[1] Using feeder K-Tron 20
[2] Using feeder K-Tron 35

speed (equivalent to the 5% of the drive command) has been used. Geometry of hoppers and twin screws are significantly different, as well as the initial hopper fill level. However, the model predictions are satisfactory for both cases. Both simulations involve a significant dead time, around 50 s, which is difficult to notice from the figures as the duration of the feeding operations is in the order of some hours.

At low screw speed, a significant initial delay in the mass flow rate can be observed when feeding lactose monohydrate (see Fig. 4), crosscarmellose sodium (see Fig. 6) and sodium stearyl fumarate (see Fig. 8). When the screw speed is significantly increased, the dynamic response of the system shows a marked reduction in the dead time, as can be seen in Figures 5, 7 and 9 when feeding lactose monohydrate, crosscarmellose sodium and sodium stearyl fumarate, respectively.

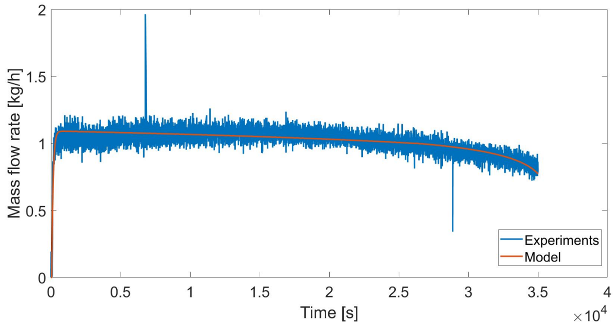

Fig. 2. Simulated and experimental mass flow rates using mannitol SD-100, feeder K-Tron 20, 7.71 rpm.

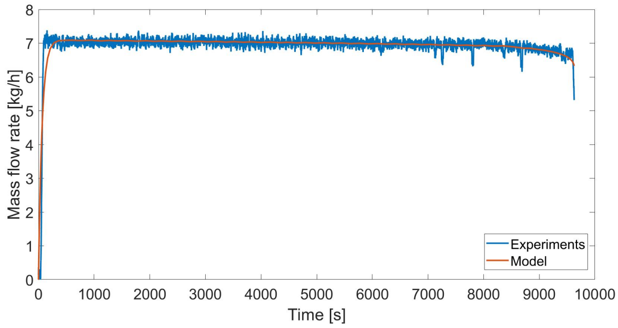

Fig. 3. Simulated and experimental mass flow rates using mannitol SD-100, feeder K-Tron 35, 6.4 rpm.

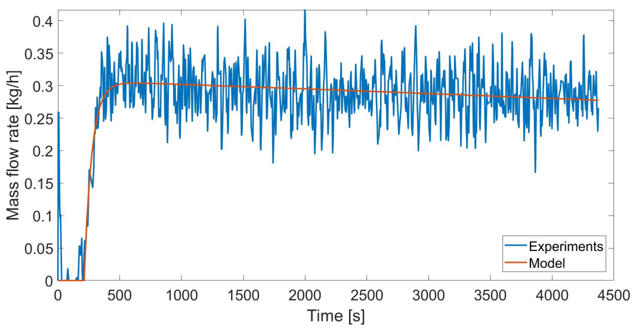

Fig. 4. Simulated and experimental mass flow rates using lactose monohydrate, feeder K-Tron 20, 7.1 rpm.

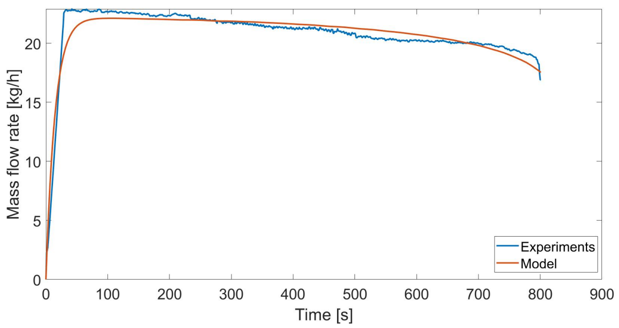

Fig. 5. Simulated and experimental mass flow rates using lactose monohydrate, feeder K-Tron 20, 77.1 rpm.

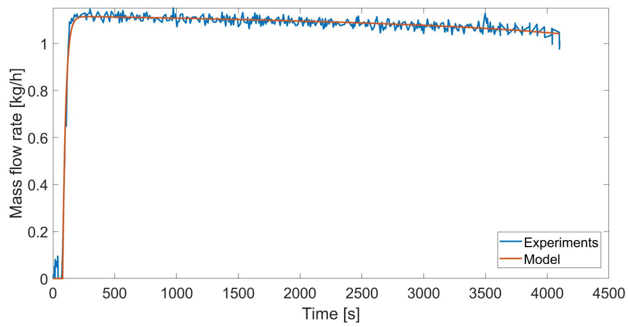

Fig. 6. Simulated and experimental mass flow rates using crosscarmellose sodium, feeder K-Tron 20, 7.71 rpm.

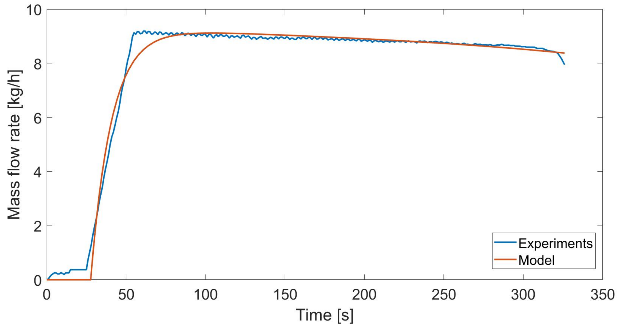

Fig. 7. Simulated and experimental mass flow rates using crosscarmellose sodium, feeder K-Tron 20, 61.7 rpm.

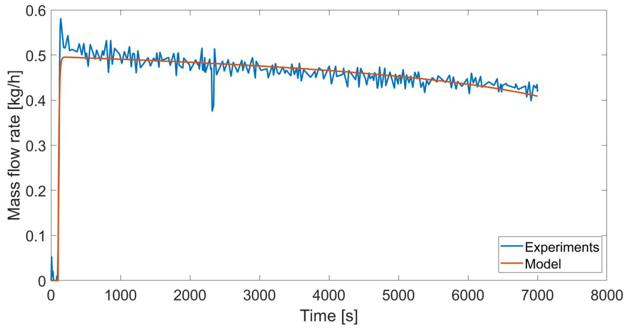

Fig. 8. Simulated and experimental mass flow rates using sodium stearyl fumarate, feeder K-Tron 20, 7.71 rpm.

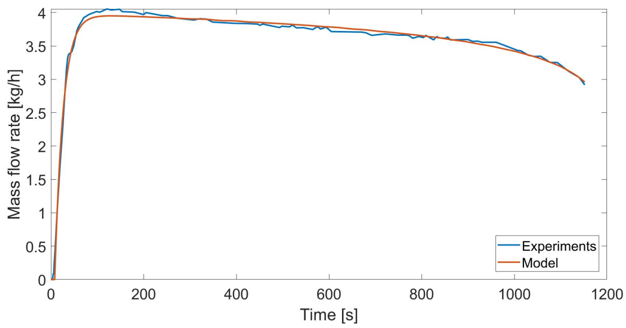

Fig. 9. Mass flow rate of sodium stearyl fumarate, feeder K-Tron 20, 61.7 rpm.

3. NONLINEAR MODEL PREDICTIVE CONTROL

NPMC can be suitable for processes with complex input-output couplings, nonlinearities and time delays (Grimard et al., 2017). The application of NMPC, to adjust the screw speed in order to maintain an accurate powder feed rate, has been investigated in this section. The cost function J used in this work can be described by the generic expression:

$$J = \sum_{i=1}^{N_P} w_y (y_{k+i} - y_{k+i}^{SP})^2 + \sum_{k=1}^{N_C} w_{\Delta u} \Delta u_{k+i}^2 + + \sum_{k=1}^{N_C} w_u (u_{k+i} - \bar{u})^2 \quad (12)$$

where y is the controlled variable, u is the manipulated variable, k is the discrete time, N_P is the horizon prediction, N_C is the horizon control, $\bar{u}$ is the nominal value of u. In this case, y and u are, respectively, mass flow rate and screw speed. The coefficients w_y, $w_{\Delta u}$ and w_u represent the weight of each term in equation (12). The first term indicates the accuracy of the setpoint tracking, the second term is used to penalises the incremental change, the third term is included to avoid large deviations from the nominal value of the actuators (Singh et al., 2013). The NMPC weights are tuned to meet setpoint tracking according to the Integral of Time Absolute Error (ITAE) criteria, i.e. minimising the following integral (Singh et al., 2012):

$$ITAE = \int_{t_0}^{t} t|y - y^{SP}|dt \quad (13)$$

Investigated bulk solid and feeder are, respectively, mannitol SD-100 and K-Tron 20. A significant setpoint step change has been considered to tune the NMPC weights, from 5 kg h^{-1} to 15 kg h^{-1}. In the continuous tablet manufacturing, when using mannitol and K-Tron 20, the screw speed can vary, approximately, in the range experimentally investigated (from 7.7 rpm to 77 rpm). This range corresponds to a mass flow rate potentially ranging from approximately 1 kg h^{-1} to 20 kg h^{-1}.

The solver *fminsearch* has been used to minimise the integral in equation (13), whereas the *fmincon* solver has been used to optimise the control input sequence in the future horizons. Horizons and control interval Δt have been chosen over a range of typical values and such that $N_P - N_C \geq \theta_{max}/\Delta t$, where θ_{max} is the maximum delay possible (Singh et al., 2013), i.e. 119.4 s (see Table 2). The resulting control parameters are listed in Table 3.

The optimal values of the NMPC weights are significantly affected by the physical properties of the powder and must be identified for each material. For example, applying the methodology described above to tune the NMPC weights considering microcrystalline cellulose Avicel PH 102, the optimal value of $w_{\Delta u}$ is 0.421, whilst the other weights are close to the values in Table 3.

The NMPC control is simulated allowing the screw speed to vary in the entire operating range experimentally investigated, to assess the performance of the NMPC during significant setpoint changes. The model parameters in Table 2, including the dead time, are assumed to vary linearly with the screw speed, between their values calculated at highest and lowest speed for fixed material and feeder.

Table 3. NMPC controller parameters.

Parameter	Value
N_P	5
N_C	2
Δt [s]	30
w_y	1
$w_{\Delta u}$	5.3×10^{-3}
w_u	6.0×10^{-4}
N_{min} [rpm]	7.71
N_{max} [rpm]	77.10

The use of mannitol SD-100 and feeder K-Tron 20 is investigated in this case study. In these conditions, the delay ranges from approximately 55 s, at the lowest screw speed experimentally investigated, to 6 s, at the highest screw speed experimentally investigated.

The effectiveness of the NPMC controller has been evaluated introducing setpoint changes and disturbances according to the following sequence:

1. from 0 s to 500 s, the setpoint is equal to 5 kg h^{-1};
2. at 500 s, the setpoint is increased to 15 kg h^{-1};
3. at 1000 s, the setpoint is decreased to the original value (5 kg h^{-1});
4. at 1500 s, the setpoint is increased to 15 kg h^{-1} and, simultaneously, the model parameter α is decreased by 10%.

Furthermore, a uniform white noise, with zero mean and 5% relative standard deviation, is added to the predicted feed rate to emulate noise measurements at t=1000 s. Setpoint changes at t= 500 s, 1000 s and 1500 s are assumed to be unpredicted events. Hence, they are not considered by the NMPC controller in the future time horizon until they occurred.

The *fmincon* optimiser has been used to solve this constrained nonlinear optimisation problem, using the *trust-region-reflective* algorithm.

The performance of the designed control is shown in Fig. 10, whilst the variation of the control input is depicted in Fig. 11. In general, the setpoint tracking performance is satisfactory. When the setpoint is significantly increased, at t=500 s, the dynamic response of the system is fast and the new sepoint is reached in approximately 100 s. When the setpoint is markedly decreased, at t=1000 s, the targeted mass flow rate is reached in approximately 250 s. The slower dynamic response, at the lower setpoint, is consistent with the larger time constant and dead time identified at lower screw speeds for this material (see Table 2). After the second setpoint increase, at t=1500 s, the desired feed rate is reached in approximately 150 s, slower when compared to the first setpoint increase (at t=500 s). This is due to the introduction of noise (at t=1000 s) and parameter uncertainty (at t=1500 s) into the system. The reduction of α leads to a reduction in the predicted mass flow rate, according to equations (5)–(9), hence an increase in the screw speed is needed. This increase, together with the simulated noise, leads to a positive peak larger than the setpoint by approximately 10%, before reaching the desired feed rate in approximately 150 s.

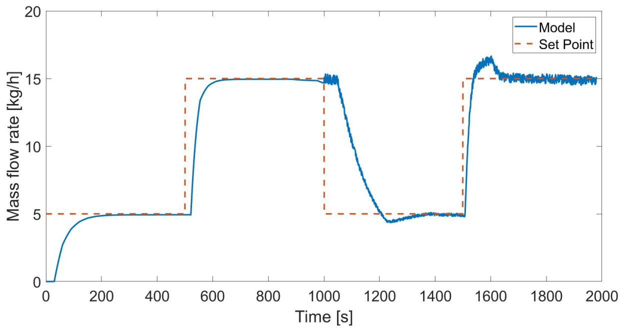

Fig. 10. Mass flow rate (output) predicted by the control system (continuous blue line) and variation of the setpoint in time (red dashed line).

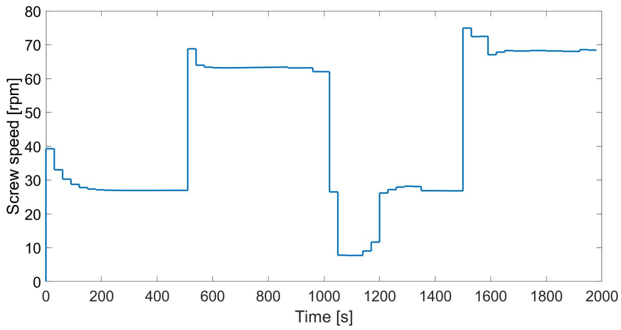

Fig. 11. Variation of the screw speed (input) in time, with the designed NPMC.

As the computational effort is not an issue (approximately 150 s with a 4-core 3.7 GHz processor), the application of this NMPC for on-line control may be further investigated.

4. CONCLUSIONS

A First Order Plus Dead Time (FOPDT) model has been proposed to predict the powder mass flow rate out of a twin screw feeder. A good agreement between predicted and experimental mass flow rate has been observed for various materials, operating conditions and feeder geometries.

Due to the presence of time delays and nonlinearities, the application of NMPC has been investigated to regulate the powder feed rate at its setpoints. The feed accuracy is essential to meet the desired drug formulation in continuous tablet manufacturing. The control input is the screw speed, the main operating variable affecting the dynamics of the system. The effectiveness of the controller has been investigated over a wide operating range, in terms of screw speed. In particular, significant setpoint changes and disturbances have been introduced into the system, such as simulated noise measurements and model uncertainties. The setpoint tracking is satisfactory, although the control input has been generated by local optimisations.

As no issues related to the computational complexity of the NMPC method have been encountered, this strategy may be further investigated for real-time control of feeders.

The developed model can be used to develop alternative and customised model-based control strategies, identify the original equipment manufacturer control system and optimise the refill operations, where the process operates in an open loop mode for a short time window.

Future works will focus on the modelling of the stochastic high frequency variations in the mass flow rate. Furthermore, the impact of the material properties on the effective density within the screws will be investigated.

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