Available online at www.sciencedirect.com

ScienceDirect

IFAC PapersOnline CONFERENCE PAPER ARCHIVE

IFAC PapersOnLine 52-1 (2019) 329–334

Lyapunov-based online parameter estimation in continuous fluidized bed spray agglomeration processes

Ievgen Golovin [*,⋆] **Eric Otto** [*] **Robert Dürr** [**] **Stefan Palis** [*,***] **Achim Kienle** [*,**]

[*] *Otto-von-Guericke University, D-39106 Magdeburg, Germany*
[**] *Max-Planck-Institute for Dynamics of Complex Technical Systems, D-39106 Magdeburg, Germany*
[***] *National Research University "Moscow Power Engineering Institute", Moscow, Russia*

Abstract: Fluidized bed spray agglomeration is a particle formation process in many industrial applications, e.g. pharmaceutical and food processing. The properties of the formed agglomerates, like characteristic volume, significantly affect the product quality and can be affected by variation of certain operating parameters. Mathematical modeling not only provides an abstract characterization of the effects of those on the product properties but also supports thorough understanding of the underlying physical and chemical mechanisms. Moreover, it enables application of advanced process analysis, control and intensification schemes. As characteristic properties underlie variations within the ensemble of agglomerates the process can be described as a distributed parameter system, where the resulting model equations are partial differential equations. Adaption to experimental data requires the solution of inverse problems, which tend to be ill-conditioned. As an alternative approach, in this contribution an adaptive identification procedure is presented. Therefore, a modified plant model is run in parallel to the process and adaption rates are chosen based on a Lyapunov-function. The approach is validated in a parametric study for two scenarios: In the first, it is assumed that the structure of the dynamics is fully known, while in the second, this assumption does not hold. It is shown that the proposed approach allows to reconstruct unknown kinetic information of the process dynamics.

Keywords: Adaptive identification, distributed parameter systems, population balance equations, partial differential equations

1. INTRODUCTION

Agglomeration is a particle formation process in which at least two primary particles are combined to form a new one. This principle is often used in many industries, e.g. pharmaceutical manufacturing and food processing. The properties of the formed agglomerates, e.g. size, shape and porosity, significantly affect its end-use properties, e.g re-hydration behavior of food powders, processability and storeability. In the industrial practice, agglomerates are often formed in drums, pans or fluidized beds. The advantages of the latter include good mixing and high heat and mass transfer between particles, liquid and gas phase. Compared to widely applied batch processes, the additional benefits of operating in continuous mode are constant product quality and higher flow rates which are more attractive for chemical, food and pharmaceutical industries. For those reasons focus in this contribution is on continuous fluidized bed spray agglomeration, which was not in the focus of research efforts so far.

The process scheme is shown in Fig. 1: Particles in the the chamber are fluidized by a stream of hot air from the bottom, liquid binder is sprayed on the particles in the form of small droplets to make them wet and sticky. Due to random collisions liquid bridges between particles are formed. These can become solid by drying and thereby agglomerate particles consisting of different numbers of individuals are formed. The formation of the agglomerates and thereby the product properties can be influenced by variation of different operating parameters and process configurations, like feed rate, binder concentration and temperature of the drying/fluidizing air.

Parameterization of process models is an important part within the interplay of process analysis, model-based control and process intensification. It is well-known that the individual properties, like characteristic size or porosity, differ from particle to particle in the studied process. The emerging heterogeneity significantly affects the overall product properties. It can be accounted for in the framework of population balance modeling (PBM) (Ramkrishna, 2000). The resulting model equations generally represent nonlinear integro partial differential equations, which are usually discretized and numerically solved with established techniques (see e.g. Kumar et al. (2006), Bück et al. (2012) and the references therein). Commonly, reliable first principles models that include detailed models on the underlying kinetic processes on the microscopic

⋆ Correponding author: ievgen.golovin@ovgu.de

2405-8963
Peer review under responsibility of International Federation of Automatic Control.
10.1016/j.ifacol.2019.06.083

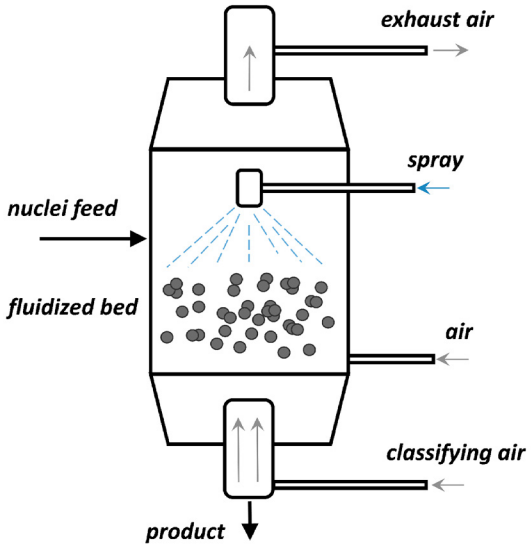

Fig. 1. *Schematic representation of fluidized bed spray agglomeration process*

scale are rarely found and thus kinetics are described in a more mechanistic fashion. This requires the estimation of unknown parameters from experimental data. The resulting inverse problems often tend to be ill-conditioned (Chakraborty et al., 2015). In order to overcome these problems a parameter identification based on the nonlinear optimization (Golovin et al. (2018)) as well as an online parameter estimation approach featuring a parallel model can be applied (Dürr et al., 2015; Palis and Kienle, 2013, 2017).

In this contribution, a new adaptive online estimation approach for fluidized bed spray agglomeration processes is developed. In particular, focus is on identification of the agglomeration kernel containing information on the effects of process conditions and characteristic agglomerate size on formation of new agglomerates.

Section 2 presents the modeling of the fluidized bed spray agglomeration process. The proposed Lyapunov-based adaptive approach applied for the agglomeration kernel estimation is described in section 3. In section 4 the presented method is validated within two simulation studies.

2. POPULATION BALANCE MODELING OF FLUIDIZED BED SPRAY AGGLOMERATION

In particle formation processes, significant heterogeneities with respect to the individual particle properties like size or shape emerge. Population balance modeling represents an established concept to describe such distributed parameter systems. Instead of describing a large number of particles and their interactions, PBM describes the dynamics of the particles via the number density distribution function (NDF) $n(t, \mathbf{x})$ representing information of the number of particles within an infinitesimal section of the particle property state space $\mathbf{x} \in \mathbb{R}^{N_x}$. In the following, it is assumed that individual particles do only differ w.r.t. characteristic volume v such that $\mathbf{x} = v$ and $N_x = 1$. In course of the process, the particle distribution underlies change, which is given by the solution of the so called population balance equation (PBE)

$$\frac{\partial n(t,v)}{\partial t} = \dot{n}_{\text{feed}}(t,v) - \dot{n}_{\text{prod}}(t,v) + \dot{n}_{\text{agg}}(t,v)\,. \tag{1}$$

The corresponding initial NDF is given as

$$n(0,v) = N_\Sigma \frac{\exp(\frac{-(v-\mu_1)^2}{2\sigma_1^2})}{\int_0^\infty \exp(\frac{-(v-\mu_1)^2}{2\sigma_1^2})\,\mathrm{d}v}\,, \tag{2}$$

where N_Σ is the mass normalizing parameter.

The left hand side of (1) accounts for temporal evolution while the first two elements of the right hand side describe feeding new seed particles to and removal of the desired product from the fluidized bed. Both are assumed to be known and given as

$$\dot{n}_{\text{prod}}(t,v) = N_{out} K(v) n(t,v)\,, \tag{3}$$

$$\dot{n}_{\text{feed}}(t,v) = N_{in} \frac{\exp\left(\frac{-(v-\mu_2)^2}{2\sigma_2^2}\right)}{\int_0^\infty \exp\left(\frac{-(v-\mu_2)^2}{2\sigma_2^2}\right)\,\mathrm{d}v}\,, \tag{4}$$

where N_{out} and N_{in} denote the time-invariant removal and feed rates of particles, respectively while $K(v)$ represents the separation function. The last element of the right hand side denotes the formation of new particles of volume v by agglomeration of two particles with volumes u and $v-u$

$$\begin{aligned}\dot{n}_{agg}(t,v) &= \dot{n}^+_{agg}(t,v) - \dot{n}^-_{agg}(t,v)\\ &= \frac{1}{2}\int_0^v \beta(t,u,v-u)n(t,u)n(t,v-u)\mathrm{d}u\\ &\quad - \int_0^\infty \beta(t,u,v)n(t,v)n(t,u)\mathrm{d}u\,.\end{aligned} \tag{5}$$

Here, the agglomeration kernel $\beta(t,u,v)$ contains information about the probability of forming a new agglomerate and is usually separated in volume and time-dependent parts

$$\beta(t,v,u) = \beta_0(t)\beta(v,u)\,. \tag{6}$$

For modeling of the volume-dependent part, called coalescence kernel, different approaches exist (see e.g. (Eisenschmidt et al., 2017) and (Le Borne et al., 2015)). Two possibilities are the Brownian kernel, which is derived from the Brownian motion,

$$\beta(u,v) = (u^{1/3} + v^{1/3})(u^{-1/3} + v^{-1/3}) \tag{7}$$

or a more general kernel structure approximation using a Laurent-polynomial

$$\beta(u,v) = \sum_{i=-N_L}^{N_L}\sum_{j=-N_L}^{N_L} k_{i,j} v^i u^j\,, \tag{8}$$

where $N_L \in \mathbb{N}$ denotes the rank of the polynomial and $k_{i,j}$ are the associated polynomial coefficients.

In contrast, the time dependent part $\beta_0(t)$, also called the agglomeration efficiency, mirrors the effects of the process conditions and operating parameters and is mostly not known beforehand. Moreover, it is frequently assumed that the time dependency of the agglomeration efficiency can be neglected, such that $\beta_0(t) = const.$

3. LYAPUNOV-BASED ADAPTIVE IDENTIFICATION

In this section the online parameter identification of the agglomeration kernel is introduced. In order to derive an adaptation law for the unknown parameters the Lyapunov-based approach is applied (Krstic, 2006; Palis and Kienle,

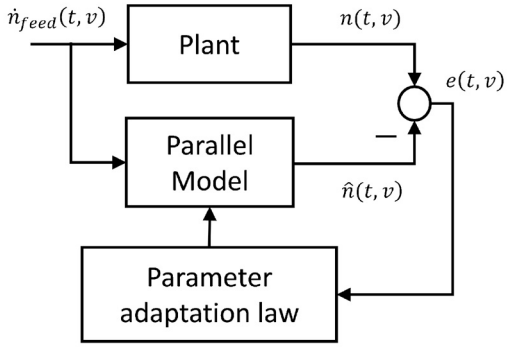

Fig. 2. *Adaptive online parameter identification scheme*

2013; Dürr et al., 2015; Palis and Kienle, 2017). The parameter identification scheme consisting of a modified plant model, which runs parallel to the actual plant and the parameter adaptation algorithm is represented in Fig. 2.

In this work two scenarios for the parameter estimation are studied. In the first scenario, the modified plant model includes the volume-dependent Brownian kernel function with unknown agglomeration efficiency β_0, which should be estimated. In the second scenario, it is considered that the structure of the coalescence kernel $\beta(u,v)$ is also unknown. In order to approximate it, the Laurent polynomial with its unknown coefficients is included in the modified plant model.

3.1 Estimation of the agglomeration efficiency

In the first scenario, the estimation of the agglomeration efficiency β_0 is considered. For this reason, the modified parallel plant model with an additional observer term can be represented as follows

$$\begin{aligned}\frac{\partial \hat{n}(t,v)}{\partial t} &= \dot{n}_{\text{feed}}(t,v) - \dot{n}_{\text{prod}}(t,v) + \dot{n}_{\text{agg}}(t,v) \\ &\quad + l\,(\hat{n}-n)\,, \qquad (9)\\ \dot{n}_{agg}(t,v) &= \frac{1}{2}\int_0^v \hat{\beta}_0\beta(u,v-u)n(t,u)n(t,v-u)\mathrm{d}u \\ &\quad - \int_0^\infty \hat{\beta}_0\beta(u,v)n(t,v)n(t,u)\mathrm{d}u\,, \qquad (10)\end{aligned}$$

where $\hat{n}$ and $\hat{\beta}_0$ are the particle size distribution and the agglomeration efficiency estimated from the modified plant model and l is an additional tuning parameter.

The related estimation errors are given by

$$e = \hat{n} - n\,, \qquad \tilde{\beta}_0 = \hat{\beta}_0 - \beta_0\,. \qquad (11)$$

Taking into account the plant model equations (1), (5) and the modified parallel model equations (9), the error dynamics can be derived as

$$\begin{aligned}\frac{\partial e}{\partial t} &= \frac{1}{2}\int_0^v \tilde{\beta}_0\beta(u,v-u)n(t,u)n(t,v-u)\mathrm{d}u \\ &\quad - \int_0^\infty \tilde{\beta}_0\beta(u,v)n(t,v)n(t,u)\mathrm{d}u + l\,e\,. \qquad (12)\end{aligned}$$

For the adaptation of the model parameters the following Lyapunov functional is chosen

$$V = \frac{1}{2}\int_0^\infty e^2\mathrm{d}v + \frac{1}{2\gamma}\tilde{\beta}_0^2\,, \qquad (13)$$

where γ is a positive real tuning parameter. It can be easily seen that the Lyapunov functional V is positive definite and it vanishes if the considered estimation errors (11) are zeros. According to the Lyapunov stability theory the stability of the proposed identification scheme can be achieved if the first time derivative of the Lyapunov functional is negative semi-definite along the state trajectories. This time derivative can be derived as follows

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}t} &= \int_0^\infty l\,e^2\mathrm{d}v \\ &\quad + \int_0^\infty e\Big(\frac{1}{2}\int_0^v \tilde{\beta}_0\beta(u,v-u)n(t,u)n(t,v-u)\mathrm{d}u \\ &\quad - \int_0^\infty \tilde{\beta}_0\beta(u,v)n(t,v)n(t,u)\mathrm{d}u\Big)\mathrm{d}v \\ &\quad + \frac{1}{\gamma}\tilde{\beta}_0\dot{\tilde{\beta}}_0\,. \qquad (14)\end{aligned}$$

Therefore, choosing the adaptation law $\dot{\hat{\beta}}_0$ as follows

$$\begin{aligned}\dot{\hat{\beta}}_0 &= -\gamma\int_0^\infty e\Big(\frac{1}{2}\int_0^v \beta(u,v-u)n(t,u)n(t,v-u)\mathrm{d}u \\ &\quad - \int_0^\infty \beta(u,v)n(t,v)n(t,u)\mathrm{d}u\Big)\mathrm{d}v \qquad (15)\end{aligned}$$

yields in the negative semi-definiteness of the time derivative of V

$$\frac{\mathrm{d}V}{\mathrm{d}t} = \int_0^\infty l\,e^2\mathrm{d}v \qquad (16)$$

for the observer parameter $l < 0$.

3.2 Estimation of the Laurent polynomial

In the second scenario, the estimation of the volume-dependent agglomeration kernel function is proposed. In general, the aggregation kernel $\beta(u,v)$ is a non-negative symmetric function of two variables. In order to approximate such types of functions, Laurent polynomials (8) can be used (Eisenschmidt et al., 2017). A reasonable approximation can be achieved with the rank $N_L = 1$ resulting in

$$\begin{aligned}\beta_{est}(u,v) &= k_1 + k_2\,v^{-1}u^{-1} + k_3\,vu + k_4\,(v^{-1}+u^{-1}) \\ &\quad + k_5\,(vu^{-1}+v^{-1}u) + k_6\,(v+u)\,. \qquad (17)\end{aligned}$$

Here, k_1 to k_6 are unknown polynomial coefficients that should be identified. The modified parallel model with the polynomial is given by

$$\begin{aligned}\frac{\partial \hat{n}(t,v)}{\partial t} &= \dot{n}_{\text{feed}}(t,v) - \dot{n}_{\text{prod}}(t,v) + \dot{n}_{\text{agg}}(t,v) \\ &\quad + l\,(\hat{n}-n)\,, \qquad (18)\end{aligned}$$

where

$$\begin{aligned}\dot{n}_{agg}(t,v) &= \frac{1}{2}\int_0^v \beta_{est}(u,v-u)n(t,u)n(t,v-u)\mathrm{d}u \\ &\quad - \int_0^\infty \beta_{est}(u,v)n(t,v)n(t,u)\mathrm{d}u\,. \qquad (19)\end{aligned}$$

Analogous to the aforementioned design procedure, the adaptation law for the polynomial coefficients can be derived as

$$\begin{aligned}\dot{\hat{k}}_i &= -\gamma_i\int_0^\infty e\Big(\frac{1}{2}\int_0^v f_i(u,v-u)n(t,u)n(t,v-u)\mathrm{d}u \\ &\quad - \int_0^\infty f_i(u,v)n(t,v)n(t,u)\mathrm{d}u\Big)\mathrm{d}v\,, \qquad (20)\end{aligned}$$

where $f_i(u,v)$ is the volume dependent part associated with i-th coefficient of (17).

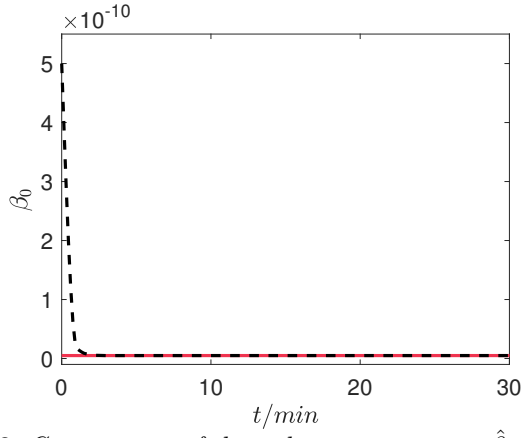

Fig. 3. *Convergence of the unknown parameter $\hat{\beta}_0$ (dotted, black) to the actual parameter β_0 (solid, red)*

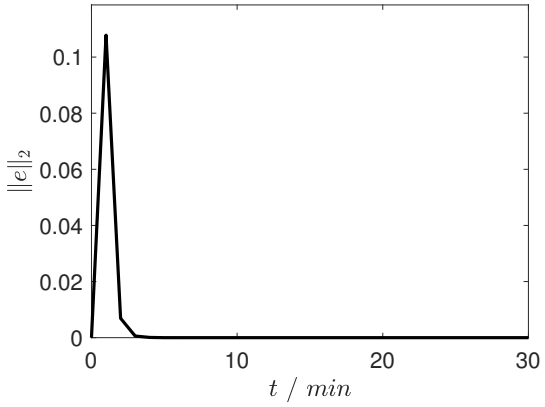

Fig. 4. *L_2 - norm of the error in time*

Table 1. *Model parameters used for simulation*

Parameter	Value	Parameter	Value
μ_1	$3.6 \cdot 10^{-12}$	σ_1	$1 \cdot 10^{-12}$
N_Σ	$7.5 \cdot 10^{8}$	σ_2	$1 \cdot 10^{-12}$
μ_2	$3.6 \cdot 10^{-12}$	N_{out}	$5 \cdot 10^{-4}$
N_{in}	$4 \cdot 10^{5}$		

4. RESULTS

The proposed parameter estimation approach has been implemented for numerical computations in MATLAB. For the solution of the population balance equations the method of lines is applied. Here, the internal coordinate, i.e. the particle volume, is lumped using the cell-average method (Kumar et al., 2006) on a logarithmic grid with $n_v = 55$ grid points. In order to solve the set of the ordinary differential equations and to overcome the stiffness problems the *ode15s* solver has been used. For the simulations the actual plant model with the Brownian motion coalescence kernel (7) and the scalar agglomeration efficiency $\beta_0 = 5 \cdot 10^{-12}$ is considered. The model parameters used for simulations are represented in Table 1.

4.1 Estimated agglomeration efficiency

In the first instance, the performance of the proposed online identification approach is shown for the scenario of agglomeration efficiency estimation. Here, the modified plant model with Brownian kernel runs simultaneously with the actual process plant. The same initial conditions from (2) are applied for the particle size distributions in

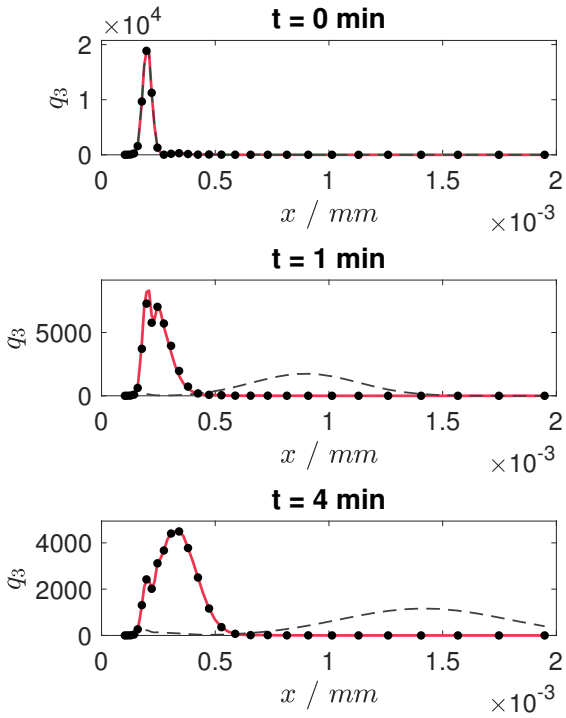

Fig. 5. *Particle size distributions q_3 of the actual plant (solid, red), parallel plant model with (points, black) and without online estimation (dotted, grey)*

the parallel model. The initial value for the estimate is chosen $\hat{\beta}_0 = 5 \cdot 10^{-10}$. Both tuning parameters γ and l have a strong impact on the estimation dynamics. Therefore, assigning of their values is an iterative procedure where trade-offs between different design specifications, e.g. fast parameters convergence rates, oscillating behaviour and attenuation of possible measurements noise, should be taken into account. For this scenario the tuning parameters are chosen as follows

$$\gamma = 1 \cdot 10^{-18}\,, \qquad l = -0.1\,. \tag{21}$$

The obtained simulation results are represented in Fig. 3, Fig. 4 and Fig. 5. Here, in Fig. 3 the convergence of the estimated $\hat{\beta}_0$ and actual β_0 is depicted. It can be seen that the unknown parameter converges within approximately three minutes, which is sufficiently fast related to the process dynamics. It is also clear from the Fig. 4 that corresponding L_2 - norm of the estimation error between particle size distributions n and $\hat{n}$ converges towards zero within the same time. In order to compare the process dynamics the additional particle size distributions

$$q_3(t,x) = \frac{x^3 n(t,x)}{\int_0^\infty x^3 n(t,x)\mathrm{d}x} \tag{22}$$

of the actual plant, the parallel model with and without online parameter estimation for different time points are depicted in Fig. 5. A significant divergence of the process dynamics with and without online parameter estimation, i.e. with roughly known initial guesses, can be observed already in a short period of time.

4.2 Estimated Laurent polynomial parameters

In the second scenario, the proposed method is applied to estimate the agglomeration kernel. Here, the modified

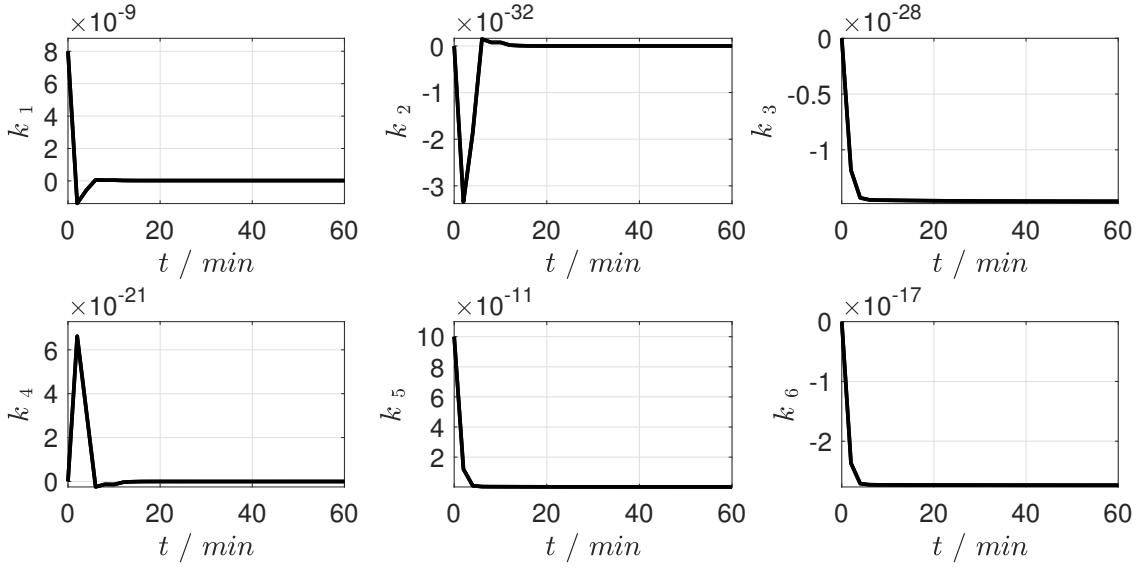

Fig. 6. *Convergence of the Laurent-polynomial coefficients for identification of coalescence kernel*

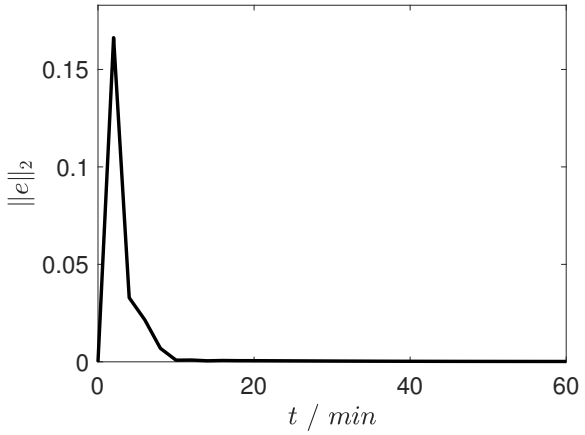

Fig. 7. L_2 - *norm of the error in time*

Table 2. *Initial estimates and tuning parameters for identification of Laurent-kernel*

Parameter	Value	Parameter	Value
$\hat{k}_1(0)$	$8 \cdot 10^{-9}$	γ_1	$5 \cdot 10^{-41}$
$\hat{k}_2(0)$	0	γ_2	$1 \cdot 10^{-41}$
$\hat{k}_3(0)$	0	γ_3	$5 \cdot 10^{-41}$
$\hat{k}_4(0)$	0	γ_4	$7 \cdot 10^{-41}$
$\hat{k}_5(0)$	$1 \cdot 10^{-10}$	γ_5	$7 \cdot 10^{-46}$
$\hat{k}_6(0)$	0	γ_6	$5 \cdot 10^{-41}$
		l	-0.022

plant model, which includes the Laurent polynomial with six unknown parameters (17), runs simultaneously to the actual process plant. In this case, the same initial conditions for the parallel model and the actual plant are used. The initial values for the polynomial parameters and chosen tuning parameters are given in Table 2.

The corresponding simulations results are shown in Fig. 6, Fig. 7, Fig. 8 and Fig. 9. From Fig. 6 it is clear that parameters converge with a different rate. Moreover, the simulation studies indicated that only two polynomial addends associated with parameters k_1 and k_5 make a significant contribution in the overall estimation dynamics. In the Fig. 7 a corresponding L_2 - norm of the estimation error

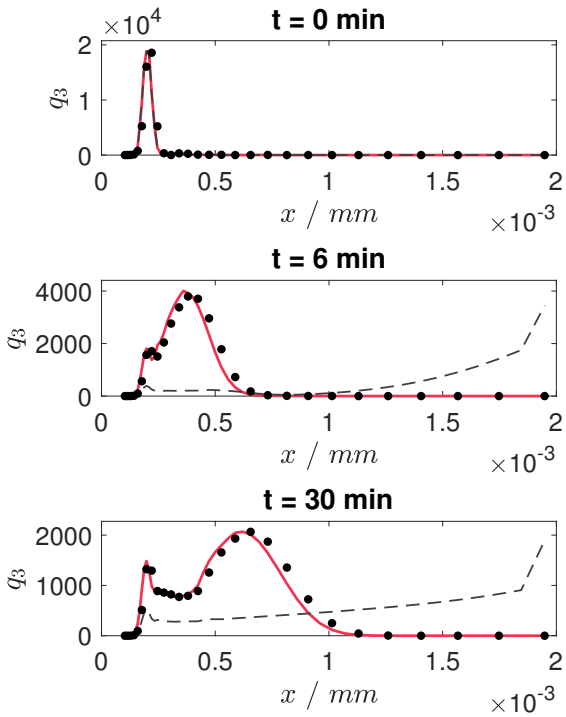

Fig. 8. *Particle size distributions q_3 of the actual plant (solid, red), parallel plant model with (points, black) and without online estimation (dotted, grey)*

between particle size distributions n and $\hat{n}$ is depicted. It can be seen that a sufficient convergence is achieved within approximately 10 minutes, which is reasonably fast related to the slow process dynamics. However, from the Fig. 8, the sufficient accuracy of the distributions can be observed after approximately 6 minutes.

The estimate of the Brownian kernel using the proposed Laurent polynomial and the relative error between both kernels are shown in Fig. 9. It can be seen that the relative error is below 5 %.

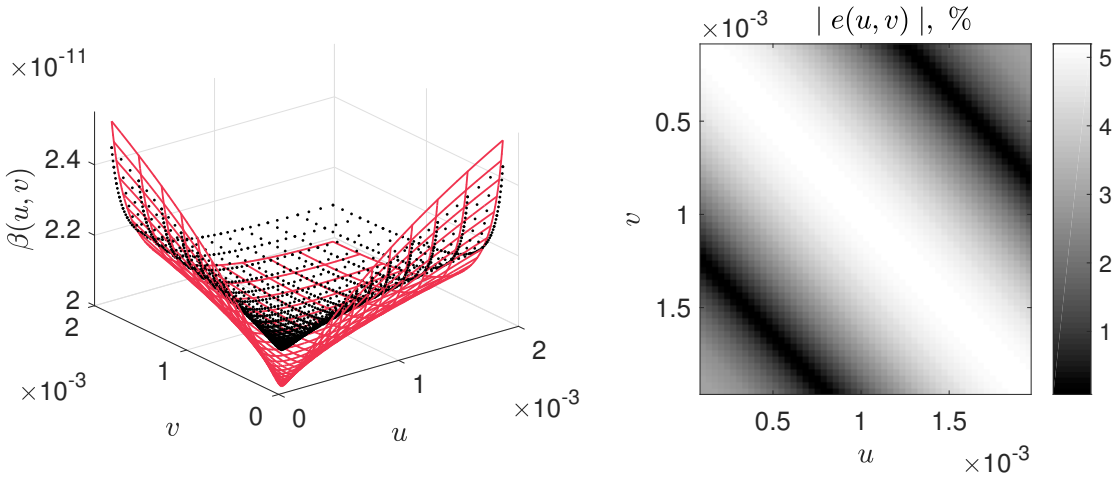

Fig. 9. *Brownian kernel (red, at the left), estimated kernel (black, at the left) and relative error between kernels (at the right)*

5. CONCLUSION

In this work the online parameter estimation for the continuous fluidized bed spray agglomeration process has been demonstrated. For the identification of the agglomeration kernel the Lyapunov-based adaptive approach has been proposed. The presented methodology has been studied for two different identification scenarios. In the first scenario, this method has been applied for the agglomeration efficiency estimation assuming that the agglomeration kernel is perfectly known. In the second scenario, the proposed approach has been applied for the volume-dependent agglomeration kernel estimation. For the kernel structure approximation a low-order Laurent polynomial has been used. It has been shown that this approach allows a sufficiently fast parameter estimation for both cases in the case of noiseless measurements. Future work will be concerned with the robustness analysis in presence of measurement noise and parameter uncertainties as well as application of this approach to real plant measurements.

ACKNOWLEDGEMENTS

This work is funded by the European Regional Development Fund (ERDF) project "Center of Dynamic Systems". The financial support is hereby gratefully acknowledged.

REFERENCES

Bück, A., Klaunick, G., Kumar, J., Peglow, M., and Tsotsas, E. (2012). Numerical simulation of particulate processes for control and estimation by spectral methods. *AIChE Journal*, 58, 2309–2319.

Chakraborty, J., Kumar, J., Singh, M., Mahoney, A., and Ramkrishna, D. (2015). Inverse problems in population balances. determination of aggregation kernel by weighted residuals. *Industrial & Engineering Chemistry Research*, 54(42), 10530–10538.

Dürr, R., Palis, S., and Kienle, A. (2015). Online parameter identification of facet growth kinetics in crystal morphology population balance models. *Procedia Engineering*, 102(0), 1336–1345. Proceedings of The 7th World Congress on Particle Technology.

Eisenschmidt, H., Soumaya, M., Bajcinca, N., Le Borne, S., and Sundmacher, K. (2017). Estimation of aggregation kernels based on Laurent polynomial approximation. *Computers and Chemical Engineering*, 103, 210–217.

Golovin, I., Strenzke, G., Dürr, R., Palis, S., Bück, A., Tsotsas, E., and Kienle, A. (2018). Parameter Identification For Continuous Fluidized Bed Spray Agglomeration. *Processes*, 6(12), 246. doi:10.3390/pr6120246. URL `http://www.mdpi.com/2227-9717/6/12/246`.

Krstic, M. (2006). Systematization of approaches to adaptive boundary stabilization of PDEs. *International Journal of Robust Nonlinear Control*, 16, 801–818.

Kumar, J., Peglow, M., Warnecke, G., Heinrich, S., and Mörl, L. (2006). Improved accuracy and convergence of discretized population balance for aggregation: The cell average technique. *Chemical Engineering Science*, 61, 3327–3342.

Le Borne, S., Shahmuradyan, L., and Sundmacher, K. (2015). Fast evaluation of univariate aggregation integrals on equidistant grids. *Computers and Chemical Engineering*, 74, 115–127.

Palis, S. and Kienle, A. (2013). Online parameter identification for continuous fluidized bed spray granulation. In *5th International Conference on Population Balance Modelling, PBM 2013*.

Palis, S. and Kienle, A. (2017). Online parameter identification for continuous fluidized bed spray granulation with external sieve-mill cycle. In *2nd International Conference on Methods and Models in Automation and Robotics, MMAR 2017*, 594–598.

Ramkrishna, D. (2000). *Population Balances: Theory and Applications to Particulate Systems in Engineering*. Academic Press, San Diego.