Supporting Information
Model based process optimization for nanoparticle precipitation

Andrea Gilch,[⋆,a] Adeel Muneer,[⋆,b] Jana Dienstbier,[a] and Lukas Pflug[b]

Fixed point mapping

S1 Compact form

The fixed point equation for $k \in \{2,\dots,N_t\}$ is given by:

$$F_k(\bar{C},C) = C_k - C_{k-1} - \left(\bar{C}_k - \bar{C}_{k-1}\right) + \tfrac{\pi\rho}{6M_P}\mathcal{N}(C_{k-1})\delta_{k-1}\mathsf{G}^3_{k-1,k-1} + \tfrac{\pi\rho}{6M_P}\sum_{\ell=1}^{k-2}\mathcal{N}(C_\ell)\delta_\ell\left(\mathsf{G}^3_{\ell,k-1} - \mathsf{G}^3_{\ell,k-2}\right) \tag{S1}$$

and, for $k=1$,

$$F_1(\bar{C},C) = C_1 - M_1. \tag{S2}$$

S2 Derivative of the fixed point mapping

The derivative of the fixed point mapping F w.r.t concentration C reads as follows:

$$\partial_{C_i}F_k(\bar{C},C) = \begin{cases} 0 & \text{for } i>k,\\ 1 & \text{for } i=k,\\ -1 + \tfrac{\pi\rho}{6M_P}\left(\delta_{k-1}\mathcal{N}'_i\mathsf{G}^3_{k-1,k-1} + 3\delta^2_{k-1}\mathcal{N}_{k-1}\mathcal{G}'_i\mathsf{G}^{2+n}_{k-1,k-1} + 3\sum_{\ell=1}^{k-2}\mathcal{N}_\ell\delta_\ell\mathcal{G}'_i\delta_i\mathsf{G}^{2+n}_{\ell,k-1}\right) & \text{for } i=k-1,\\ \tfrac{\pi\rho}{6M_P}\mathcal{N}'_i\delta_i\left(\mathsf{G}^3_{i,k-1} - \mathsf{G}^3_{i,k-2}\right) + 3\tfrac{\pi\rho}{6M_P}\sum_{\ell=1}^{i}\mathcal{N}_\ell\delta_\ell\mathcal{G}'_i\delta_i\left(\mathsf{G}^{2+n}_{\ell,k-1} - \mathsf{G}^{2+n}_{\ell,k-2}\right) & \text{for } i<k-1, \end{cases} \tag{S3}$$

where $\mathcal{N}_k = \mathcal{N}(C_k), \mathcal{N}'_k = \mathcal{N}'(C_k), \mathcal{G}_k = \mathcal{G}_0(C_k), \mathcal{G}'_k = \mathcal{G}'_0(C_k)$ and, as already defined in (26),

$$\mathsf{G}_{\ell,k} := \left(x_{\mathrm{n}}^{1-n} + (1-n)\sum_{m=\ell}^{k}\mathcal{G}_m\delta_m\right)^{\frac{1}{1-n}}.$$

S3 Objective functional

In general, by considering the x^m weighted PSD, the objective functional as stated in (1) can be written in terms of moments as follows:

$$\hat{J}(Y_m,Y_{m+1},Y_{m+2}) = \tfrac{Y_{m+2}}{Y_m} - \left(\tfrac{Y_{m+1}}{Y_m}\right)^2. \tag{S4}$$

The constraint in (1) is defined as:

$$h(C) := E[q(T,\cdot)] - \mu_d = 0. \tag{S5}$$

In terms of moments, the constraint (S5) is written as:

$$h(C) = \hat{h}(Y_m,Y_{m+1}) = \tfrac{Y_{m+1}}{Y_m} - \mu_D. \tag{S6}$$

For $m=0$, the number weighted PSD, whereas for $m=3$, the volume-weighted PSD is considered.

S4 Derivative of the objective functional

The derivative of the objective functional stated in S3 is given as follows:

$$\begin{aligned}\partial_{C_i}\hat{J}(Y_m,Y_{m+1},Y_{m+2}) = {}& \tfrac{Y_m\partial_{C_i}Y_{m+2} - Y_{m+2}\partial_{C_i}Y_m}{Y_m^2}\\ & - 2\left(\tfrac{Y_{m+1}}{Y_m}\right)\tfrac{Y_m\partial_{C_i}Y_{m+1} - Y_{m+1}\partial_{C_i}Y_m}{Y_m^2}.\end{aligned} \tag{S7}$$

In addition, the derivative of the constraint S6 is given by:

$$\partial_{C_i}\hat{h}(Y_m,Y_{m+1}) = \tfrac{Y_m\partial_{C_i}Y_{m+1} - Y_{m+1}\partial_{C_i}Y_m}{Y_m^2}. \tag{S8}$$

[⋆] *These authors contributed equally to this manuscript.*

[a] *Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Department of Data Science (DDS), Professorship of Optimization under Uncertainty & Data Analysis, Nürnberger Straße 74, 91052 Erlangen, Germany. E-mail: {jana.dienstbier,andrea.gilch}@fau.de*

[b] *Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Department of Mathematics, Chair of Applied Mathematics (Continuous Optimization), Cauerstraße 11, 91058 Erlangen, Germany; Competence Center Scientific Computing (FAU CSC), Martensstrasse 5a, 91058 Erlangen, Germany. E-mail: {adeel.muneer,lukas.pflug}@fau.de*