Parameter and uncertainty identification for a multidimensional population balance model for granulation

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A methodology for the estimation of model parameters and their uncertainties for a multivariate population balance model for granulation is presented. The outcome of the detailed population balance model is locally approximated by response surfaces in order to allow quick computation in the parameter estimation approach, using three different objective functions.

1. Background and idea

The evolution of the particles during a wet granulation process is described by a multidimensional population balance framework with following particle model and incorporated transformations [1]:

Image 1: Diagram of particle model and transformations

- Coalescence
- Compaction
- Breakage
- Penetration
- Chemical reaction

2. Theory

Choice of “universal” parameters

- model response with parameters $x$
  $$\eta = \eta(x) \quad \text{with} \quad x = (x_1, ..., x_i)$$
- experimental datum
  $$\eta^{\text{exp}} = \eta^{\text{opt}} + \epsilon$$
- each parameter $x$ can be represented by
  $$x = x_i + c_i \xi$$
  $$\xi \sim N(0,1)$$

For a simple linear model, $K=1$:

$$\eta(x) = A + Bx$$

$$\mu(x_i) = E[\eta(x_i, c_i)] = A + Bx_i$$

$$\sigma(c) = \sqrt{\text{Var}(\eta(x_i, c_i))} = \sqrt{Bc^2}$$

*optimal values for unknown parameters $x_i$ and associated uncertainties $c_i$*:

$$(x_i^{*}, c_i^{*}) = \text{arg min}[\eta(x_i, c_i)]$$

*with objective function (moment matching)*:

$$\Phi(x_i, c_i) = \sum_{i=1}^{N} |\mu_i - \mu_i^{*}|^2 + |\sigma_i - \sigma_i^{*}|^2$$

*and constraints*

$$x_{\text{low}} \leq x_i \leq x_{\text{high}} \quad (i = 1, ..., K)$$

$$0 \leq c \leq c^{(u)}$$

Where do we get model response $\eta(x)$ and $\mu(x, c), \sigma(x, c)$ respectively from?

- directly from model: numerically expensive
- local model approximation: response surface
  - e.g. 2nd order response surface
  $$\eta(x) = \beta_0 + \sum_{i=1}^{K} \beta_i x_i + \sum_{i=1}^{K} \sum_{j=i+1}^{K} \beta_{ij} x_i x_j$$

Alternative objective function

- expected least squares
  $$\Phi(x_i, c_i) = \sum_{i=1}^{N} |\mu_i - \mu_i^{*}|^2 + |\sigma_i - \sigma_i^{*}|^2$$
  $$+ \sum_{i=1}^{N} 2\sigma_i^{2} c_{i}^{2} + \sum_{i=1}^{K} \beta_i x_i c_i + \sum_{i=1}^{K} \sum_{j=i+1}^{K} \beta_{ij} x_i x_j$$

- weighted expected least squares: experimental uncertainties as weights [2]

3. Results

Experimental system

- wet granulation of sugar panels with aqueous PEG4000 solution in food mixer operated with impeller speed of 900 and 1200 rpm [3]
- determination of mass of agglomerates at 4 different process times

1st order vs. 2nd order approximation

- moment matching objective function (impeller speed of 900 rpm)

Different objective functions

- 2nd order response surfaces (impeller speed of 900 rpm)

4. Conclusions

- estimation of unknown model parameters and associated uncertainties for multivariate population balance model
- choice of moment-matching objective function recommend as number of experimental points is independent of number of unknown parameters
- use of methodology for falsification of models in future work

References


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