# Population balance modelling for struvite formation

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## 1. Introduction

Behaviour of systems where new particles are forming due to either chemical or physical processes is of much interest in pharmaceutical and chemical engineering industries. Computational fluid dynamics can be used to model the outcomes of a specific reactor, but in order to do that a correct mathematical formulation is needed. There are two approaches that can be applied - Lagrangian or Eulerian. Slightly different mathematical structure is needed for each of the approaches. Lagrangian models are usually applied to model dispersed phase system evolution where each particle is assigned an individual transport equation. This is useful if one is interested in learning specifics of physics that affects each particle in the dispersed phase. An alternative is to treat the dispersed phase as a continuous field which can then be evolved through time and space. Both approaches have it's own advantages and disadvantages.
Currently the system in question is struvite formation inside a vessel, where crystal formation is induced through the means of reactive crystallisation (precipitation). Struvite crystallisation process is mainly governed by nucleation and growth processes. The system such as this where new particulates are forming can be modelled in Lagrangian formulation, though an alternative approach is possible, where a crystal size distribution function is regarded as a continuous field in space and time and therefore is evolved in an Eulerian manner.

## 2. Population balance model

### 2.1. Number density function

Starting point is to introduce a number density function $n(\underline{\xi}, \mathbf{x}, t)$ which is dependant on a set of internal variables $\underline{\xi}$, space $\mathbf{x}$ and time $t$. The set of internal variables is chosen freely, but most commonly a univariate approach is chosen where it is either the radius $\xi = L$ or the volume $\xi = V$ of the particles; the set can be multivariate (e.g. length and width of the particles), though this increases the complexity of the solution algorithm.

A population balance equation is used to model the evolution of the NDF in time and space. Considering a case where internal coordinates are univariate $\underline{\xi} = L$, an evolution equation is formed:

$$\frac{\partial n(L, \mathbf{x}, t)}{\partial t} + \nabla\big(\mathbf{u} n(L, \mathbf{x}, t)\big) = J(S, \theta_b)\delta(L_0, L) - \frac{\partial G(L, S, \theta_b) n(L, \mathbf{x}, t)}{\partial L} \tag{1}$$

$S(S, t, \theta_b)$ - nucleation source term; $G(L, S, \theta_g)$ - growth source term; with $S$ - supersaturation of the solute, $\theta_b$ - vector of nucleation kinetic parameters, $\theta_g$ - vector of growth kinetic parameters.

### 2.2. Statistical moments of the distribution

In order to extract quantitative measure about a particular distribution function one can use moments of the distribution. Moments of a smooth function are defined as:

$$\mu_j = \int_0^\infty L^j n(L, \mathbf{x}, t) dL, \quad j = 0, 1, 2, ..., \infty \tag{2}$$

Depending on what are the internal variables of the distribution each moment would represent a different quality of the distribution. From statistical analysis if function $n$ represents distribution of some random variable $X$ then the moments of the distribution would represent the following measures:

- $\mu_0$ - mean;
- $\mu_1$ - variance;
- $\mu_2$ - skewness;
- $\mu_3$ - historical kurtosis (or flatness);
- $\mu_4$ - hyperskewness;
- $\mu_5$ - hyperflatness.

If $n$ represents size distribution of the particles in the system then the analogous information can be extracted using moments:

- $N_t = \mu_0$ - total number particle density;
- $A_t = k_a \mu_2$ - total particle area;
- $V_t = k_v \mu_3$ - total solids volume

Mean crystal size is defined as:

$$d_{43} = \frac{\mu_4}{\mu_3}$$

### 2.3. Moments transformation of PBE

We can apply moment transformation to population balance equation to obtain transport equations in terms of distribution moments.

$$\frac{d\mu_j(t)}{dt} = J(S, t, \theta_b)\delta(L_0, L) + \int_0^\infty jL^{j-1} G(L, S, \theta_b) n(L, \underline{x}, t) dL \tag{3}$$

### 2.4. Gaussian quadrature

Gaussian quadrature method approximates the function in terms of a set of weighting factors $w(t)$ and abscissa functions $f(L, L_i(t))$. Applying that to a number distribution one can obtain the following expression:

$$n(L, \underline{x}, t) \approx \sum_{i=1}^{N_q} w_i(t) f_i(L, L_i(t)) \tag{4}$$

Applying the same rule to the moments of the distribution:

$$\mu_j(t) \approx \sum_{i=1}^{N_q} w_i(t) L_i^k(t) \tag{5}$$