Determination of population balance distributions by the moment method combined with a Chebyshev spline reconstruction

J.-P. Gaillard, P.O. Lamare

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Determination of population balance distributions by the moment method combined with a Chebyshev spline reconstruction

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Content of the presentation

Introduction

- Population Balance in the context of reactive precipitation,
- Method of Classes and Quadrature of Moments (QMOM),

Reconstruction from finite number of moments

- Short state of art,
- Presentation of the Chebishev Spline Reconstruction (CSR).

Validation and Results

- Nucleation and growth analytical solution,
- Nucleation, growth and agglomeration : a parametric study,
- Application to experimental tests.

Conclusion

Crystalisation/Reactive Precipitation modeling

Thermodynamics

Solubility

Driving force

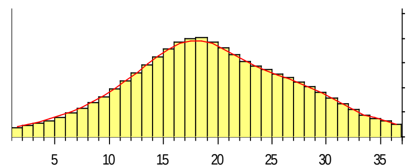
kinetics :
Nucleation/Growth
Agglomeration

Design of experiments

Mathematical treatment identification

Population balance

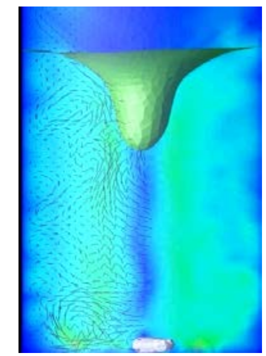
Classes methods



Moment approach

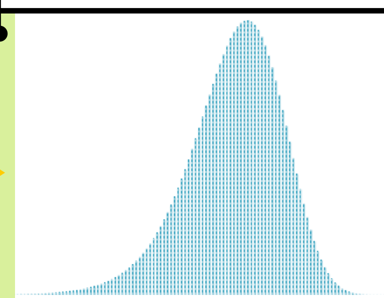
$$m_k = \int_0^\infty L^k \phi(L,t)\,dL$$

Hydrodynamic & Particle transport*



Q_i,
γ_i

Process simulation



Particle-size distribution

* : Y. Sommer de Gélicourt :PhD thesis and M. Bertrand & al. : Chem. Eng. Sc. 77(2012) 95–104

Population balance : Generalities

$$\underbrace{\frac{1}{V}\frac{\partial Vn(L,t)}{\partial t}}_{\text{Accumulation rate}} + \underbrace{\frac{\partial Gn(L,t)}{\partial L}}_{\text{Growth rate}} + \underbrace{\frac{Q_o n(L,t) - Q_i n_i(L,t)}{V}}_{\text{Inlet and outlet}} = \underbrace{R_N \, \delta(L_0)}_{\text{Nucleation rate}} + \underbrace{B(L) - D(L)}_{\text{Agglomeration rate}}$$

L : crystal size - n(L,t) : population density - δ : Kronecker symbol

The moment transformation of the population balance

$$m_k = \int_0^\infty L^k n(L,t)\,dL \quad \Rightarrow \quad \boxed{\frac{dm_k}{dt} = R_N \cdot 0^k + k\,G m_{k-1} + \overline{B_k} - \overline{D_k}} \qquad k = 0 \ldots N$$

Advantages : Only ~ 6 unknown rather than ~ 100 (interesting for CDF calculations)

ODE rather than PDE

Drawbacks : System unclosed in case of agglomeration ➔ **Quadrature**

Only statistical results (m_0 : # of particles, $L_{43} = m_4/m_3$) ➔ ***Reconstruction***

Population balance : Quadrature Moment approach "QMOM"

- Use of quadrature to compute the moment integrals :

$$m_k(t) = \int_0^{\infty} n(L,t) L^k \, dL \approx \sum_{i=1}^{N_q} \omega_i \cdot L_i^k$$

Product-Difference or Chebyshev …

- The moment's equations become :

$$\frac{dm_k}{dt} = R_N \cdot 0^k + k\,G m_{k-1} + \frac{1}{2}\sum_{i=1}^{3}\omega_i \sum_{j=1}^{3}\omega_j (L_i^3 + L_j^3)^{k/3} \beta_{ij} - \sum_{i=1}^{3}\omega_i L_i^k \sum_{j=1}^{3}\omega_j \beta_{ij}$$

- The algorithm of resolution :
  - Determination of weights w_i and abscisses L_i : knowing $m_k(t)$,
  - Calculation of $\frac{dm_k}{dt}$,
  - Update of $m_k(t+dt)$

Moments : What do you have ?

m $_0$: 2,442D+14
m $_1$: 3,065D+08
m $_2$: 4854,5069
m $_3$: 0,1800897
m $_4$: 0,0000101
m $_5$: 7,267D-10
m $_6$: 6,261D-14
m $_7$: 6,226D-18

m $_0$: number / m^3
m $_1$: m / m^3
m $_2$: m^2 / m^3
m $_3$: m^3 / m^3

$$D_{43} = \frac{m_4}{m_3}$$

$$c.v. = \sqrt{\left(\frac{m_0 m_2}{m_1^2} - 1\right)} \cong (1 - I_{agg})^{-0.3}$$

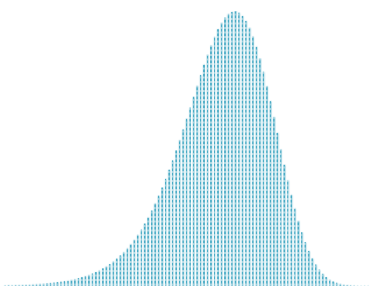
$$\frac{m_0}{\alpha\tau} = R_N - \frac{\beta}{2} m_0^2$$

$$\frac{m_3}{\alpha\tau} = 3G \cdot m_2$$

$$\frac{m_6}{\alpha\tau} = 6G \cdot m_5 + \beta m_3^2$$

Check : R_N,G,β

What we would like !



Reconstruction : bibliography

The problem of reconstructing a function from a given number of moments is known in mathematics as the *finite-moment problem :*

➔ It is severely ill-conditioned !

- A priori basic shapes function : Gauss, log-normal, beta, Rayleigh …
- Maximum entropy approach,
- Adaptive spline-based algorithm,
- Statistically most probable distribution.
- …

Chebishev Spline Reconstruction : CSR

The spline approximation of the particle size distribution

Degree of the Spline

$$s_{n,s}(L) = \sum_{i=1}^{n} p_i [L_i - L]_+^s \qquad u_+ = u\,H(u)$$

H(u) Heaviside step function :
1 : L < L_i and 0 : L > Li

n splines ➔ 2 n moments

Approximation of n(L) by $s_{n,s}$ continous, differentiable, and **so that the moment are preserved,**

$$\int_0^\infty s_{n,s}(L) L^k dL = m_k = \int_0^\infty n(L) L^k dL$$

$$\sum_{i=1}^{n} (p_i L_i^{s+1}) L_i^j = \frac{(j+1)(j+2)\ldots(j+s+1)}{s!} m_j$$

Thanks to three-term recurrence relation of the Chebyshev algorithm

Gautschi W., Orthogonal Polynomials : Computation and Approximation. Oxford Science Publications, 2004

CSR : Results and validations

Nucleation and growth in a MSMPR crystallizer :

- Steady state,
- Mixed Suspension, Mixed Product Removal.

$$n(L) = \frac{R_N}{G}\exp\left(\frac{-L}{G\tau}\right)$$

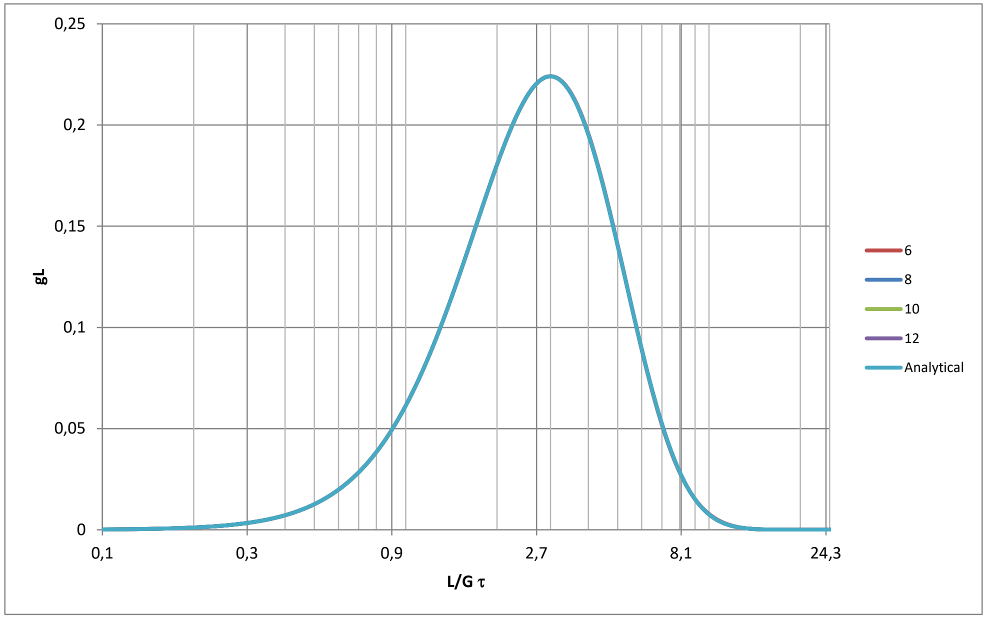
$$\frac{m_k}{\tau} = k!\,R_N(G\tau)^k$$

$$g(L) = \frac{n(L)L^3}{m_3}$$

- $R_N = 10$
- $G = 0.1$
- $\tau = 10$

- Ode (Lsode)
- Until steady state

Moment	Analytical	Calculated	Relative error
m0	100	100	0
m1	100	100	0
m2	200	200	1,421E-16
m3	600	600	1,895E-16
m4	2400	2400	3,79E-16
m5	12000	12000	6,063E-16
m6	72000	72000	6,063E-16
m7	504000	504000	6,929E-16
m8	4032000	4032000	8,084E-16
m9	36288000	36288000	8,213E-16
m10	362880000	362880000	1,15E-15
m11	3991680000	3991680000	1,075E-15



Comparison for Nucleation, growth and agglomeration

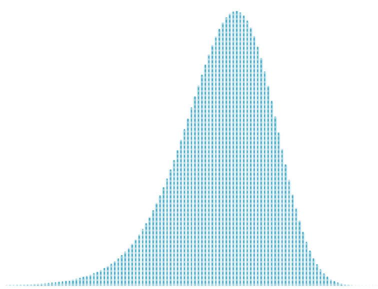
Population Balance

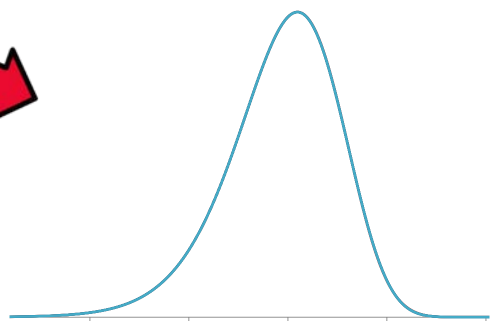
Method of classes : « Reference »

Quadrature of Moments

Moments

Spline reconstruction





Discretized moments

[Method of classes : Koren 3rd order for growth, Litster adjustable discretization q = 5 Lmin =0.001, Lmax = 30.]

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NonDimensionaliszing the Population Balance

$$x = \frac{L}{G\tau}$$

$$f(x) = \frac{G}{R_N}$$

$$\frac{df(x)}{dx} + f(x) - \delta(x) - b(x) + d(x) = 0$$

$$b(x) = K\frac{x^2}{2}\int_0^x \frac{f[(x^3-\lambda^3)^{1/3}]\,f(\lambda)}{(x^3-\lambda^3)^{2/3}}d\lambda$$

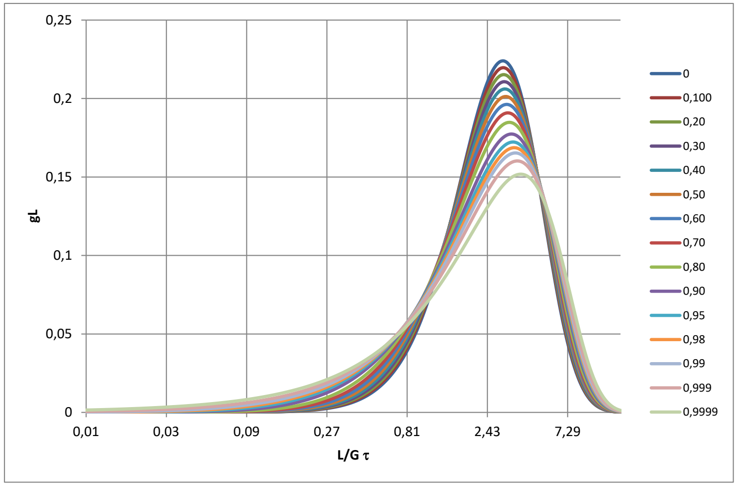
$$d(x) = Kf(x)\int_0^\infty f(\lambda)d\lambda = K\,f(x)\,\tilde{\mu}_0$$

$$K = R_N \beta_o \tau^2$$

$$I_{agg} = 1 - \frac{m_0}{R_N\tau}$$

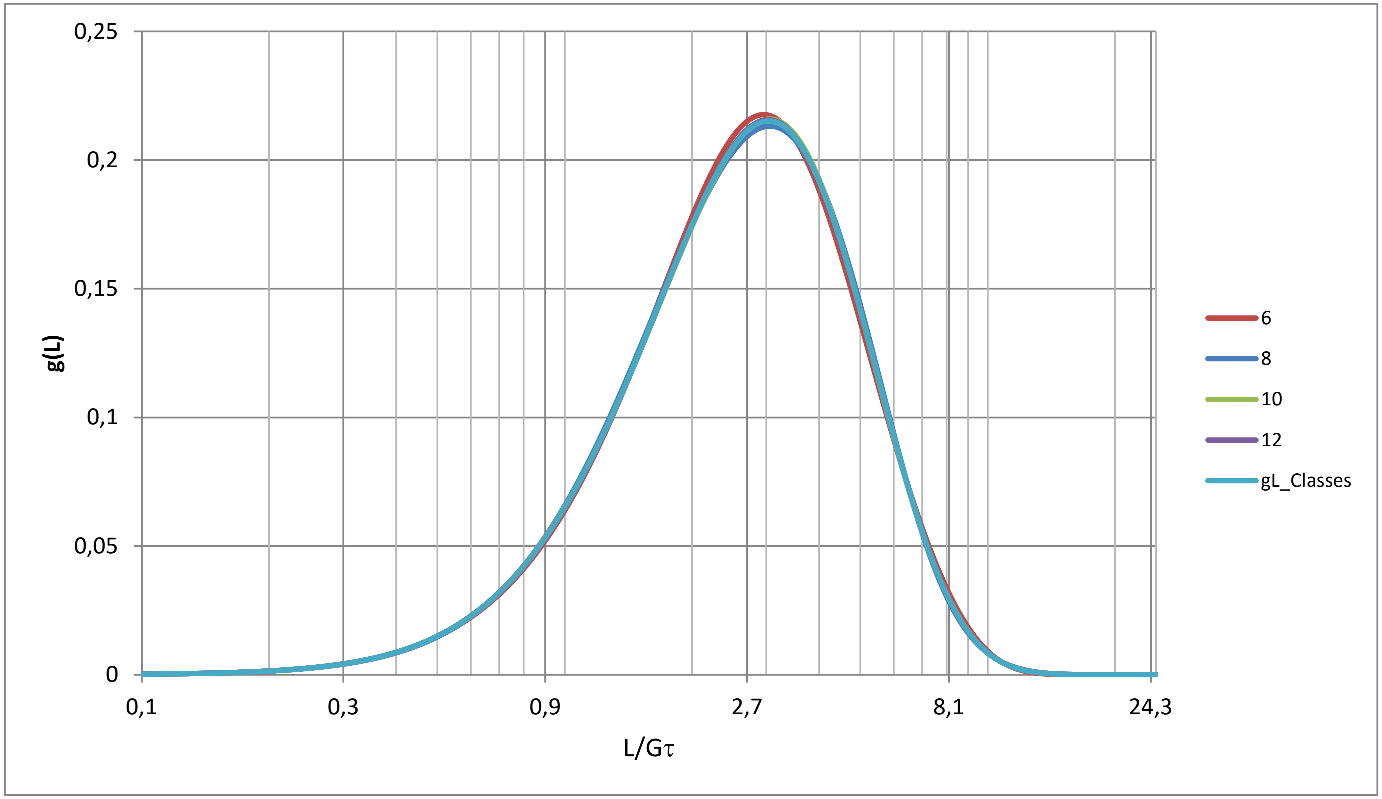
Number of particles / Number of created particles

« Reference » by method of classes



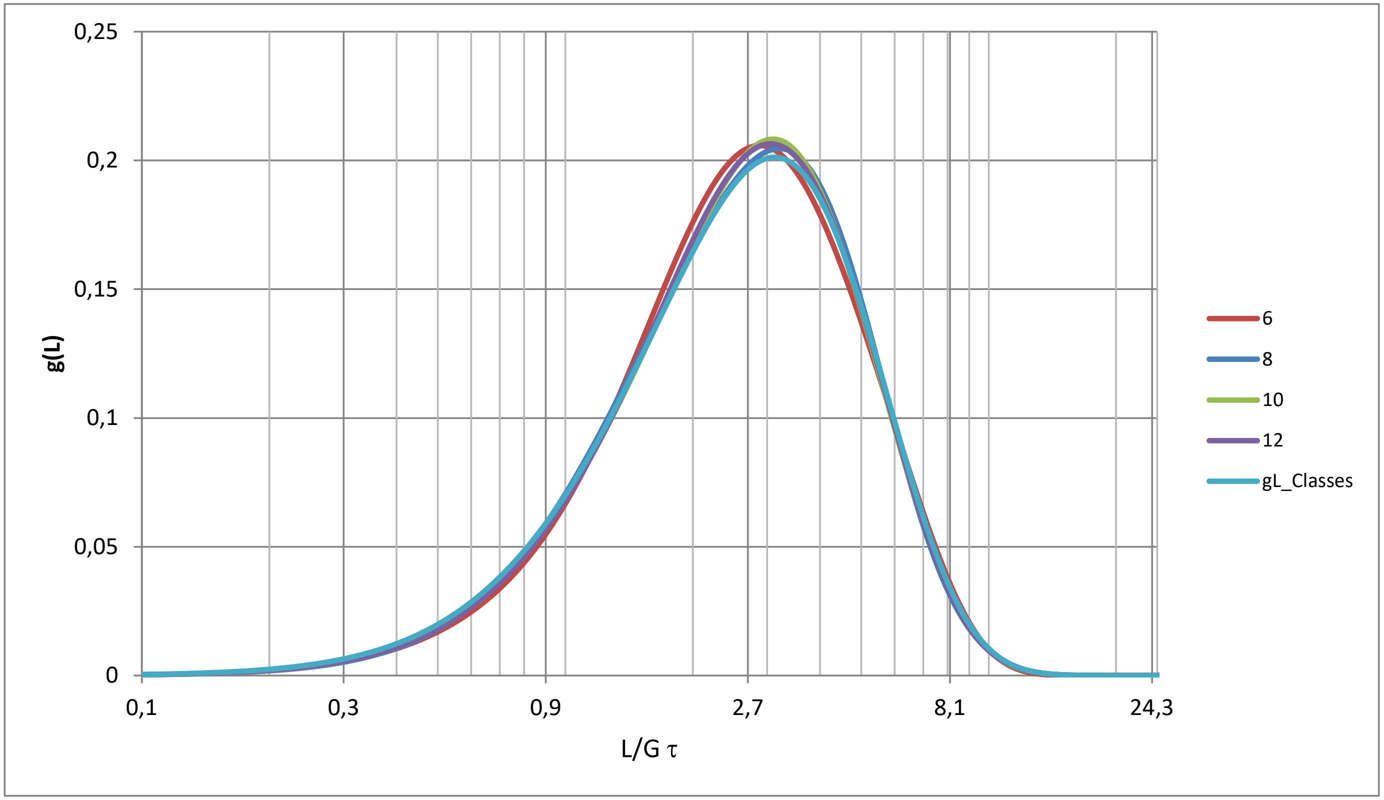
[M.J. Hounslow : Nucleation Growth and agglomeration rates from steady-state experimental data, AIChE J.,Nov 1990 Vol.36,n 11 p1748-1752]

Results : Iagg = 0.2



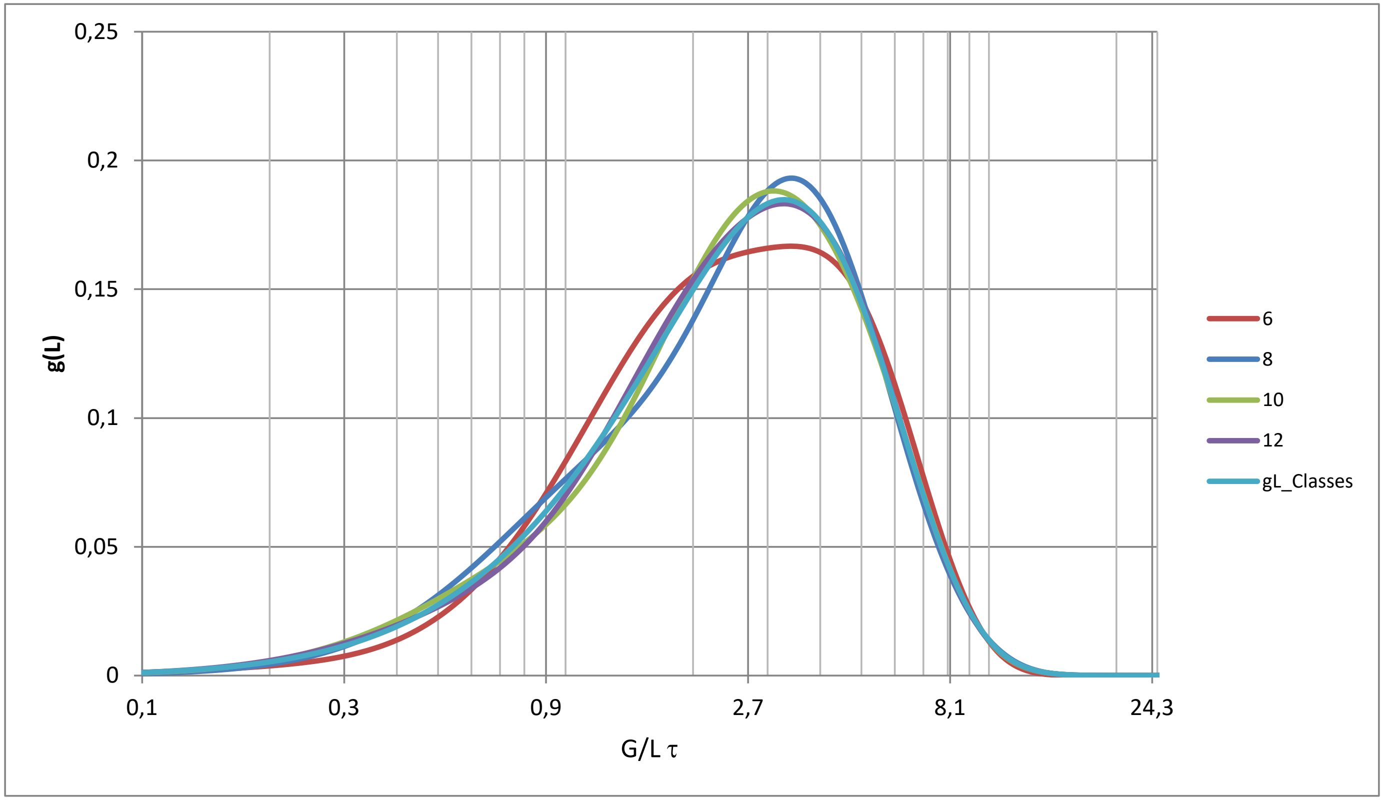
	Number of moments				
	6	8	10	12	Classes
D10	1,055	1,047	1,045	1,046	1,047
D50	2,649	2,656	2,661	2,658	2,659
D90	5,417	5,4	5,397	5,402	5,403
D43	4,062	4,061	4,060	4,060	4,061

Results : Iagg = 0.4



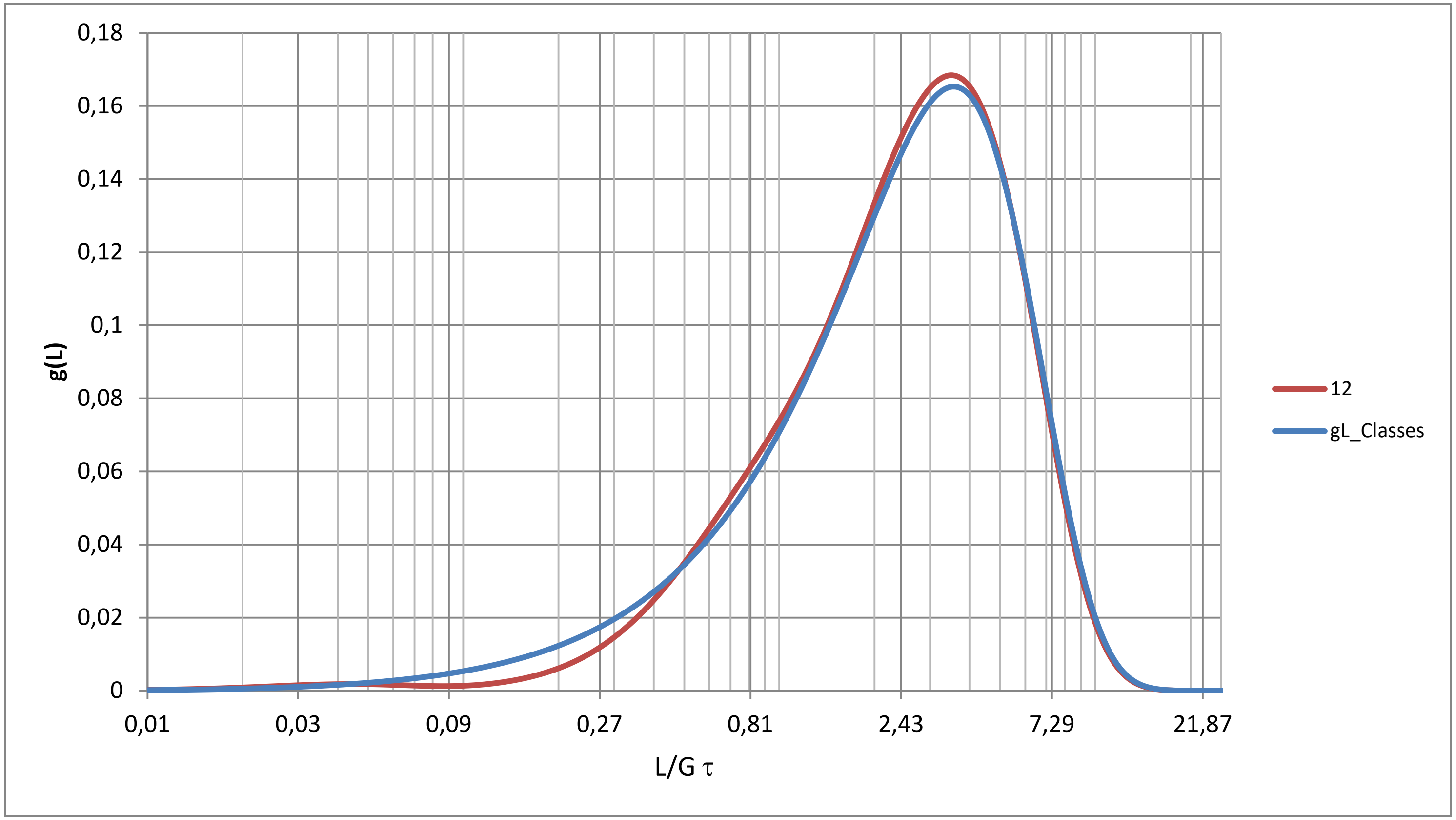
	Number of moments				
	6	8	10	12	Classes
D10	1,005	0,9787	0,9771	0,9819	0,9453
D50	2,611	2,645	2,647	2,64	2,631
D90	5,553	5,486	5,494	5,499	5,553
D43	4,136	4,133	4,132	4,131	4,134

Results : Iagg = 0.8



	Number of moments				
	6	8	10	12	Classes
D10	0,8547	0,7619	0,7685	0,8007	0,7923
D50	2,511	2,641	2,603	2,589	2,594
D90	5,867	5,709	5,761	5,754	5,762
D43	4,359	4,348	4,346	4,346	4,354

Results : Iagg = 0.99



	Number of moments				
	6	8	10	12	Classes
D10	0,6567	0,4675	0,6285	0,6623	0,5545
D50	2,509	2,651	2,555	2,572	2,534
D90	6,107	5,931	6,04	6,038	6,091
D43	4,604	4,584	4,587	4,595	4,658

Results : Iagg = 0.99 : some insights

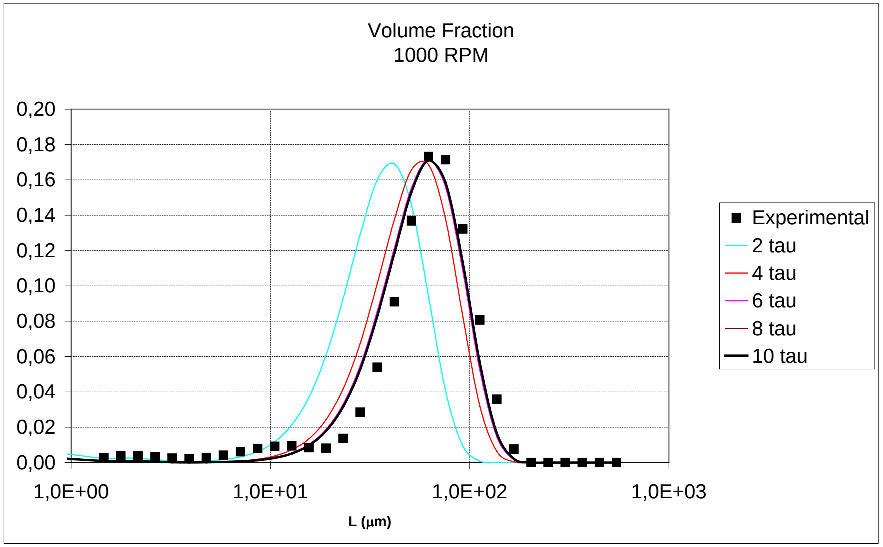
	Number of moments				
	6	8	10	12	Classes
m0	1,000	1,000	1,000	1,000	0,999
m1	0,034	0,039	0,042	0,044	0,057
m2	0,044	0,047	0,048	0,049	0,055
m3	0,132	0,140	0,145	0,148	0,166
m4	0,606	0,641	0,664	0,682	0,773
m5	3,534	3,756	3,914	4,029	4,648
m6		26,404	27,638	28,531	33,458
m7		214,129	224,987	232,872	277,336
m8			2061,847	2139,298	2583,791
m9			20934,394	21767,871	26611,184
m10				242516,417	299335,014
m11				2932733,601	3642944,196
G		0,1	0,1	0,1	0,1
RN		10	10	10	10,17
Beta		19,8	19,8	19,8	20,16
Iagg		0,9900	0,9900	0,9900	0,9902

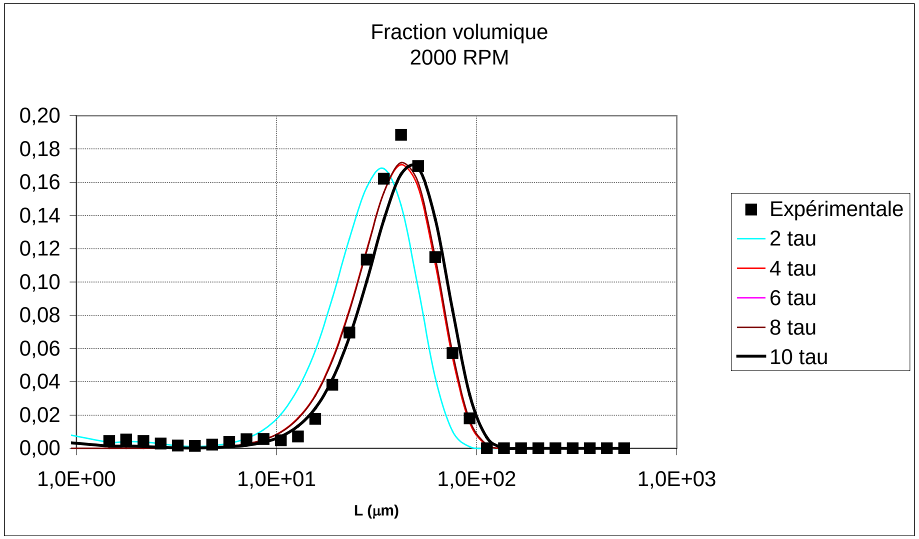
$$\frac{m_0}{\alpha\tau} = R_N - \frac{\beta}{2} m_0^2$$

$$\frac{m_3}{\alpha\tau} = 3G \cdot m_2$$

$$\frac{m_6}{\alpha\tau} = 6G \cdot m_5 + \beta m_3^2$$

Application to transient experiments





1000 rpm

2000 rpm

[S. Lalleman : Study of Neodymium Oxalate Precipitation in a Continuous MSMPR]

Conclusion

- ✓ Using the algorithm of Chebyshev, a spline reconstruction preserving the moments, gives access to the distribution of particle sizes,
- ✓ The CSR has been validated against analytical and results obtained with the method of classes, in a non dimensional formulation,
- ✓ It has been also used to model experimental runs,
- ✓ In that case, the comparisons between the experimental and the reconstructed distributions show very good agreement,
- ✓ The QMOM coupled the moment together so other moment approaches, might be tested in the futur.

Thank You

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