Population Balance Modeling

JMBC-Particle Technology 2015

Pieter Vonk
Advanced Chemical Engineering Solutions
March 6th, 2015

DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

HEALTH · NUTRITION · MATERIALS

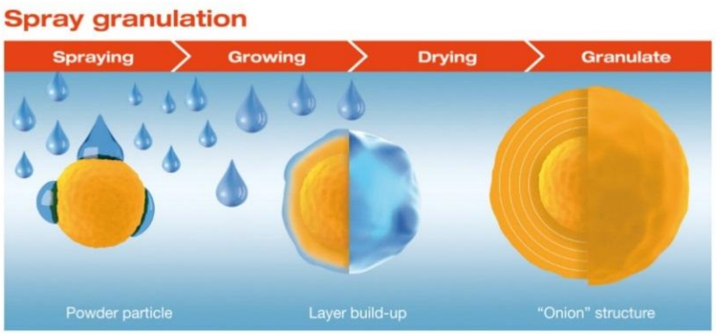
Overview

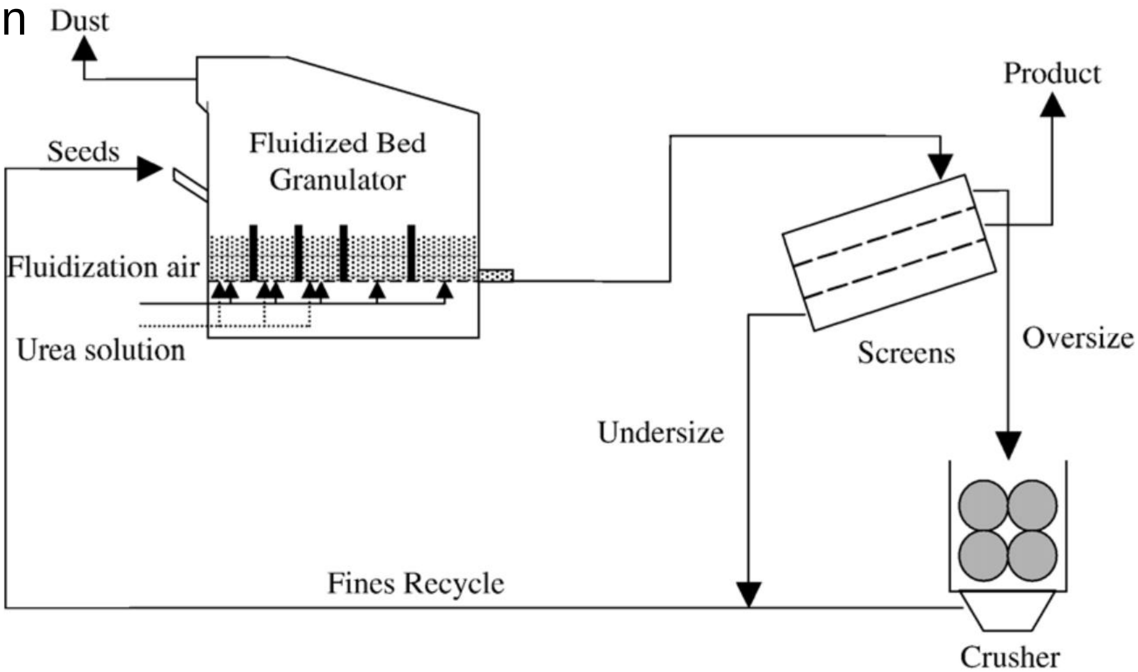
- Introduction & Industrial challenges
  - Granulation processes
  - Crystallization processes
- Population Balance Equation
  - General population balance
    - Nucleation
    - Growth
    - Agglomeration
    - Breakage
- Solution methods/Tools
  - Matrix methods (steady state solution)
  - Moment methods
  - Method of lines
  - Class methods

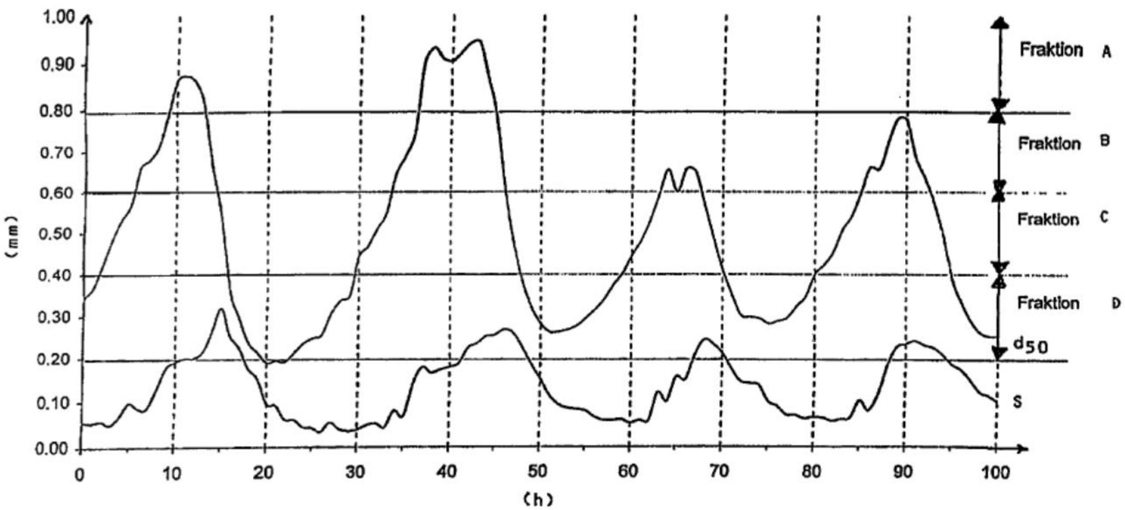
DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

Fertilizer production

- Urea fluid bed granulation
  - Oscillations
  - Variable production
  - Variable costs



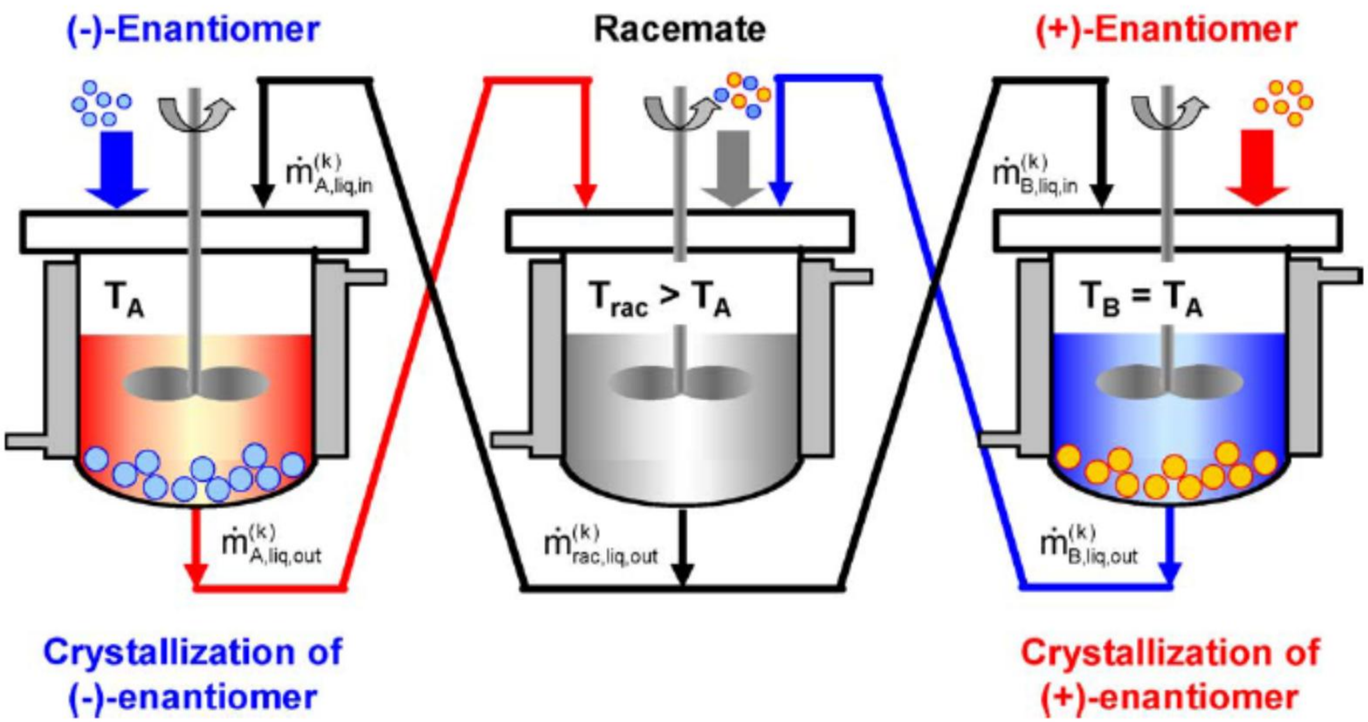




DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

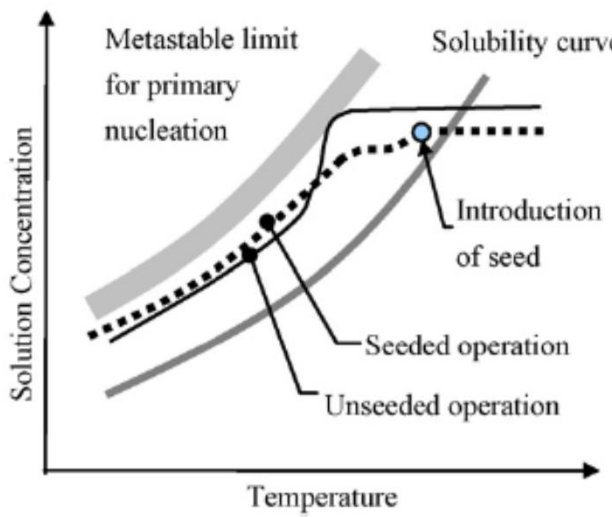
Batch crystallization

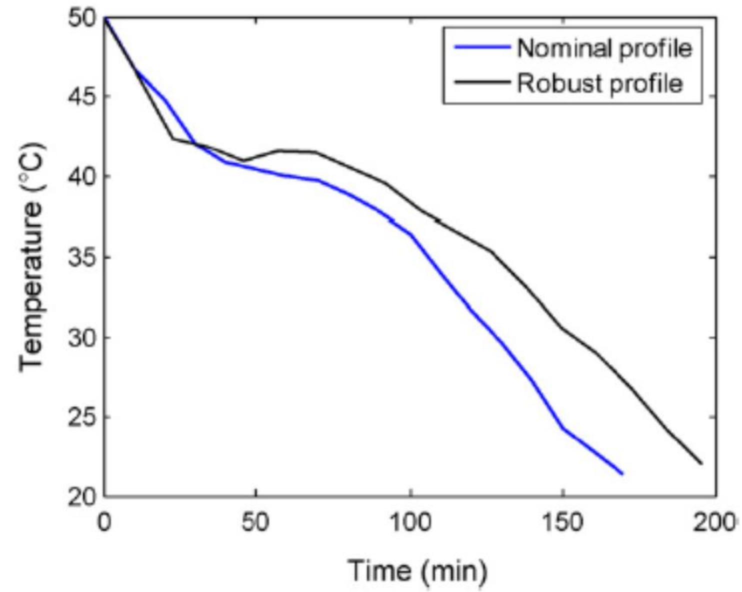
- Enantiomer separation



Batch crystallization

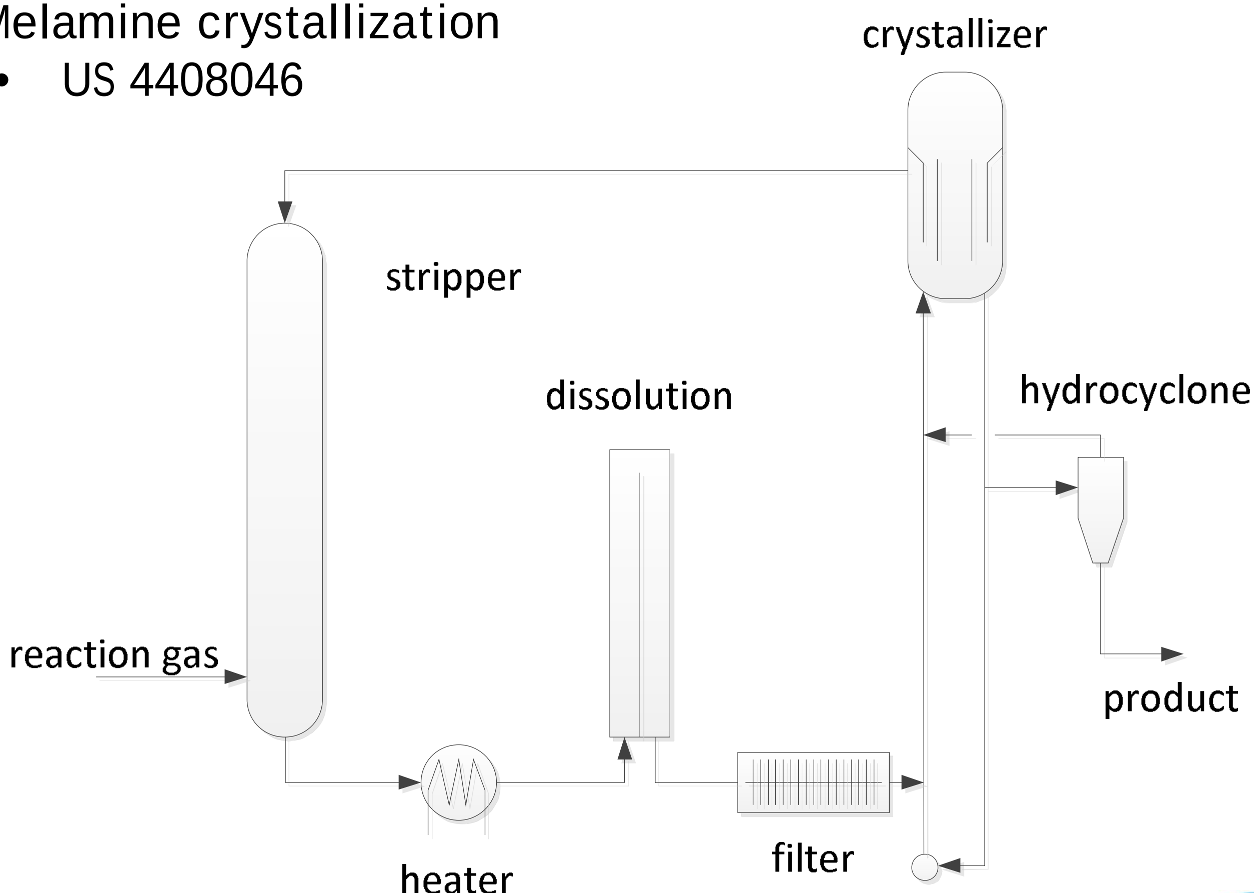
- Optimal cooling profile





Continuous crystallization

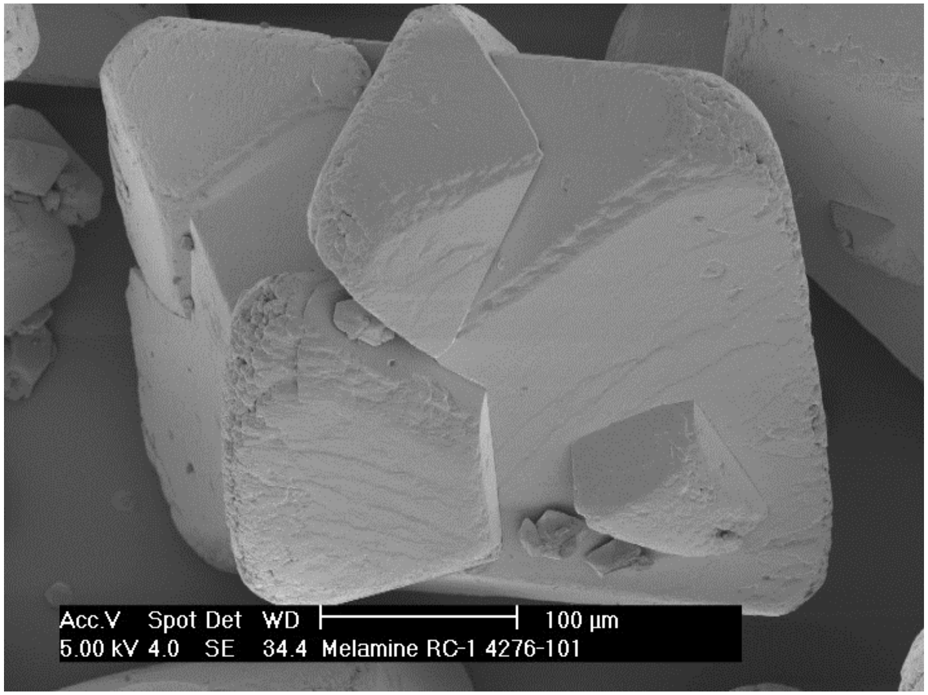
- Melamine crystallization
  - US 4408046



DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

Continuous crystallization

- Melamine particle
  - Agglomerate of crystals
- Effect on properties
  - Sensitive to attrition
    - Dust formation
  - Inclusion mother lye
    - Caking possible



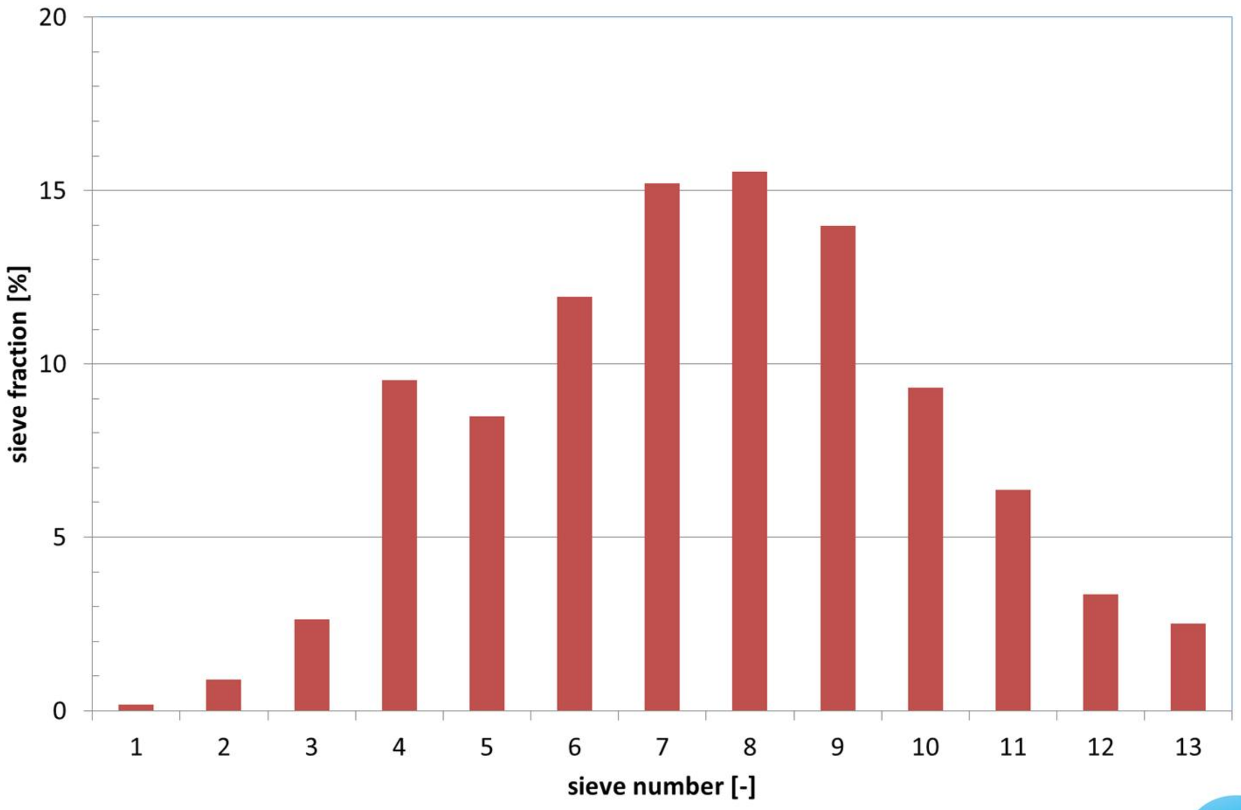
Industrial challenges

- Design of plant/operation
  - Estimation of recycles & required equipment
  - Feed rate & cooling profile
  - Size of equipment
- Troubleshooting/optimization
  - Flexibility in product size
  - production of fines/too small particles
  - Unwanted agglomeration
  - Strong oscillations
  - Energy reduction
- Debottlenecking
  - Increase capacity

DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

Population density

- Results sieve analysis

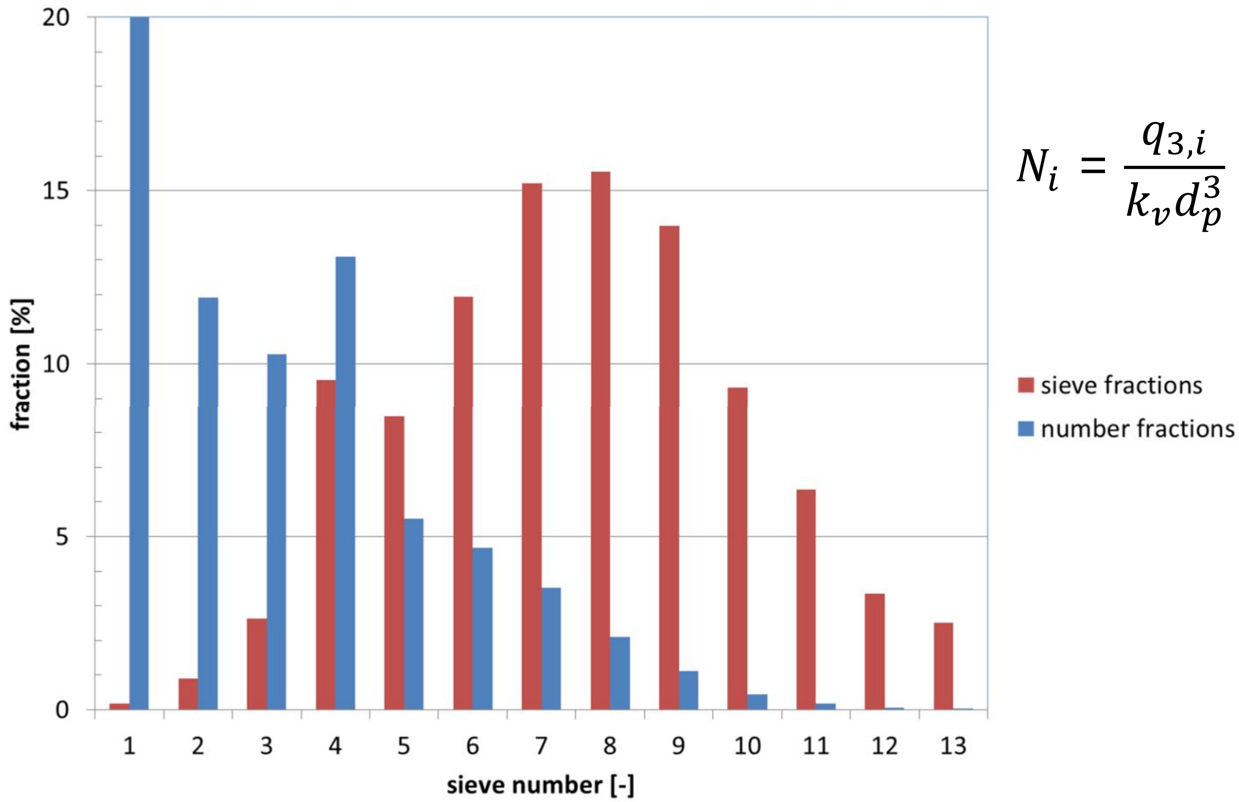


d_{sieve}	q_3
[mm]	[%]
0.6	0.19
1	0.91
1.4	2.64
2	9.54
2.36	8.49
2.8	11.95
3.35	15.22
4	15.55
4.75	13.97
5.6	9.32
6.7	6.37
8	3.36
10	2.51

DSM BRIGHT SCIENCE. BRIGHTER LIVING.

Population density

- From sieve data to number data



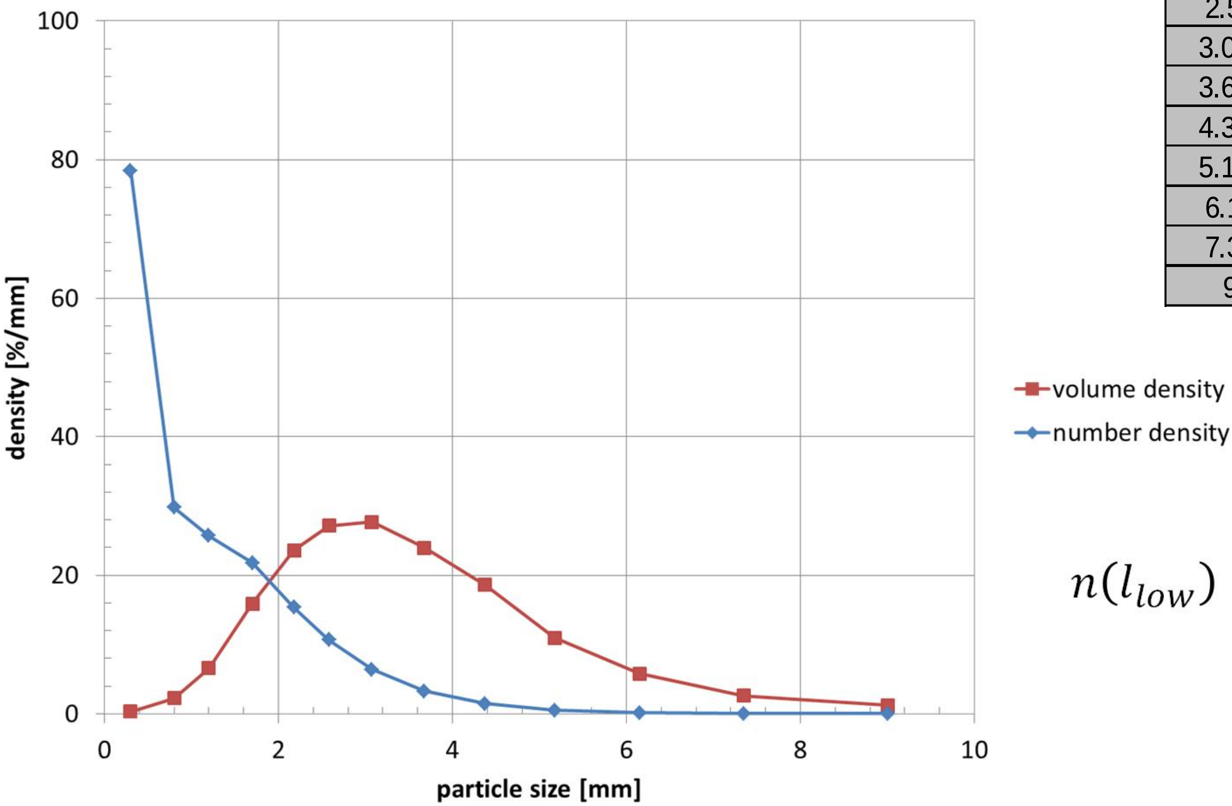
$$N_i = \frac{q_{3,i}}{k_v d_p^3}$$

d_{sieve}	q_3	d_{avg}	N_i	N_i/N_{tot}
[mm]	[%]	[mm]	[#]	[%]
0.6	0.19	0.3	13.33	47.03
1	0.91	0.8	3.38	11.91
1.4	2.64	1.2	2.91	10.28
2	9.54	1.7	3.71	13.08
2.36	8.49	2.18	1.56	5.52
2.8	11.95	2.58	1.33	4.69
3.35	15.22	3.075	1.00	3.53
4	15.55	3.675	0.60	2.11
4.75	13.97	4.375	0.32	1.12
5.6	9.32	5.175	0.13	0.45
6.7	6.37	6.15	0.05	0.18
8	3.36	7.35	0.02	0.06
10	2.51	9	0.01	0.02

Population density

- Particle size distribution

d_{avg}	N_i	N_i/N_{tot}	n_i	v_i
[mm]	[#]	[%]	[%/mm]	[%/mm]
0.3	13.33	47.03	78.39	0.31
0.8	3.38	11.91	29.79	2.26
1.2	2.91	10.28	25.71	6.59
1.7	3.71	13.08	21.80	15.90
2.18	1.56	5.52	15.33	23.58
2.58	1.33	4.69	10.65	27.15
3.075	1.00	3.53	6.41	27.67
3.675	0.60	2.11	3.25	23.92
4.375	0.32	1.12	1.50	18.63
5.175	0.13	0.45	0.53	10.97
6.15	0.05	0.18	0.17	5.79
7.35	0.02	0.06	0.04	2.58
9	0.01	0.02	0.01	1.25



$$n(l_{low}) = \lim_{l_{up} \to l_{low}} \frac{N_i}{l_{up} - l_{low}}$$

DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

Population balance

- Conversation law on particles
  - Similar to mass & heat balance
  - Describes changes of particle ensembles

- Phenomena to describe
  - Nucleation & Growth
  - Agglomeration
  - Breakage

- One-dimensional PBE for compartment

$$\frac{\partial n}{\partial t} + \frac{\partial Gn}{\partial l} = B - D \pm \sum \Phi_{in/out}$$

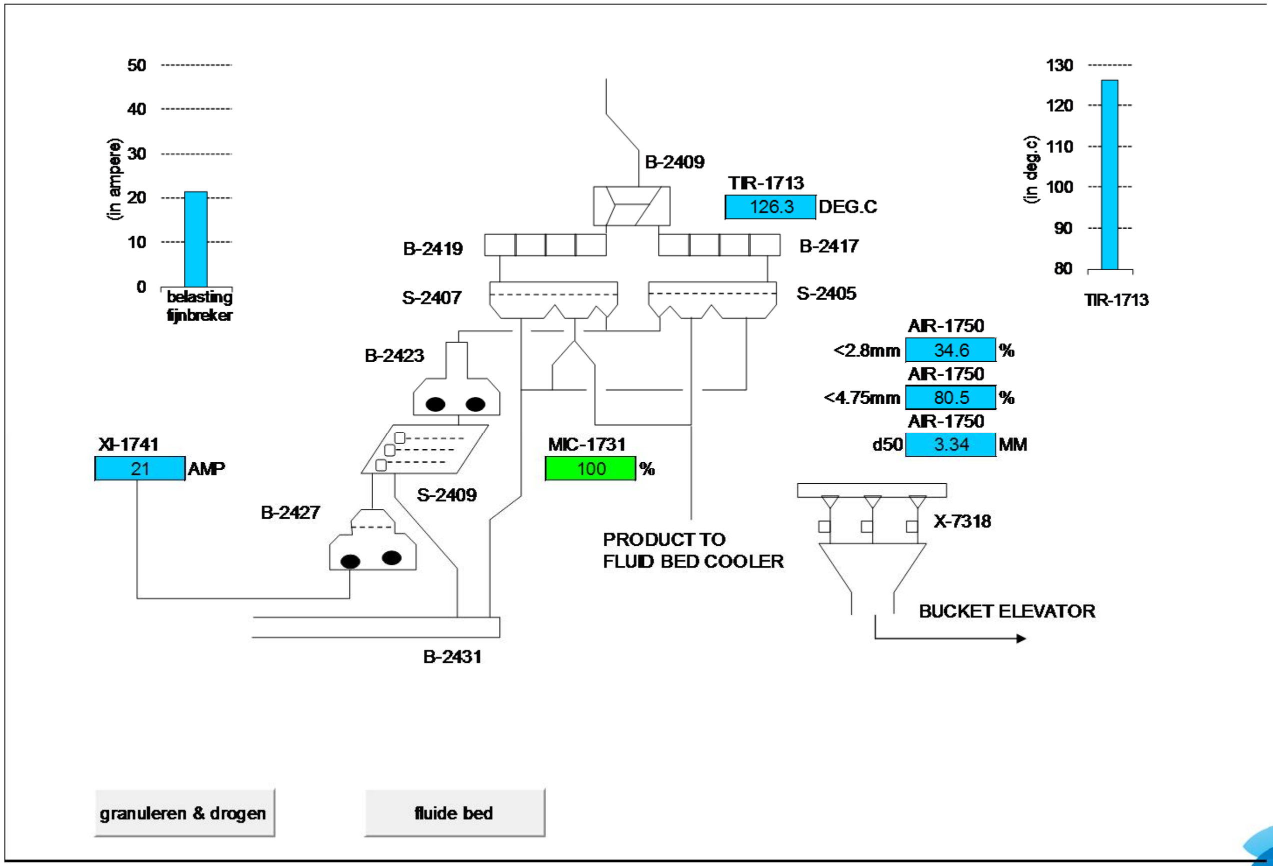
BRIGHT SCIENCE. BRIGHTER LIVING.

Population balance

- Solution methods
  - Steady state solutions
    - Matrix approach
    - Analytical solutions
  - Dynamic solutions
    - Moment methods
    - Method of lines
    - Class methods
  - Commercial tools
    - SolidSim/Aspen plus
    - gCrystal/gSolid
  - Experimental verification

Matrix approach towards population balance

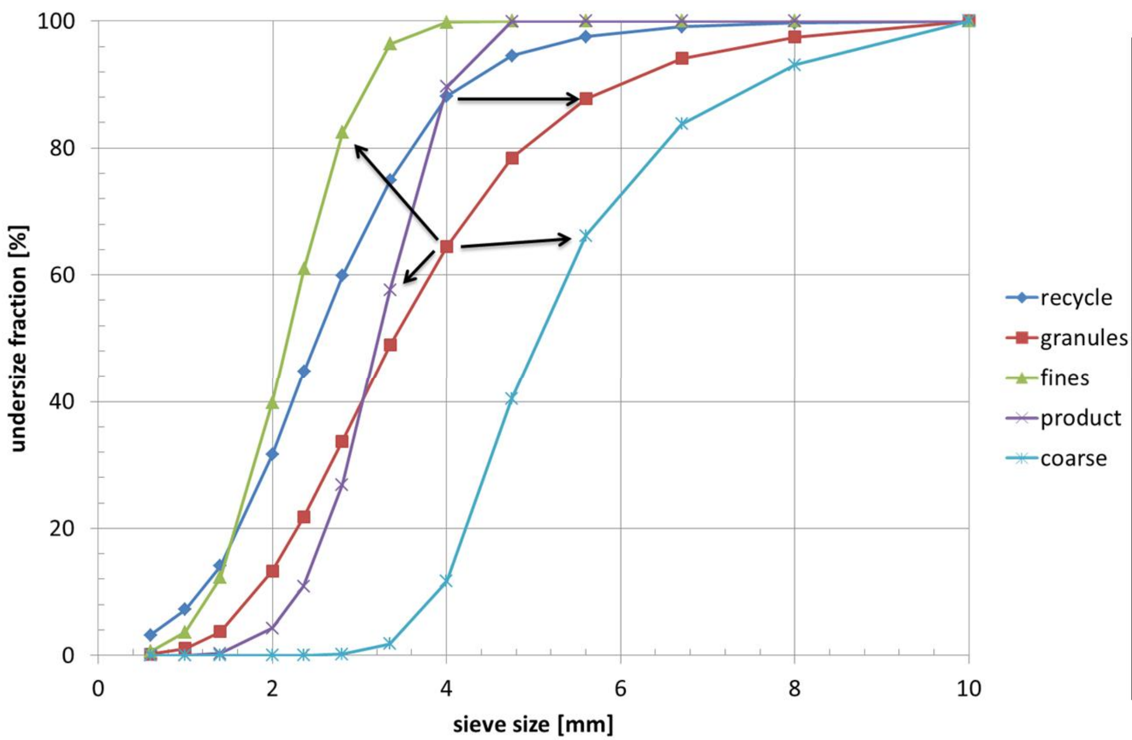
- Milling & sieving



DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

Milling & sieving

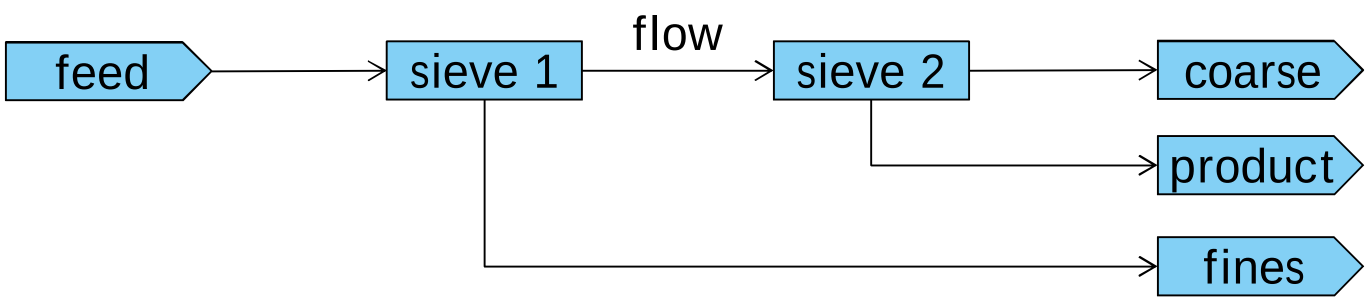
- Process data



	recycle	granules	fines	product	coarse
d_{sieve}	Q_3	Q_3	Q_3	Q_3	Q_3
[mm]	[%]	[%]	[%]	[%]	[%]
0.6	3.19	0.19	0.64	0.00	0.00
1	7.21	1.09	3.67	0.02	0.00
1.4	14.09	3.73	12.27	0.29	0.00
2	31.63	13.27	39.86	4.30	0.00
2.36	44.75	21.76	60.93	10.86	0.02
2.8	59.94	33.70	82.54	26.90	0.17
3.35	74.88	48.92	96.39	57.64	1.80
4	88.18	64.47	99.82	89.69	11.65
4.75	94.51	78.44	100.00	99.95	40.42
5.6	97.54	87.77	100.00	100.00	66.15
6.7	99.10	94.13	100.00	100.00	83.77
8	99.71	97.49	100.00	100.00	93.06
10	100.00	100.00	100.00	100.00	100.00
d_{50}	2.51	3.40	2.17	3.21	5.07

Sieve operation

- Process sequence



- Sieve/Tromp curve
  - Sieve curve: T = flow/feed

- Mass balance

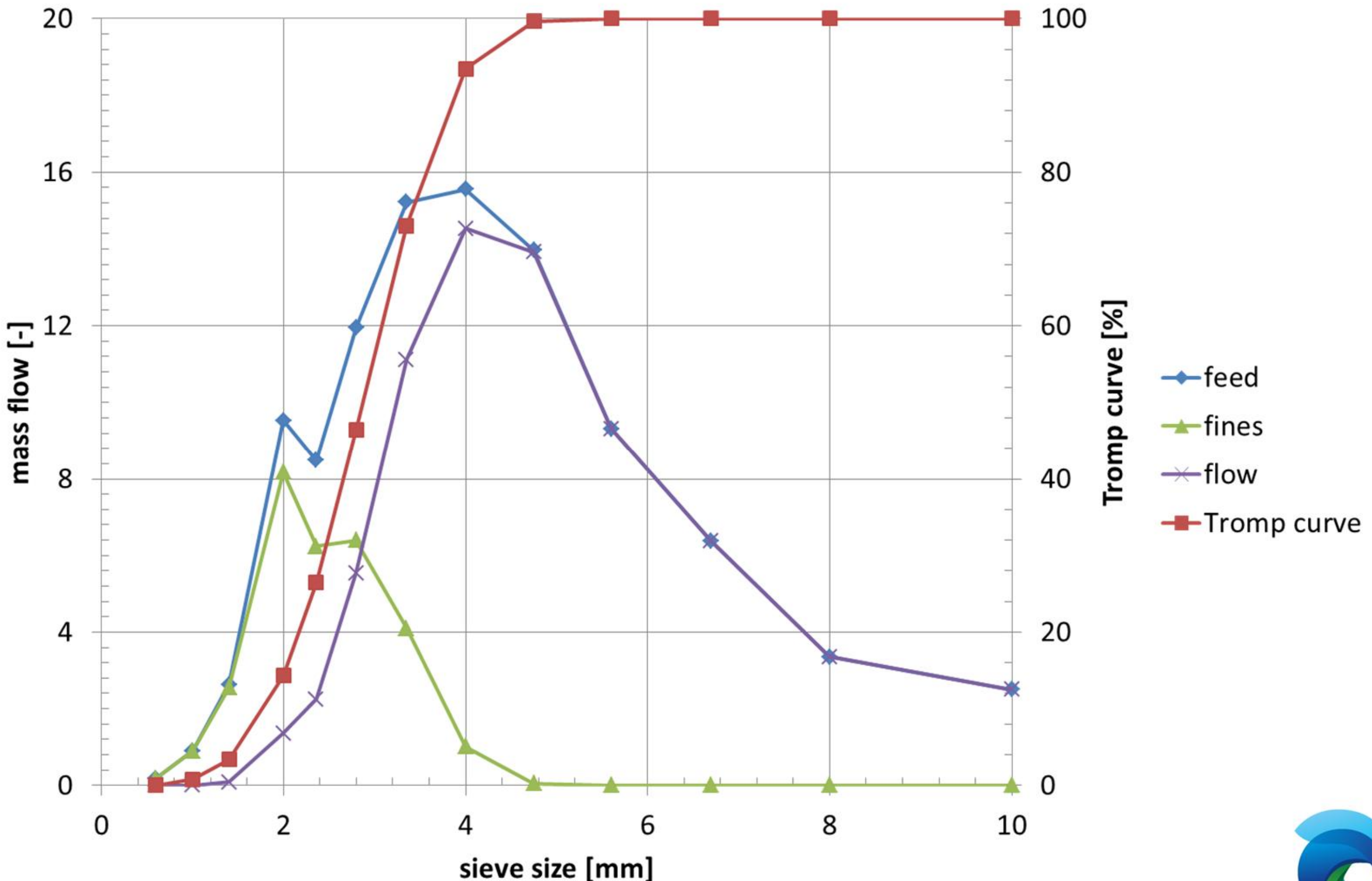
$$\begin{bmatrix} flow\ 1 \\ \vdots \\ flow\ N \end{bmatrix} = \begin{bmatrix} T\ 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & T\ N \end{bmatrix} \begin{bmatrix} feed\ 1 \\ \vdots \\ feed\ N \end{bmatrix}$$

$$\begin{bmatrix} feed\ 1 \\ \vdots \\ feed\ N \end{bmatrix} = \begin{bmatrix} fines\ 1 \\ \vdots \\ fines\ N \end{bmatrix} + \begin{bmatrix} flow\ 1 \\ \vdots \\ flow\ N \end{bmatrix}$$

Sieve operation

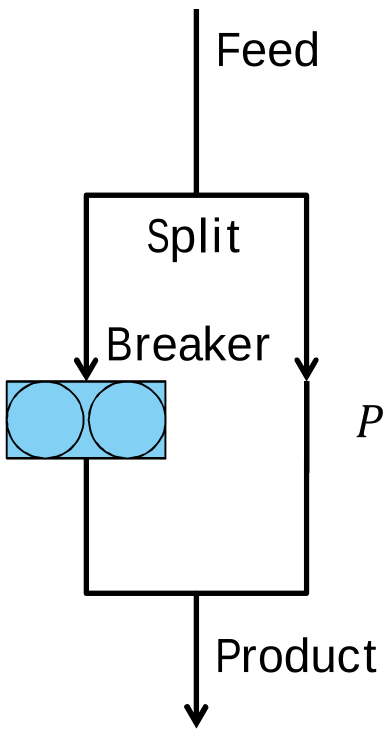
$$T(d_p) = \frac{1}{1 + \left(\frac{d_{cutoff}}{d_p}\right)^2 exp\left[k_s\left(1 - \left(\frac{d_2}{d_{cutoff}}\right)^2\right)\right]}$$

- Sieve performance

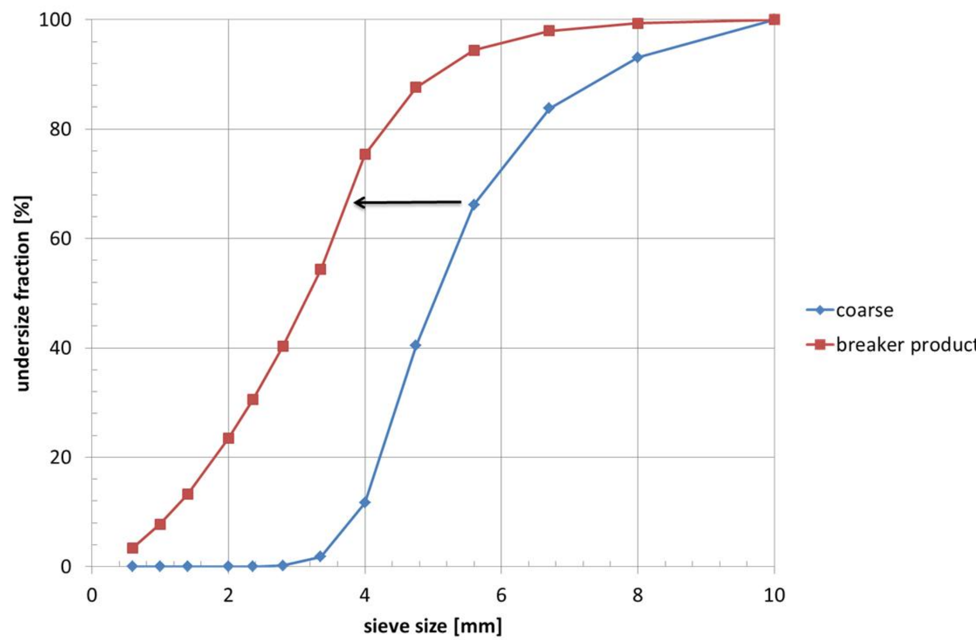


Milling operation

- flowsheet



$$P = (1 - S)F + BSF$$



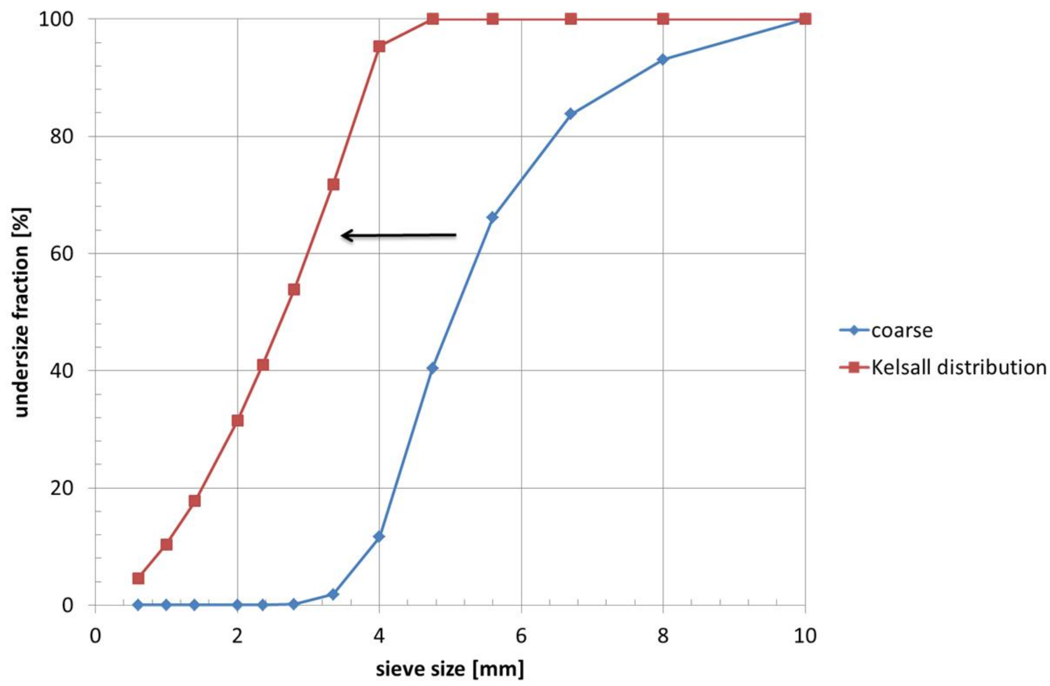
Milling operation

- Kelsall breaking model

$$Q_{3,frag} = \left(\frac{d}{d_{mill}}\right)^k$$

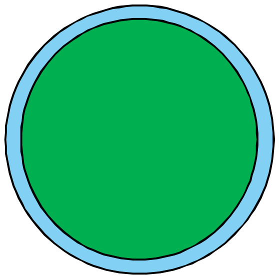
$$q_{3,i} = \left(\frac{d_i}{d_{mill}}\right)^k - \left(\frac{d_{i-1}}{d_{mill}}\right)^k$$

$$B = \begin{bmatrix} q_{3,1} & 0 & 0 \\ q_{3,1} & q_{3,2} & 0 \\ q_{3,1} & q_{3,2} & q_{3,N} \end{bmatrix}$$



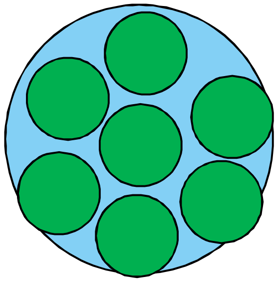
granulation

- Two mechanisms
  - Growth by layering

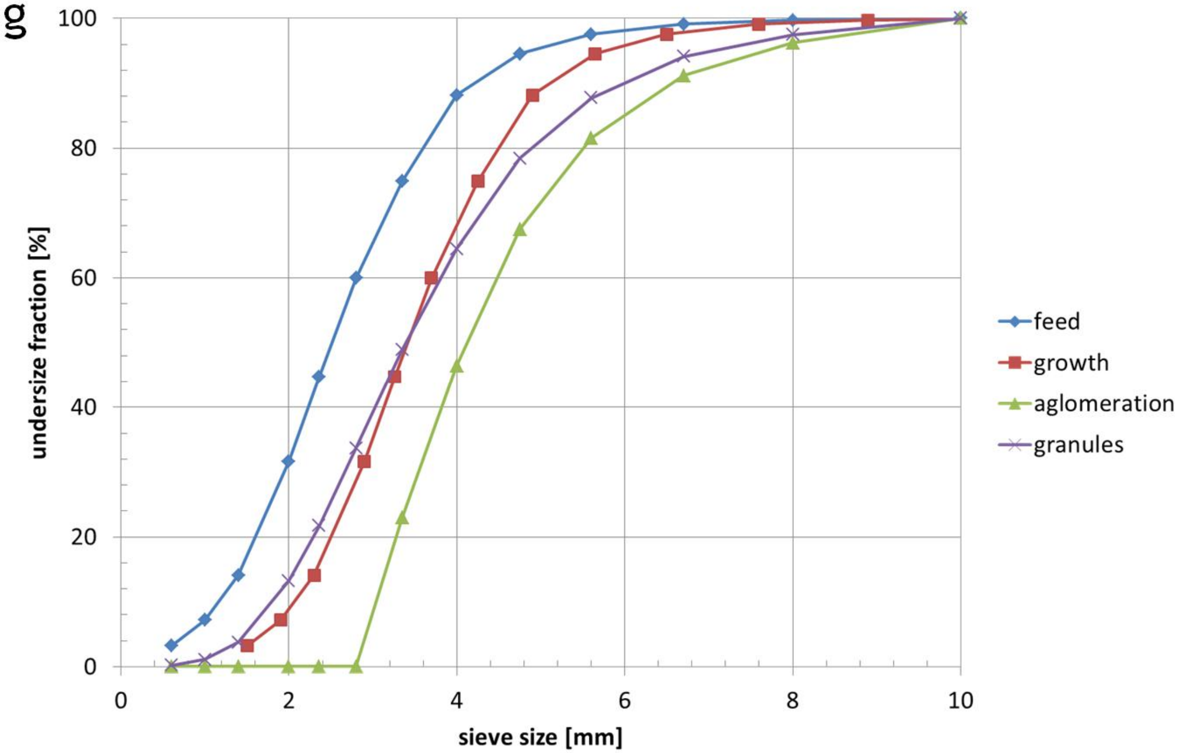


$$d_{new} = \beta d_{old}$$

  - Agglomeration

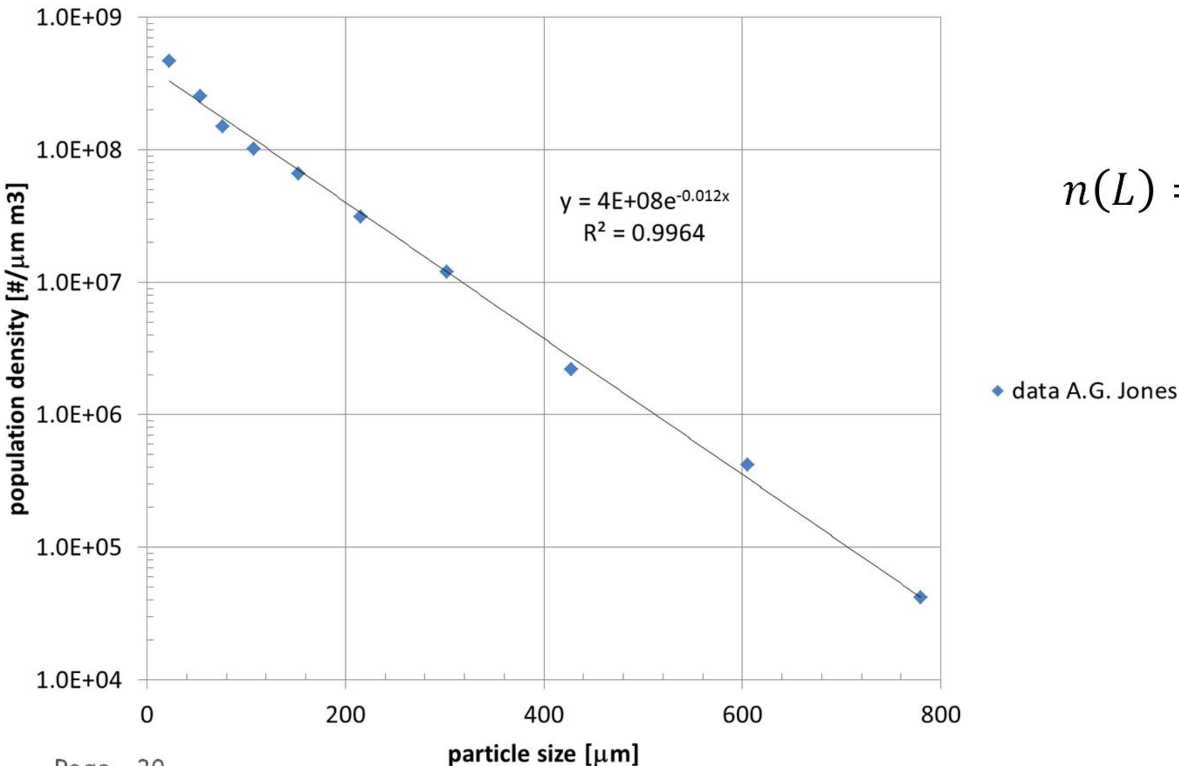


$$Q_{3,new} = \frac{Q_{3,old} - Q_{3,crit}}{1 - Q_{3,crit}}$$



MSMPR crystallizer

- Mixed suspension, mixed product removal
  - Continuous system
  - Size independent crystal growth
  - No agglomeration/attrition



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

Method of moments

- Moments of distribution

$$m_i = \int_0^{\infty} n(L) L^i dL$$

- Zeroth moment: number of particles
- First moment: total length of particles
- Second moment: total area of particles
- Third moment: total volume of particles
- Crystal growth:

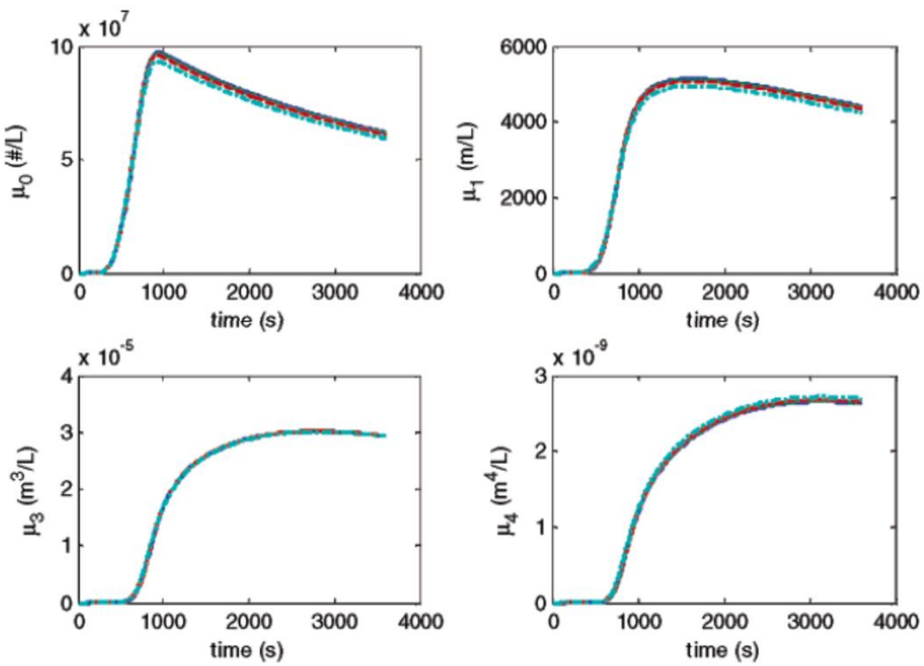
$$\frac{dm_0}{dt} = BV \qquad \frac{dm_i}{dt} = i m_{i-1} G$$

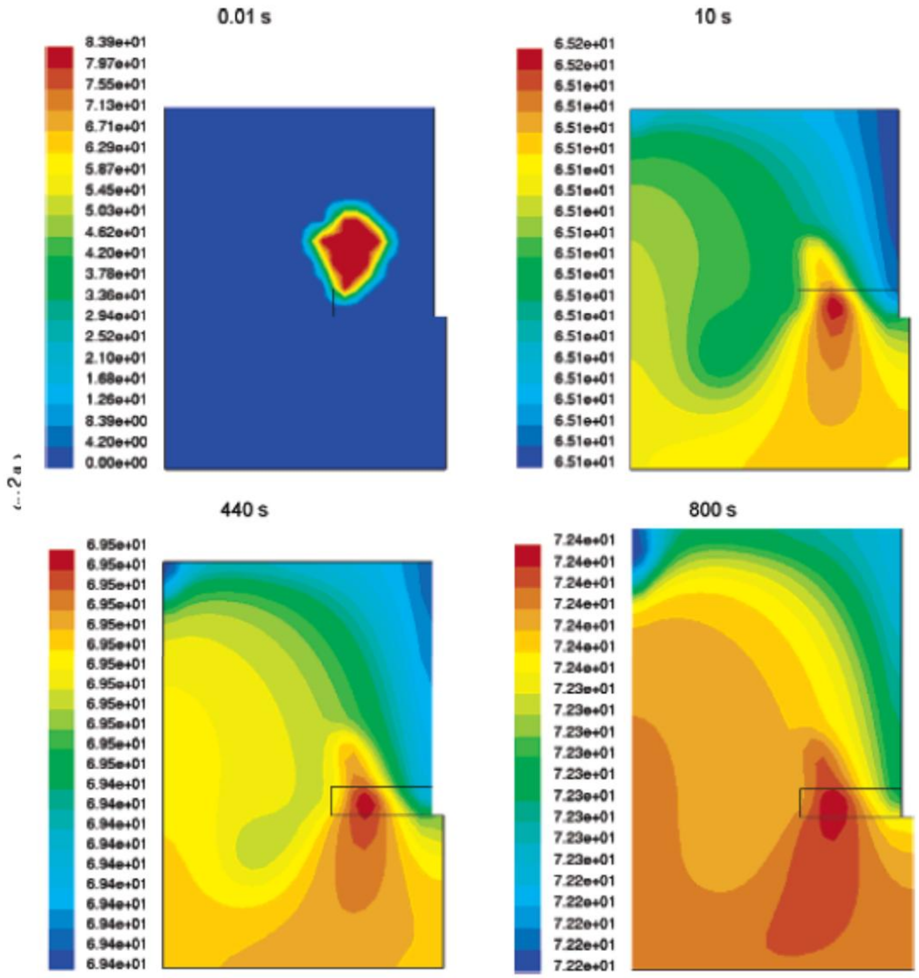
- Applied in CFD applications

DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

Method of moments & CFD

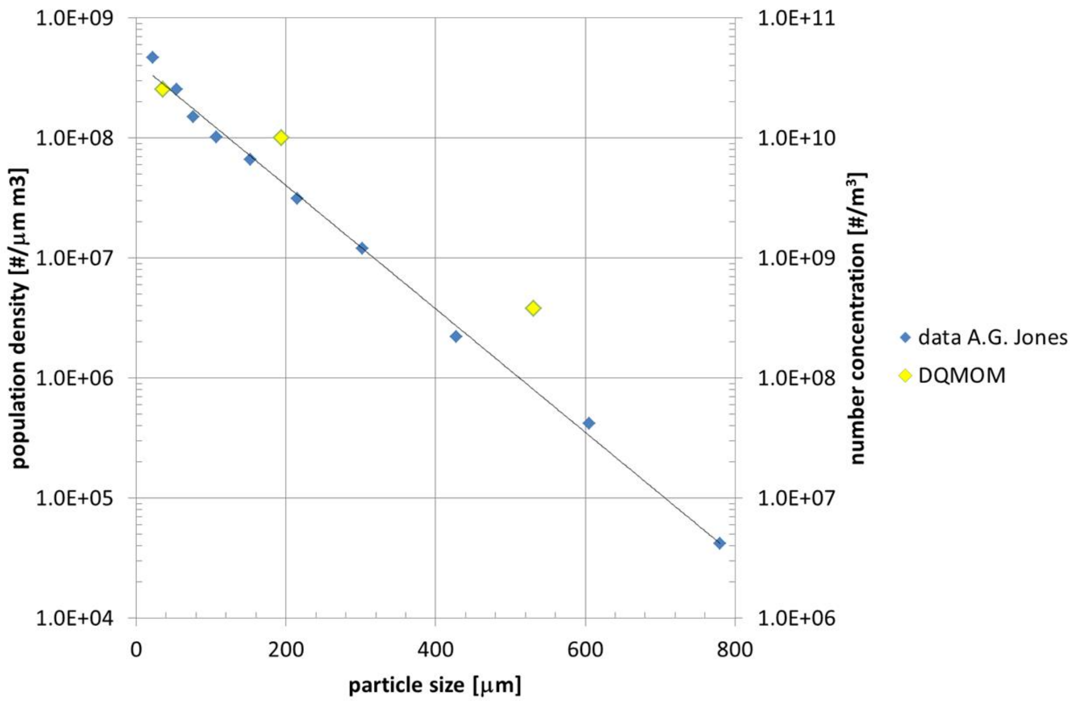
- Anti-solvent crystallization
  - Crystal Growth & Design
  - 6 (2006), 1291 - 1303





Discrete Quadrature Method Of Moments

- Aerosol Science, 36 (2005), 43 – 73
- Discretization of population density with Dirac functions
  - Variable number concentration and particle size

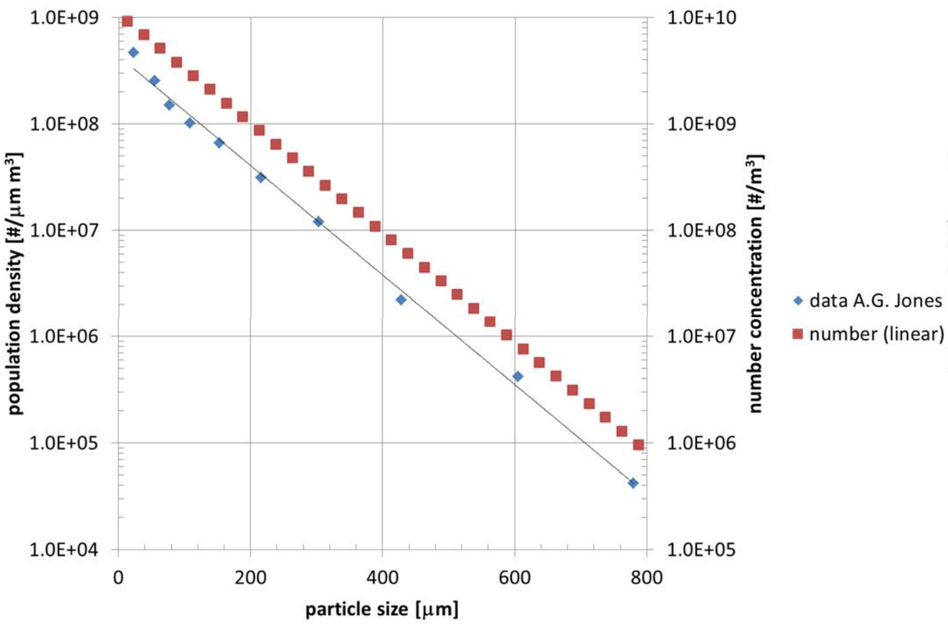


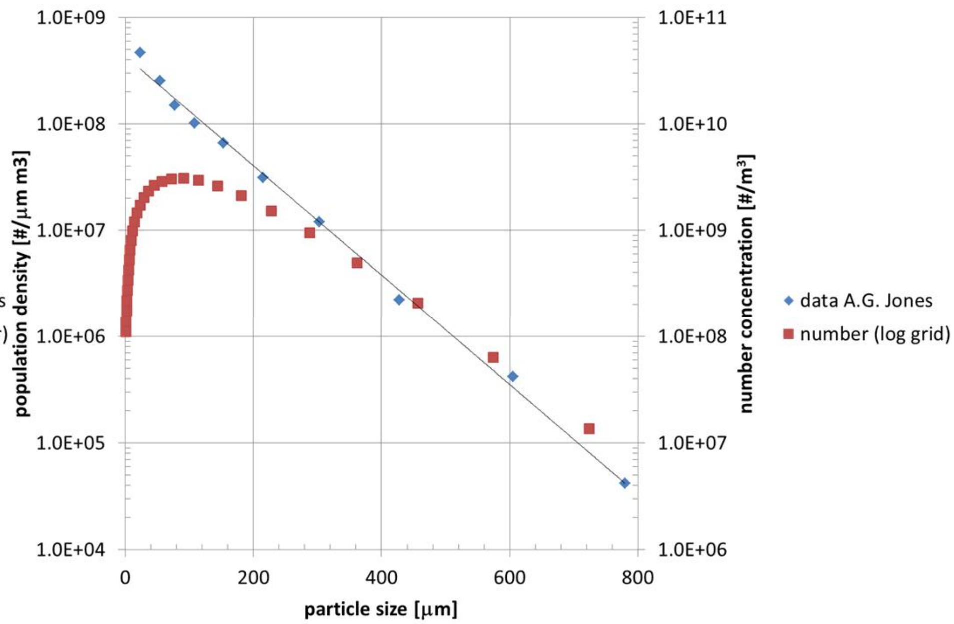
BRIGHT SCIENCE. BRIGHTER LIVING.

Class method for PBE

- Transformation from partial differential equation to set of ordinary differential equations
  - From density to number concentrations
  - Discretization of size domain

$$N_i = n(L_i)\Delta L$$



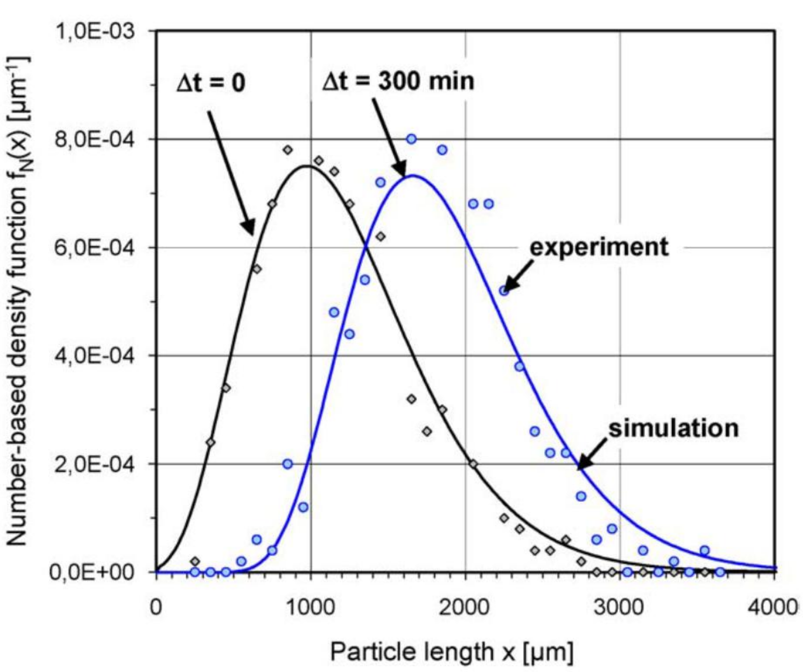


DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

Class method for PBE

- Transformation from partial differential equation to set of ordinary differential equations
  - From density

$$\frac{\partial n}{\partial t} + \frac{\partial Gn}{\partial l} = B - D \pm \sum \Phi_{in/out} \Rightarrow$$



  - to number concentrations

$$\frac{dN_i}{dt} = \frac{aG_iN_i + bG_{i-1}N_{i-1}}{L_i} + B_i - D_i \pm \sum \Phi_{i,in/out}$$

DSM BRIGHT SCIENCE. BRIGHTER LIVING.

Class method for PBE

- Incorporation of agglomeration
  - Hounslow et al, AIChE J., 34 (1988), 1821 - 1832

$$\frac{dN_i}{dt} = N_{i-1}\sum_{j=1}^{i-1} 2^{j-i+1}\beta_{i-1,j}N_j + \frac{1}{2}\beta_{i-1,i-1}N_{i-1}^2 - N_i\sum_{j=1}^{i-1} 2^{j-i}\beta_{i,j}N_j - N_i\sum_{j=i}^{\infty}\beta_{i,j}N_j$$

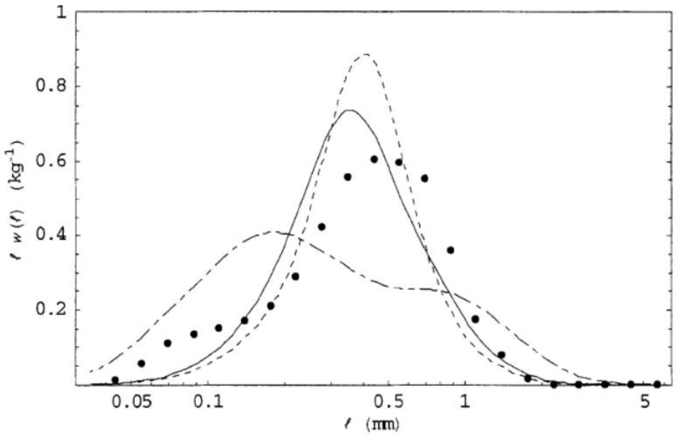


Figure 5. Granule-size distribution results of initial simulations using SIK (dotted line), SSK (chain-dashed line) and EKK (continuous line).

Size-independent kernel SIK	$\beta_0(t)$
Smoluchowski's shear kernel SSK	$\beta_0(t)(l+\lambda)^3$
Equipartition of kinetic energy kernel EKK	$\beta_0(t)(l+\lambda)^2\sqrt{\frac{1}{\lambda^3}+\frac{1}{l^3}}$

Class method for PBE

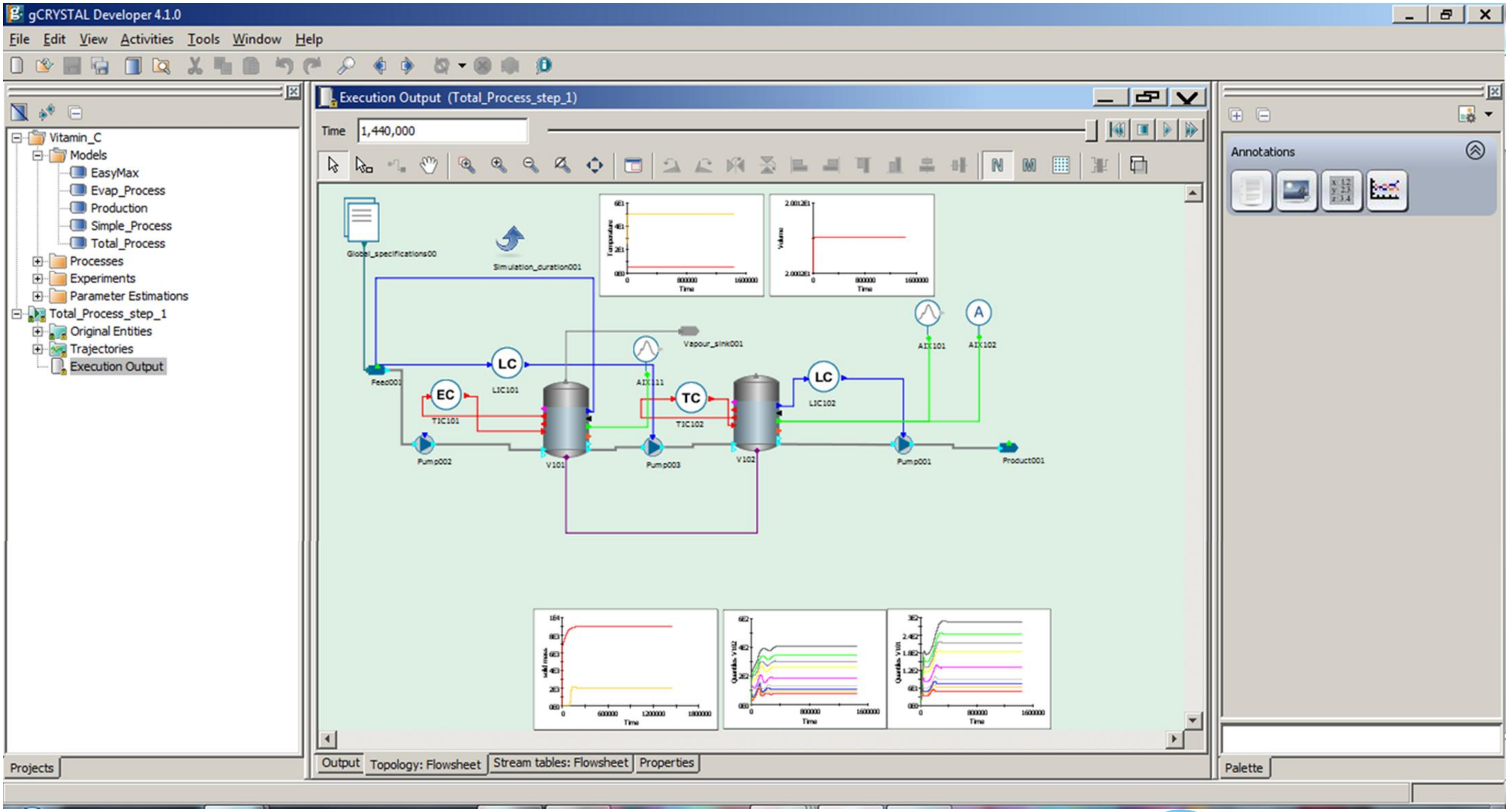
- Other methods possible
  - Higher order discretization
  - Logarithmic densities
  - Pivot method (variable size grid)

- Population Balances, D. Ramkrishna, Academic Press, San Diego, USA, ISBN 0-12-576970-9

BRIGHT SCIENCE. BRIGHTER LIVING.

Commercial tools

- gCrystal



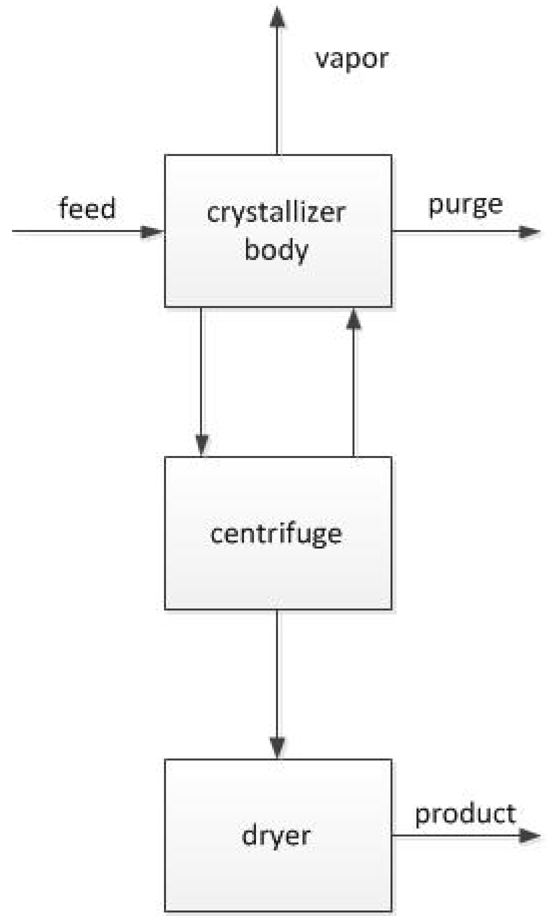
DSM
BRIGHT SCIENCE. BRIGHTER LIVING.

References

- Population Balances, D. Ramkrishna, Academic Press, San Diego, USA, ISBN 0-12-576970-9
- Crystallization Process Systems, A.G. Jones, Butterworth-Heinemann, Oxford, UK, ISBN 0-7506-5520-8
- A Discretized Population Balance for Nucleation, Growth, and Aggregation, M.J. Hounslow et al, AIChE J, 34 (1988), 1821 – 1832.

Exercise

- Design vitamin C crystallization plant
  - Specifications for Vitamin C product:
    - Ascorbic acid content > 99 wt-%
    - organic impurities < 0.2 wt-%
    - Particle size distribution
      - Max 20 % < 75 mm,
      - Max 30 % > 150 mm
  - Specification for Vitamin C process:
    - Requested production:
      - 3 kta
    - Feed stream:
      - 20 wt-% ascorbic acid in water
      - 0.1 wt-% KGA present
    - Centrifuge:
      - Cake liquid content: 10 wt-%
  - Cryst. Res. Technol. 43 (2008), 381 – 389



BRIGHT SCIENCE. BRIGHTER LIVING.™