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Models based on population balance approach

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Population Balance models

The population balance equation (PBE) is a statement of continuity for particulate systems, originally derived in 1964.

Population balances are of key relevance to a very diverse group of scientists, including astrophysicists, high-energy physicists, geophysicists, colloid chemists, biophysicists, materials scientists, meteorologists and chemical engineers.

Chemical engineers have put population balances to most use, with applications in the areas of crystallization; gas-liquid, liquid-liquid, and solid-liquid dispersions; liquid membrane systems; fluidized bed reactors; aerosol reactors; and microbial cultures.

Engineers encounter particles in a variety of systems. The particles are either naturally present or engineered into these systems. In either case these particles often significantly affect the behavior of such systems.

This modeling approach provides a framework for analyzing these dispersed phase systems and describes how to synthesize the behavior of the population particles and their environment from the behavior of single particles in their local environments

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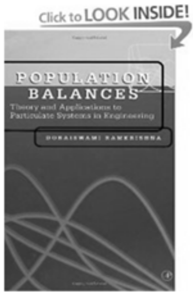
Population Balance models

Ramkrishna provides a clear and general treatment of population balances with emphasis on their wide range of applicability. New insight into population balance models incorporating random particle growth, dynamic morphological structure, and complex multivariate formulations with a clear exposition of their mathematical derivation is presented. **Population Balances** provides the only available treatment of the solution of inverse problems essential for identification of population balance models for breakage and aggregation processes, particle nucleation, growth processes, and more. This book is especially useful for process engineers interested in the simulation and control of particulate systems. Additionally, comprehensive treatment of the stochastic formulation of small systems provides for the modeling of stochastic systems with promising new areas of applications such as the design of sterilization systems and radiation treatment of cancerous tumors.



Doraiswami Ramkrishna,
Purdue University, West Lafayette, Indiana, U.S.A.
“**Population Balances. Theory and Applications to Particulate Systems in Engineering**”, Academic Press, ISBN: 0-12-576970-9,
Pages: 355, Publication Date: 8 August 2000, Price: £83.99

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Population Balances

Formulation

The Population Balance Equation was originally derived in 1964, when two groups of researchers studying crystal nucleation and growth recognized that many problems involving change in particulate systems could not be handled within the framework of the conventional conservation equations only, see Hulburt & Katz (1964) and Randolph (1964) .

They proposed the use of an equation for the continuity of particulate numbers, termed population balance equation, as a basis for describing the behavior of such systems.

This balance is developed from the general conservation equation:

Input - Output + Net Generation = Accumulation

🕮 § 4.4 in Himmelblau D.M. and Bischoff K.B., “Process Analysis and Simulation”, John Wiley & Sons Inc., 1967 (**Collocazione: 660.281 HIM 1**)

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Elements necessary for a population balance Model

Element	General description	Example
ENTITY	• *specific of each "particulate system";* • *crystallization, biochemical processes, polymerization, leaching, comminution, and aerosols are just some examples;* • entities are "discrete" and not continuous; • entities are "countable", but may be infinite in number	Yeast cell in a fermenter
PROPERTIES of ENTITY	• *in general, entities have a specified set of m properties* $\boldsymbol{\zeta_i}$ with i = 1,2...m • *the properties* ζ_i *will depend on the application;* • *typical examples are the entity's size diameter, entity's chemical composition, entity's age*	Cell mass, cell age, etc.
ENTITY DISTRIBU-TION	• *the function* $\boldsymbol{\psi(t, x, y, z, \zeta_1, \zeta_2, ..., \zeta_m)}$ *represents the entity distribution* • **t** *is time* • **x, y, z** *are the spatial coordinates* • *it is similar to a probability density function*	Number of cells per unit fermenter volume, unit cell mass, unit cell age, etc.

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Entity distribution function

Physical meaning

$$\psi(x, y, z, \zeta_1, \ldots, \zeta_m, t)dx\, dy\, dz\, d\zeta_1 \ldots d\zeta_m$$

is the fraction of entities at time **t** that are:

- contained in the infinitesimal volume $dV = dxdydz$
- characterized by values of properties in the ranges $\zeta_1 \div \zeta_1 + d\zeta_1, \ldots, \zeta_m \div \zeta_m + d\zeta_m$

Congruence constraint

$$\int_\Omega \psi(x, y, z, \zeta_1, \ldots, \zeta_m, t)dx\, dy\, dz\, d\zeta_1 \ldots d\zeta_m = 1$$

where Ω is the (3+m)-dimensional space of the independent variables:

3 spatial or external coordinates (**x, y, z**)

m properties or internal coordinates ($\boldsymbol{\zeta_i}$ with i = 1,2...m)

ⓘ time **t** may be one additional independent variable

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Conservation law

Generation

Positive and Negative terms are defined as:

$$\mathrm{N} = \frac{Entity\ born}{(time\ unit)(volume\ unit)(unitary\ variation\ of\ the\ \text{"i"}\ property}$$

$$\mathrm{M} = \frac{Entity\ disappearance}{(time\ unit)(volume\ unit)(unitary\ variation\ of\ the\ \text{"i"}\ property}$$

Hypotheses:

- large, arbitrary, time-varying sub-space $R(t) \subseteq \Omega$
- closed sub-space, with no input or output of entities

Balance equation

Accumulation = Net Generation

$$\frac{d}{\mathrm{dt}}\int_{R(t)} \psi dR = \int_{R(t)} (N - M)\, dR \qquad \text{(I)}$$

$$dR = dxdydzd\zeta_1 \ldots d\zeta_m$$

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Leibnitz formula

One dimension

a(t) b(t)

------ |——| ----->

x

$$\frac{d}{dt}\int_{a(t)}^{b(t)} f(x,t)dx = \int_{a(t)}^{b(t)}\left\{\frac{\partial f(x,t)}{\partial t} + \frac{d}{dx}\left[\frac{dx}{dt} f(x,t)\right]\right\}dx = \int_{a(t)}^{b(t)}\frac{\partial f(x,t)}{\partial t}dx + f\left[b(t),t\right]\frac{db(t)}{dt} - f\left[a(t),t\right]\frac{da(t)}{dt}$$

Multi-dimensional

$$\frac{d}{dt}\int_{R(t)} f dR = \int_{R(t)}\left[\frac{\partial f}{\partial t} + \sum_{l} \frac{\partial}{\partial l}\left(\frac{dl}{dt} f\right)\right]dR = \int_{R(t)}\left[\frac{\partial f}{\partial t} + \nabla \bullet \left(\dot{l} f\right)\right]dR$$

where:

R(t) is a time-variable region of the space Ω

f(•) is a scalar function

l stands for any of the non-time variables x, y, z, ζ_1, ζ_2….,

the sum Σ is over all such variables

$\dot{l}$ = is the column vector of all $\frac{dl}{dt}$

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Generalized population balance model on «microscopic scale»

The total derivates with respect to time included in the Leibnitz formula can be explained in a physical way:

$$\frac{dx}{dt} = v_x ; \frac{dy}{dt} = v_y ; \frac{dz}{dt} = v_z ; \frac{d\zeta_i}{dt} = v_i$$

v_i is the change rate with respect to the time or kinetics of the property ζ_i

The Equation (I) becomes:

$$\int_{R(t)} \left\{ \frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}(v_x \psi) + \frac{\partial}{\partial y}(v_y \psi) + \frac{\partial}{\partial z}(v_z \psi) + \sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}(v_i \psi) + M - N \right\} dR = 0$$

As the region R(t) is arbitrary, the necessary condition for that equation to be true is that the integrating term is null

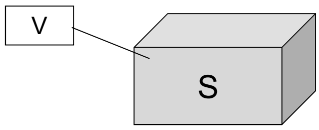
$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}(v_x \psi) + \frac{\partial}{\partial y}(v_y \psi) + \frac{\partial}{\partial z}(v_z \psi) + \sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}(v_i \psi) + M - N = 0$$

This is the **generalized population balance model on <u>microscopic scale</u>**

(in x, y, z coordinates)

Switch to «macroscopic scale»

Often ψ spatial dependence is not known or not desired, while only averaged value on system geometric volume V is requested.
The volume-averaged entity distribution is:



$$\overline{\psi} = \frac{1}{V} \int_V \psi dV \qquad dV = dxdydz$$

Integrating over the whole volume the **generalized population balance model**:

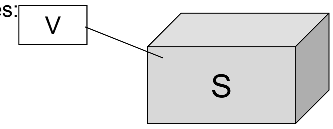
$$\int_V \left\{ \overset{\boxed{\mathrm{I}}}{\frac{\partial \psi}{\partial t}} + \overset{\boxed{\mathrm{II}}}{\nabla \bullet (\vec{v}\psi)} + \overset{\boxed{\mathrm{III}}}{\sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}(v_i \psi)} + \overset{\boxed{\mathrm{IV}}}{(M - N)} \right\} dV = 0$$

Let's examine the various terms:
The term (I) can be obtained by an inversion of the multi-dimensional Leibnitz formula, restricted to the spatial coordinates only:

$$\int_V \frac{\partial \psi}{\partial t} dV = \frac{d}{dt} \int_V \psi dV - \int_V \overset{\boxed{\mathrm{V}}}{\nabla \bullet (\vec{v}_s \psi)} dV$$

Where $\vec{v}_s$ indicates the speedness of the surface S which containes the volume V translating and varying

According to **Gauss divergence theorem**, the term ***V*** becomes:



$$\int_V \nabla \bullet \left(\overrightarrow{v_s}\psi\right) dV = \int_S \vec{n} \bullet \left(\overrightarrow{v_s}\psi\right) dS$$

vector $\vec{v}_s$ indicates the speedness for every point of the surface S containing control volume V

$\vec{n}$ is the normal versor to S directed toward the external

The term ***II*** is transformed by the same **Gauss theorem**

$$\int_V \nabla \bullet \left(\vec{v}\,\psi\right) dV = \int_S \vec{n} \bullet \left(\vec{v}\psi\right) dS$$

The terms ***I*** and ***II*** (included V) can be combined together:

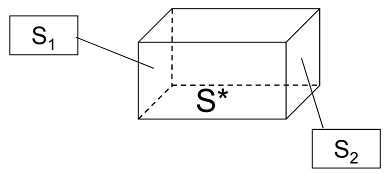
$$\int_V \left\{ \overset{\boxed{I}}{\frac{\partial \psi}{\partial t}} + \overset{\boxed{II}}{\nabla \bullet \left(\vec{v}\psi\right)} \right\} dV = \frac{d}{dt}\int_V \psi dV + \overset{\boxed{VI}}{\int_S \vec{n} \bullet \left(\vec{v} - \overrightarrow{v_S}\right) \psi dS}$$

In the term ***VI*** the surface S is considered as the sum of three contributions:

$S = S_1 + S_2 + S^*$

Where:

- S_1 is inlet surface to the system
- S_2 is the outlet surface from the system
- S^* is the remaining part of the surface (impenetrable)



The term ***VI*** becomes :

$$\int_S \vec{n} \bullet \left(\vec{v} - \overrightarrow{v_s}\right) \psi dS =$$

$$= \int_{S_1+S_2} \vec{n} \bullet \left(\vec{v} - \vec{v}_S\right)\psi dS + \overset{\boxed{VII}}{\int_{S^*} \vec{n} \bullet \left(\vec{v} - \vec{v}_S\right) \psi dS^*} = \overset{\boxed{VIII}}{-\int_{S_1} V_1 \psi_1 dS_1} + \overset{\boxed{IX}}{\int_{S_2} V_2 \psi_2 dS_2} + 0$$

Where :

- v_1 is the relative speedness in the inlet section (directed toward the opposite verse to the normal $\vec{n}$) $\quad \vec{n} \cdot (\vec{v} - \vec{v}_s) = 0$
- v_2 is the relative speedness in the outlet section
- Term ***VII*** is null because on S* $\quad \vec{n} \bullet \left(\vec{v} - \vec{v}_S\right) = 0$

Further Hypothesis:
ψ_1 and ψ_2 are averaged and, therefore, constant, respectively on S_1 and S_2

The terms ***VIII*** and ***IX*** can be simplified as follows:

$$\int_{S_1} v_1 \psi_1 dS_1 = \overline{\psi}_1 \int_{S_1} v_1 dS_1 = \overline{\psi}_1 Q_1 \quad ; \quad \int_{S_2} v_2 \psi_2 dS_2 = \overline{\psi}_2 \int_{S_2} v_2 dS_2 = \overline{\psi}_2 Q_2$$

where Q_1 and Q_2 are volumetric flowrates through S_1 and S_2, respectively.

The term ***III*** is integrated over the volume V and yields:

$$\int_V \sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}(v_i \psi) dV = \sum_{i=1}^{m} \int_V \frac{\partial}{\partial \zeta_i}(v_i \psi) dV =$$

$$= \sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i} \int_V v_i \psi dV = \sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}\left[v_i \int_V \psi dV\right] = V \sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}\left(v_i \overline{\psi}\right)$$

The term ***IV*** yields:

$$\int_V (M - N) dV = V\left(\overline{M} - \overline{N}\right)$$

Population balance model on «macroscopic scale»

After replacing all the terms:

$$V \frac{\partial}{\partial t}\left(\overline{\psi}\right) + V \sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}\left(v_i \overline{\psi}\right) + V\left(\overline{M} - \overline{N}\right) - Q_1 \overline{\psi}_1 + Q_2 \overline{\psi}_2 = 0$$

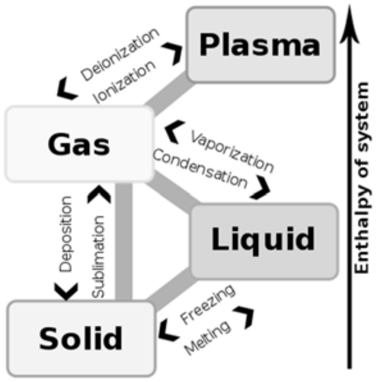
Dividing by V:

$$\underbrace{\frac{\partial}{\partial t}\left(\overline{\psi}\right)}_{\text{ACC}} + \underbrace{\sum_{i=1}^{m} \frac{\partial}{\partial \zeta_i}\left(v_i \overline{\psi}\right)}_{\text{PSEUDO/CONV}} + \underbrace{\overline{M} - \overline{N}}_{\text{GEN}} = \left[\underbrace{Q_1 \overline{\psi}_1}_{\text{IN}} - \underbrace{Q_2 \overline{\psi}_2}_{\text{OUT}}\right] \frac{1}{V}$$

This is the **population balance model on «macroscopic scale»**

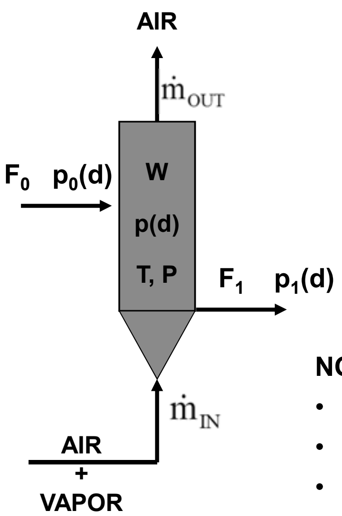
(without x, y, z coordinates)

Example No. 1
Vapor Deposition in a gas-solid fluidized bed



ch.14 pag.136, Daizo Kunii and Octave Levenspiel, Fluidization Engineering , 2nd. ed. Butterworth-Heinemann, 1991

Hypotheses



scheme
of the fluidized bed

- Steady state
- Macroscopic approach
- Constant inventory of particles in the fluidized bed
- All particles having the same chemical composition
- Particles having spherical geometry
- Particles having constant density
- No new particle formed directly by vapor deposition
- Negligible elutriation
- Negligible solid-solid and solid-wall attrition

NOMENCLATURE

- W = bed mass (inventory of particles)
- F_0 = mass feed rate of fresh particles
- F_1 = mass discharge rate of processed particles

O. Levenspiel, D. Kunii, T. Fitzgerald
The processing of solids of changing size in bubbling fluidized beds
Powder Technology, Volume 2, Issue 2, December 1968, Pages 87-96

Vapor Deposition
in a gas-solid fluidized bed

Entity: solid particles

Property: particle diameter d

Objective: → **p(d) [=] m^{-1}**

p(d)*d*d is the mass fraction of particles with diameter between d and d+*d*d

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Population Balance approach:
the generation term

No. particles in [d; d+dd] • rate of particle volume change • particle density / particle size interval

$$\overline{N}(d) = \frac{W \cdot p(d)\,\mathit{d}d}{\rho_p \cdot \frac{\pi}{6} \cdot d^3} \cdot \frac{dV_p}{dt} \cdot \rho_p \cdot \frac{1}{\mathit{d}d} = \frac{W \cdot p(d)\,\mathit{d}d}{\rho_p \cdot \frac{\pi}{6} \cdot d^3} \cdot \frac{\pi}{6} 3d^2 \frac{\mathit{d}d}{\mathit{d}t} \cdot \rho_p \cdot \frac{1}{\mathit{d}d} =$$

$$= \frac{3 \cdot W \cdot p(d) \cdot \Re(d)}{d} [=] \frac{\text{mass}}{(\text{time}) \cdot (\text{unit property change})}$$

$\Re(d)$ is the rate of particle size change with time (property kinetics)

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The overall generation

$$\bar{N}_{tot} = \int_0^{\infty} \bar{N}(d)\,dd =$$
$$= \int_0^{\infty} \frac{3 \cdot W \cdot p(d) \cdot \Re(d)}{d}\,dd \, [=] \, \frac{\text{generated mass}}{\text{time}}$$

Overall Mass Balances

IN – OUT + GEN = 0

on the solid phase with ref. to the whole fluid bed:

1. $$F_0 - F_1 + \bar{N}_{tot} = 0$$

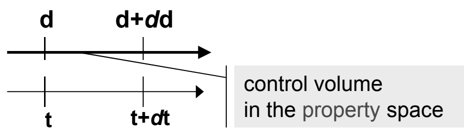
ⓘ This is NOT a Population Balance eq.

on the gas phase with ref. to the whole fluid bed:

1 bis. $$\dot{m}_{IN} - \dot{m}_{OUT} - \bar{N}_{tot} = 0$$

Population Balance approach:
the mass balance

per unit time
and
with ref. to the size interval [d;d+*d*d]:



IN with feed	OUT with discharge	entering the control volume [d; d+*d*d] from a lower size	leaving the control volume [d; d+*d*d] to a larger size	generation in the interval [d; d+*d*d]

$$F_0 \cdot p_0(d)\,dd - F_1 \cdot p_1(d)\,dd + \left[W \cdot p(d) \cdot \frac{dd}{dt}\right]_d - \left[W \cdot p(d) \cdot \frac{dd}{dt}\right]_{d+dd} + \frac{3 \cdot W \cdot p(d) \cdot \Re(d)\,dd}{d} = 0$$

$$\boxed{F_0 \cdot p_0(d) - F_1 \cdot p_1(d) - W \cdot \Re(d)\frac{dp(d)}{dd} - W \cdot p(d)\frac{d\Re(d)}{dd} + \frac{3 \cdot W \cdot p(d) \cdot \Re(d)}{d} = 0}$$

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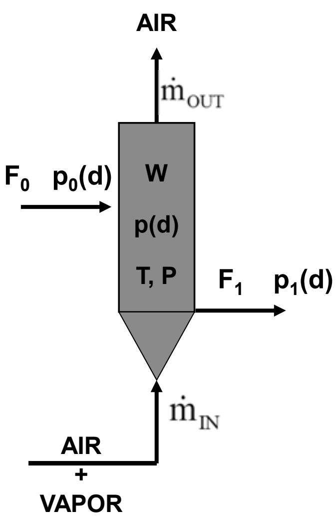
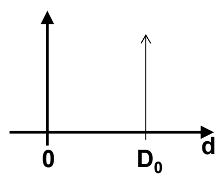
Further Hypotheses



- ✓ Back mixing: $p_1(d) = p(d)$
- ✓ “monosize” feed: $p_0(d) = \delta(d-D_0)$



DIRAC DELTA FUNCTION
(UNIT IMPULSE)

$\delta(d)=0$ for $d \neq D_0$
$\delta=\infty$ for $d=D_0$

$$\int_0^\infty \delta(d - D_0)\,dd = 1$$

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Population Balance approach: integration of mass balance eq.

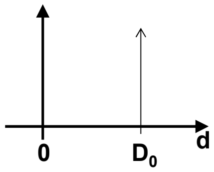
with ref. to an infinitesimal size interval located immediately below the feed size D_0: [D_0; D_0-dd]

$$F_0 \cdot p_0(d) - F_1 \cdot p(d) - W \cdot \Re(d)\frac{dp(d)}{dd} - W \cdot p(d)\frac{d\Re(d)}{dd} + \frac{3 \cdot W \cdot p(d) \cdot \Re(d)}{d} = 0$$

$$F_0 \cdot p_0(d)dd - \cancel{F_1 \cdot p(d)dd} - W \cdot \Re(d) \cdot dp(d) - \cancel{W \cdot p(d)dd} \cdot \frac{d\Re(d)}{dd} + \frac{3 \cdot W \cdot \Re(d)}{d}\cancel{p(d)dd} = 0$$

$$\frac{F_0 \cdot p_0(d)dd}{\Re(d)} - W dp(d) = 0$$

→ p(d)*d*d = 0



integration over [0, D_0] gives p(D_0):

$$\int_0^{D_0} \frac{F_0 \cdot p_0(d)}{\Re(d)} dd - \int_{p(0)=0}^{p(D_0)} W dp(d) = 0$$

$$F_0 \cdot \int_0^{D_0} \frac{p_0(d)}{\Re(d)} dd = W \cdot \int_{p(0)=0}^{p(D_0)} dp(d)$$

$$\Rightarrow \; p_0(d) = \delta(d - D_0)$$

$$\Rightarrow \; \int_0^{D_0} \frac{\delta(d - D_0)}{\Re(d)} dd = \frac{1}{\Re(D_0)}$$

4. $$p(D_0) = \frac{F_0}{W \cdot \Re(D_0)} \neq 0$$

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Population Balance approach: integration of mass balance eq.

with ref. to an infinitesimal size interval [d;d+*d*d] located above the feed size D_0:

$$\cancel{F_0 \cdot p_0(d)dd} - F_1 \cdot p(d)dd - W \cdot \Re(d) \cdot dp(d) - W \cdot p(d)dd \cdot \frac{d\Re(d)}{dd} + \frac{3 \cdot W \cdot \Re(d)}{d}p(d)dd = 0$$

manipulation and integration over [D_0, d] with d>D_0 give:

$$-\int_{D_0}^{d} \frac{F_1}{W \cdot \Re(d)} dd - \int_{p(D_0)}^{p(d)} \frac{dp(d)}{p(d)} - \int_{\Re(D_0)}^{\Re(d)} \frac{d\Re(d)}{\Re(d)} + 3 \cdot \int_{D_0}^{d} \frac{dd}{d} = 0$$

⇓

$$-\frac{F_1}{W}\int_{D_0}^{d} \frac{dd}{\Re(d)} + \ln\frac{p(D_0)}{p(d)} + \ln\frac{\Re(D_0)}{\Re(d)} + 3 \cdot \ln\frac{d}{D_0} = 0$$

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Population Balance approach: entity distribution eq. p(d)

$$-\frac{F_1}{W}\int_{D_0}^{d}\frac{d\mathrm{d}}{\Re(\mathrm{d})}=\ln\left[\frac{D_0^3}{d^3}\frac{\Re(\mathrm{d})}{\Re(D_0)}\frac{p(\mathrm{d})}{p(D_0)}\right]$$

Taking the exponential,
replacing eq. 4
and then solving for p(d) gives:

4. $$p(D_0)=\frac{F_0}{W\cdot\Re(D_0)}$$

3. $$\boxed{p(\mathrm{d})=\frac{F_0}{W\cdot\Re(\mathrm{d})}\cdot\frac{\mathrm{d}^3}{D_0^3}\cdot e^{-\frac{F_1}{W}\int_{D_0}^{d}\frac{d\mathrm{d}'}{\Re(\mathrm{d}')}}}$$

where d’ is an integration variable

Population Balance approach: congruence condition for p(d)

$$\int_{D_0}^{\infty}p(\mathrm{d})\,d\mathrm{d}=1$$

$$\int_{D_0}^{\infty}\frac{F_0}{W\cdot\Re(\mathrm{d})}\cdot\frac{\mathrm{d}^3}{D_0^3}\cdot e^{-\frac{F_1}{W}\int_{D_0}^{d}\frac{d\mathrm{d}'}{\Re(\mathrm{d}')}}\,d\mathrm{d}=1$$

2. $$\boxed{W=\frac{F_0}{D_0^3}\cdot\int_{D_0}^{\infty}\frac{\mathrm{d}^3}{\Re(\mathrm{d})}\cdot e^{-\frac{F_1}{W}\int_{D_0}^{d}\frac{d\mathrm{d}'}{\Re(\mathrm{d}')}}\,d\mathrm{d}}$$

Population Balance approach:
Final equations

1. $$F_1 - F_0 = 3W \int_{D_0}^{\infty} \frac{p(d)\cdot \Re(d)}{d} dd$$

2. $$W = \frac{F_0}{D_0^3} \cdot \int_{D_0}^{\infty} \frac{d^3}{\Re(d)} \cdot e^{-\frac{F_1}{W}\int_{D_0}^{d} \frac{dd'}{\Re(d')}} dd$$

3. $$p(d) = \frac{F_0}{W\cdot \Re(d)} \cdot \frac{d^3}{D_0^3} \cdot e^{-\frac{F_1}{W}\int_{D_0}^{d} \frac{dd'}{\Re(d')}}$$

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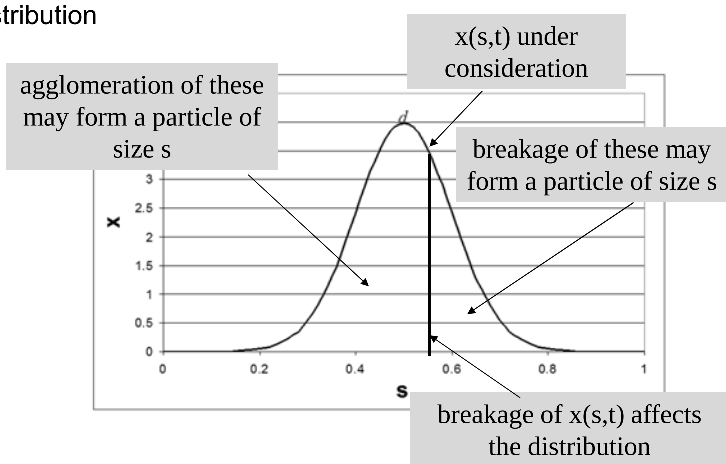
Population Balance approach:
Integro-differential equations

More generally, size distributions are time dependent.
Ex.:
rate of change of the distribution (shape) depends on the whole distribution



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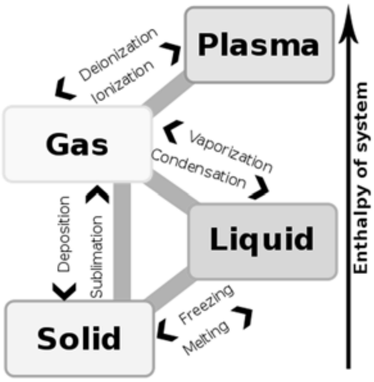
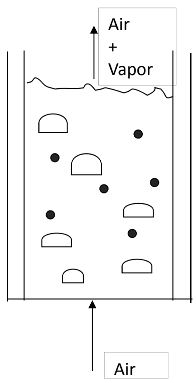
Example No. 2
Sublimation in a gas-solid fluidized bed



Hypotheses



scheme
of the fluidized bed

- Macroscopic approach
- Batch operation (dynamical system)
- “Active” particles (i.e., sublimating particles) different from the particles constituting the fluidized bed
- Perfect mixing
- All “Active” particles maintain the same composition
- Particles having spherical geometry
- Particles having constant density
- Negligible elutriation
- Negligible solid-solid and solid-wall attrition

NOMENCLATURE

- W_0 = overall mass of sublimating solid particles at time 0
- W(t) = overall mass of sublimating solid particles at time t

Population Balance approach: batch sublimation in fluidized bed

Entity: mass of sublimating solid particles

Property: particle diameter d

Objective: → **m(d,t) [=] kg/m**

m(d,t)Δd is the mass of sublimating particles in the bed with diameter between d and d+ Δd at the time t

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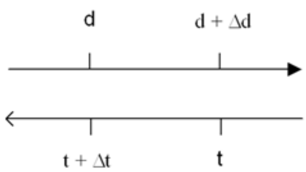
Population Balance approach: batch sublimation in fluidized bed

control volume in the "property space"



mass Balance
on the size interval Δd **and in the time interval Δt**

$$m(d+\Delta d,t)\left.\frac{dd}{dt}\right|_{d+\Delta d}\Delta t - m(d,t)\left.\frac{dd}{dt}\right|_{d}\Delta t - \frac{3m(d,t)\Delta d\,\Re(d)}{d}\Delta t = \left\{[m(d,t)]_{t+\Delta t} - [m(d,t)]_{t}\right\}\Delta d$$

$$\left[\frac{kg}{m}\,m\,\frac{m}{s}\,s\,m^{-1}\right]$$

where: $\Re(d) = \frac{dd}{dt} \; [=] \frac{m}{s}$

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Population Balance approach: batch sublimation in fluidized bed

Let us divide by Δt
For $\Delta t \rightarrow 0$

$$m(d+\Delta d,t)\left.\frac{dd}{dt}\right|_{d+\Delta d} - m(d,t)\left.\frac{dd}{dt}\right|_{d} - \frac{3m(d,t)\Delta d\Re(d)}{d} = \frac{\partial m(d,t)}{\partial t}\Delta d$$

Let us divide by Δd

$$\frac{m(d+\Delta d,t)\left.\frac{dd}{dt}\right|_{d+\Delta d} - m(d,t)\left.\frac{dd}{dt}\right|_{d}}{\Delta d} - \frac{3m(d,t)\Re(d)}{d} = \frac{\partial m(d,t)}{\partial t}$$

For $\Delta d \rightarrow 0$

$$\boxed{\frac{\partial[m(d,t)\Re(d)]}{\partial d} - \frac{3m(d,t)\Re(d)}{d} = \frac{\partial m(d,t)}{\partial t}}$$

PDE subject to:

IC:	for t=0	$m(d,0) = m_o(d)$
BC:	for d=0, $\forall t$	$m(0,t) = 0$

Population Balance approach: batch sublimation in fluidized bed

Comparison with the **population balance model on «macroscopic scale»**

$$\frac{\partial \overline{\Psi}}{\partial t} \Rightarrow \frac{\partial m(d,t)}{\partial t}$$

$$\sum_{i=1}^{m}\frac{\partial(v_i\overline{\Psi})}{\partial \zeta_i} \Rightarrow \frac{\partial[m(d,t)\Re(d)]}{\partial d}$$

$$\overline{M} \Rightarrow \frac{3m(d,t)\Re(d)}{d}$$

Total mass at time t:

$$W(t) = \int_0^{d_{max}} m(d,t)\,dd$$

Population Balance approach: batch sublimation in fluidized bed

Particular cases for sublimation kinetics

1. Volume

$$\frac{dm_p}{dt} = \rho_p \frac{\pi}{6}\frac{dd^3}{dt} = -b\pi d^3 \quad [=]\frac{kg}{s}$$

$$\rho_p \frac{3\pi d^2}{6}\frac{dd}{dt} = -b\pi d^3$$

$$\Re(d) = -hd$$

$$-hd\frac{\partial m(d,t)}{\partial d} - hm(d,t) + 3hm(d,t) = \frac{\partial m(d,t)}{\partial t}$$

2. Surface

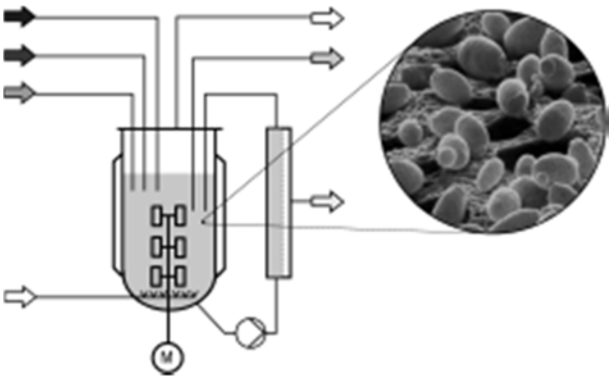
$$\frac{dm_p}{dt} = \rho_p \frac{\pi}{6}\frac{dd^3}{dt} = -c\pi d^2 \quad [=]\frac{kg}{s}$$

$$\rho_p \frac{3\pi d^2}{6}\frac{dd}{dt} = -c\pi d^2$$

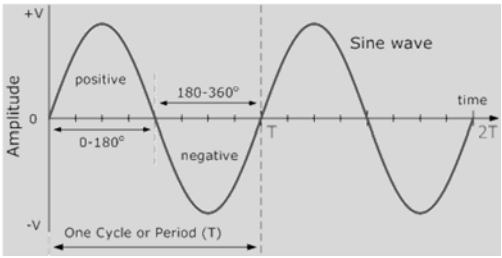
$$\Re(d) = -k$$

$$-k\frac{\partial m(d,t)}{\partial d} + \frac{3km(d,t)}{d} = \frac{\partial m(d,t)}{\partial t}$$

Yeast cell distribution in a fermenter



Example of sine wave



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