An Introduction to Population Balance Modeling

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Outline

• PBM? What’s that?
• Flocculation theory
  – Equations
  – Numerical methods
  – Solution techniques
• Examples
  – Mixing Tank
  – Secondary clarifier
Particle Collision and Coagulation Kinetics

• If particles in air or water are unstable, collisions can result in agglomeration or “Flocculation”

• Examples:
  ✓ Coagulation of aerosols
  ✓ Growth of rain droplets in clouds
  ✓ Precipitation Kinetics (Inorganics)
  ✓ Flocculation – Both double layer compression and charge neutralization

How do we describe the collision rate between particles, aerosols, droplets etc.?
Particle Collision and Coagulation Kinetics

• DOUBLE LAYER COMPRESSION
Particle Collision and Coagulation Kinetics

- Slightly Negative Colloid
- Stern Layer
- Diffuse Layer
- Ions In Equilibrium With Solution

• CHARGE NEUTRALIZATION
Particle Collision and Coagulation Kinetics

- Let's consider a box full of lots of high school sharks and one little fish (moving randomly)

The rate that seniors collide with fish is classically given by:

\[ N \propto n_s \]

- Now, if there are actually \( n_F \) fishes, the overall rate of collision between fishes and sharks is:

\[ N \propto n_F n_s \]
Particle Collision and Coagulation Kinetics

- Simplest expression for collision rate between two particle classes \( i \) and \( j \):
  \[
  N_{ij} = \beta(r_i, r_j) n_i n_j \tag{3.30}
  \]
  \( \beta \) is the collision frequency function.

- This assumes fast flocculation (no resistance to collisions).

- Now consider a discrete distribution of particle sizes:

  \[\text{Lets assume } V_2 = 2 V_1, V_3 = 3 V_1, V_4 = 4 V_1, \ldots, V_i = i V_1\]
Particle Collision and Coagulation Kinetics

- Assumption: Coalescing drop ⇒ $V_k = V_i + V_j$

- We can now define a rate equation for particle collision (Smoluchowski)

\[
\frac{dn_k}{dt} = \frac{1}{2} \sum_{i+j=k} \beta(r_i, r_j)n_i n_j - \sum_{i=1}^{\infty} \beta(r_i, r_k)n_i n_k
\]

(3.31)

**GENERAL DYNAMIC EQUATION**
Particle Collision and Coagulation Kinetics

- Laminar Shear (2D):

Collision can only occur for particles entering the sphere

⇒ Mass Transfer Rate of \( r_j \) particles into collision sphere \( r_i + r_j \)
Particle Collision and Coagulation Kinetics

- This is a mass balance problem:

\[
\frac{\partial}{\partial t} \iiint_{C.V.} n_j \, dV = - \iiint_{C.S.} n_j \, \vec{n} \cdot \vec{u} \, dA
\]
Particle Collision and Coagulation Kinetics

\[ \vec{n} \cdot \vec{u} = |n| |u| \cos \alpha \]

\[ \cos \alpha = - \sin(\alpha - 90) = -\sin \phi \]

\[ \vec{n} \cdot \vec{u} = (1) |u| (-\sin \phi) \]

\[ |u| = (r_i + r_j) \cos \phi \frac{du}{dx} \]

\[ \text{Location} \]

\[ \text{Slope} \]

\[ \vec{n} \cdot \vec{u} = (-\sin \phi)(r_i + r_j) \cos \phi \frac{du}{dx} \]
Particle Collision and Coagulation Kinetics

Figure 3.12. Three-dimensional collision sphere in two-dimensional velocity field.
Particle Collision and Coagulation Kinetics

Need to determine $dA$:

$$dA = (2)(r_i + r_j) \sin \phi (r_i + r_j) d\phi$$

Mass transferrate $= - \iiint_C (\vec{n} \cdot \vec{u}) n_j dA$

$$= (\frac{2}{\pi})(2)(r_i + r_j)^3 \frac{du}{dx} \int_0^{\pi/2} \sin^2 \phi \cos \phi \, d\phi$$

$2$ quadrants for collision differential strip
Particle Collision and Coagulation Kinetics

$$\int_{0}^{\pi/2} \sin^2 \phi \cos \phi \, d\phi$$

$$u = \sin^2 \phi \quad dv = \cos \phi \, d\phi$$

$$du = 2 \sin \phi \cos \phi \, d\phi \quad v = \sin \phi$$

Use Integration by Parts:

$$\int uv = \int vdu$$

$$\int \sin^2 \phi \cos \phi = \sin^3 \phi - 2 \int \sin^2 \phi \cos \phi \, d\phi$$

$$3 \int_{0}^{\pi/2} \sin^2 \phi \cos \phi = \sin^3 \phi \bigg|_{0}^{\pi/2} = 1 - 0 = 1$$

$$\frac{\pi}{2} \int_{0}^{\pi/2} \sin^2 \phi \cos \phi = 1/3$$
Particle Collision and Coagulation Kinetics

Mass transfer rate = \( \frac{4}{3} (r_i + r_j)^3 \frac{du}{dx} n_j \)

Since we have \( n_i \) central particles

\( N_{ij} = n_i \times \text{Mass transfer} \)

\( \therefore N_{ij} = 4/3 (r_i + r_j)^3 \frac{du}{dx} n_i n_j \)

\( N_{ij} = \beta(r_i, r_j)n_i n_j \)

For Laminar Shear, \( \beta(r_i, r_j) = 4/3 (r_i + r_j)^3 \frac{du}{dx} \)
Other Collision Mechanisms

- **Isotropic Turbulence**: 
  \[ \beta(r_i, r_j) = 1.29 \left( \frac{r_i + r_j}{v} \right)^3 \left( \frac{\bar{\varepsilon}}{v} \right)^{1/2} \]

  \( \bar{\varepsilon} = \text{Average Mass Energy Dissipation Rate} \)
  \[ \bar{\varepsilon} = \frac{\text{Energy Dissipation}}{\text{Fluid Mass - time}} = \frac{1}{\rho v} \times \text{Power} \]

  \[ \left( \frac{\bar{\varepsilon}}{v} \right)^{1/2} = \left( \frac{\rho}{\rho v} \times \frac{1}{v} \right)^{1/2} = \left( \frac{\rho}{\rho v} \times \frac{\rho}{\mu} \right)^{1/2} = \left( \frac{\rho}{\mu v} \right)^{1/2} = "G" \]

- **G** is Camp and Stein characteristic velocity gradient
- **G** is used to describe:
  - Power in mixing vessels
  - Pressure drop in pipes
  - Velocity gradient in atmospheres
Other Collision Mechanisms

- Differential Sedimentation:
  \[ \beta(r_i, r_j) = \pi (r_i + r_j)^2 |v_i - v_j| \]

- where \( v \) = Stokes terminal settling velocity

- Brownian Motion
  \[ \beta(r_i, r_j) = \frac{2kT}{3\mu} \left( \frac{1}{r_i} + \frac{1}{r_j} \right) (r_i + r_j) \]

Focus on Brownian Motion

- \( r_i = r_j \) \( \Rightarrow \beta(r_i, r_j) = \frac{8kT}{3\mu} = K' \)

Substituting into GDE

- \[ \frac{dn_k}{dt} = \frac{K'}{2} \sum_{i+j=k} n_i n_j - n_k K' \sum_{i=1}^{\infty} n_i \]
Other Collision Mechanisms

Summing each side

\[ \sum_{i=1}^{\infty} \frac{dn_i}{dt} = \frac{K'}{2} \sum_{k=1}^{\infty} \sum_{i+j=k} n_i n_j - K \sum_{k=1}^{\infty} n_k \sum_{i=1}^{\infty} n_i \]

Let \( N_\infty = \sum_{i=1}^{\infty} n_i \) = Total no. of concentration of all particle size classes at any time

Substituting into previous equation:

\[ \frac{dN_\infty}{dt} = \frac{K'}{2} N_\infty^2 - K N_\infty^2 = - \frac{K'}{2} N_\infty^2 \]

\[ \int N_\infty^{-2} dN_\infty = \int \frac{-K'}{2} dt \]

\[ - \frac{1}{N_\infty} = - \frac{K'}{2} t + \text{const} \]
Other Collision Mechanisms

At $t = 0$, $N_\infty(t) = N_\infty(0)$

$$\frac{1}{N_\infty(t)} = \frac{K'}{2} t + \frac{1}{N_\infty(0)}$$

$$N_\infty(t) = \frac{N_\infty(0)}{1 + \frac{K'N_\infty(0)}{2} t}$$

$$\tau = \frac{2}{K'N_\infty(0)}$$
Other Collision Mechanisms

Figure 3.13: Comparison of collision frequency functions for a 1-μm-radius particle interacting with other particles in air. The x-axis refers to the size of the other particle. Source: Reproduced from Friedlander, *Smoke, Dust and Haze*, John Wiley and Sons, New York, 1977. Used with permission of S.K. Friedlander, 1995.
Other Collision Mechanisms

Fig. 7.1 The variations in $N_\infty, n_1, n_2, \ldots$ with time for an initially monodisperse aerosol. The total number concentration, $N_\infty$, and the concentration of monomer, $n_1$, both decrease monotonically with increasing time. The concentrations of the polymers pass through a maximum.
Exercise

• In the previous figure, we noted that simple expressions for \( n_1, n_2, \) and so on could be developed. Imagine that at the beginning of coagulation, all particle are of size class 1 (sometimes called the “primary particles”), that is, \( n_1(t=0) = N_\infty(t=0) \). Therefore, it follows that at \( t=0 \), the concentration of all larger-size-class particles is zero.

• Examine GDE on slide 17 and show that the differential equation for \( n_1 \) is

\[
\frac{dn_1}{dt} = -K n_1 N_\infty
\]

where

\[
K = \frac{8kt}{3\mu}
\]
Exercise

Next show that this differential equation integrates to

\[ n_1 = \frac{N_\infty(0)}{(1 + t/\tau)^2} \]

where \( \tau \) is given by

\[ \tau = \frac{2}{KN_\infty(0)} \]
Solution

Solution:

\[
\frac{dn_k}{dt} = \frac{4kT}{3\mu} \sum_{i+j=k} n_i n_j - \frac{8kT}{3\mu} \sum_{i=1}^{\infty} n_i
\]

•a) For \( k=1 \), there no smaller particles that will collide to from larger \( k=1 \) particles therefore the gain term is zero.

If we let \( K = \frac{8kT}{3\mu} \) and we know that:

\[
N_\infty = \sum_{i=1}^{\infty} n_i \text{ then,}
\]

\[
\frac{dn_1}{dt} = -K n_1 N_\infty
\]

Note that \( N_\infty \) is a function of \( t \) and was solved as:

\[
N_\infty(t) = \frac{N_\infty(0)}{1 + \frac{2}{K N_\infty(0)} t}
\]

Units are 1/time
Let it be 1/\( \tau \)

•Contd.
\[ N_\infty(t) = \frac{N_\infty(0)}{1 + t/\tau} \]

Substituting into differential equation:

\[ \frac{dn_1}{dt} = -K_n N_\infty(0) \frac{1}{1 + t/\tau} \]

Solve by separation,

\[ \int_{N_\infty(0)}^{n_1} \frac{dn_1}{n_1} = -KN_\infty(0) \int_{0}^{t} \frac{1}{1 + t/\tau} \, dt \]

\[ \ln\left( \frac{n_1}{N_\infty(0)} \right) = -KN_\infty(0) \int_{0}^{t} \frac{1}{1 + t/\tau} \, dt \]

\[ \ln\left( \frac{n_1}{N_\infty(0)} \right) = -KN_\infty(0) \tau \ln(1 + t/\tau) \]

Since \( \tau = \frac{2}{KN_\infty(0)} \) hence \( KN_\infty(0)\tau = 2 \)
Solution

\[
\ln\left( \frac{n_1}{N_\infty(0)} \right) = -2 \ln(1 + t/\tau)
\]

\[
\frac{n_1}{N_\infty(0)} = e^{-2\ln(1+t/\tau)}
\]

\[
\frac{n_1}{N_\infty(0)} = e^{\ln(1+t/\tau)^{-2}}
\]

\[
\therefore \frac{n_1}{N_\infty(0)} = \frac{1}{(1+t/\tau)^2}
\]
• Breakage of flat particles in impeller
• General one-dimensional PBM (Ramkrishna, 2000) without growth

\[ \frac{\partial n(x,t)}{\partial t} = h(x,t)_{\text{agg}} + h(x,t)_{\text{break}} \]

• Birth and death concept

\[
\begin{align*}
 h(x,t)_{\text{agg}} &= \int f(\alpha, \beta(x,x'), n(x,t), n(x',t)) \\
 h(x,t)_{\text{break}} &= \int g(S(x), \Gamma(x', x), n(x,t))
\end{align*}
\]
• **Net aggregation rate expression**
  - Aggregation frequency $\beta$
    - Describes transport of flocs towards one another
      
      \[
      \beta(x, x' - x') = \frac{G}{\pi} \left( x^{1/3} + (x' - x')^{1/3} \right)^3
      \]
      \[
      \beta(x, x' - x') = \frac{G}{\pi} v_0^{1 - \frac{3}{Df}} \left( x^{1/Df} + (x' - x')^{1/Df} \right)^3
      \]
      \[
      \int f(\alpha, \beta(x, x'), n(x, t), n(x', t))
      \]
      
      - Temperature driven
      - Velocity gradient driven
      - ‘Perikinetic flocculation’
      - ‘Orthokinetic flocculation’
      - Differential Sedimentation

  - **Spicer & Pratsinis (1996)**
  - **Lee et al. (2000)**
• Net aggregation rate expression
  – Aggregation efficiency $\alpha$
    • Expresses success of collision
  – Constant \{0,1\}
  – Adler (1981)
    \[
    \alpha_{i,j} = \alpha_0 \left[ \frac{3\pi \mu (d_i + d_j)^3}{32 A_{ham}} \right]^\frac{1}{1 - \left( \frac{1}{d_i} + \frac{1}{d_j} \right)}^{-0.18}
    \]
  – Kusters et al. (1997)
    • Shell-core model
    • Similar, but using $R_{H,i}$ instead of $d_i$
• Net breakage rate expression

• Breakage frequency $S$
  – Power law – empirical approach
  \[ S(x) = Ax^a \]
  – Shear dependent - Ducoste (2000)
  \[ S(x) = \left( \frac{4}{15\pi} \right)^{1/2} \left( \frac{K_i\bar{\epsilon}}{\nu} \right) \exp \left( \frac{-C_1}{xK_i\bar{\epsilon}} \right) \]
• PBM = Integro-differential equation
\[
\frac{\partial n(x,t)}{\partial t} = \int_{0}^{\infty} \alpha \beta(x-x',x') n(x-x',t)n(x',t)dx' - n(x,t) \int_{0}^{\infty} \alpha \beta(x,x')n(x',t)dx' \\
+ \int_{x}^{\infty} r(x',t)S(x')\Gamma(x'-x,x)dx' - n(x,t)S(x)
\]

• Analytical solutions are rarely found
• Several numerical solutions in literature
• Discretisation of property x
  – Acceptable calculation times
  – Ease of implementation
Discretisation

- Integrals become summations
- $M$ ordinary differential equations
- Only *pivots* or representative $x$ for a class
• Hounslow and fixed pivot

One equation per class \( (N_i) \)

M ordinary differential equations

\[
\begin{align*}
V_i & \quad x_i & \quad V_{i+1} & \quad x_{i+1} & \quad V_{i+2} \\
\text{class } i & \quad & \text{class } i+1
\end{align*}
\]
• moving pivot

Two equations per class ($N_i$ and $x_i$)

$2^*M$ ordinary differential equations
• Combined aggregation/breakage – steady state (Nopens et al, 2005)
Introduction:

Population Balance Modeling and the Quadrature Method of Moment

Part I
Introduction: General Background

- PBM for simulating particle aggregation-breakup typically use average turbulent quantities to account for fluid flow characteristics.

- Experimental studies have revealed the influence of the turbulence spatial heterogeneity on the behavior of flocculation dynamics (Hopkins and Ducoste 2003).

- The local influence of the turbulence could be investigated by combining a CFD model with PBM equations (Marchisio et al. 2003c, Prat and Ducoste 2006, 2007).
Introduction: *PBM for aggregation-breakup problems*

- General transport equation of particles in presence of aggregation-breakup

\[
\begin{align*}
\frac{\partial n(x,t)}{\partial t} + & \quad \langle u_i \rangle \frac{\partial n(x,t)}{\partial x_i} - \frac{\partial}{\partial x_i} \left[ \rho \left( \frac{0.09 k_b^2/\varepsilon_p}{\varepsilon_p} \right) \frac{\partial n}{\partial x_i} \right] \frac{\partial x_i}{\partial x_i} \\
& = \frac{1}{2} \int \alpha[l, (d^3 - l^3)^{1/3}] \beta[l, (d^3 - l^3)^{1/3}] n(l) n((d^3 - l^3)^{1/3}) \, dl \\
& - n(d) \int \alpha[l, (d^3 - l^3)^{1/3}] \beta[l, (d^3 - l^3)^{1/3}] n(l) \, dl \\
& + \int k_b(l) F(d \mid l) n(l) \, dl \\
& - k_b(d) n(d)
\end{align*}
\]

(I : Transient term) + (II : Convective term) – (III : Diffusion term) = (IV : Source term)

► Traditional Class Size methods => *one equation to be solved for each particle Class Size*
Introduction: Advantage of the QMOM formulation

- Method of moments appear to be an alternative approach to the PBM class size method

- QMOM (McGraw 1997):
  - Provide statistical information about the evolution of the floc size distribution
  - Does not completely capture the shape of the floc size evolution (equivalent to a 3 (or Nd) class size method)

- CFD/QMOM approach used to model the transient spatial evolution of floc size in a turbulent stirred reactor
Introduction: QMOM approach

• The QMOM approach (McGraw 1997)
  
  – Based on the theory of Orthogonal Polynomial and uses a Nd points Gaussian quadrature approximation for closure

  \[ m_k = \int n(L) L^k dL \approx \sum w_i L_i^k \]

  – The particle size evolution is tracked by solving a system of differential equation for lower order moments

  – Abscissas \((L_i)\) and Weights \((w_i)\) are extracted from the moment sequence \((m_i)\) using Wheeler’s algorithm
QMOM/PBM Methodology: Moment formulation

- QMOM Aggregation-breakup methodology
  - Moment transformation of the PBE with aggregation/breakup
    \[
    \Delta m_k = \frac{1}{2} \sum w_i \sum \alpha_{ij} w_j (L_i^3 + L_j^3)^{k/3} \beta_{ij} - \sum L_i^k w_i \sum \alpha_{ij} w_j \beta_{ij} \\
    + \sum k_{bsi} F_i(k) w_i - \sum L_i^k k_{bsi} w_i
    \]
  - 3 (Nd) points QMOM to represent the PSD
    - Involves tracking the evolution of the 6 lower order moments
      - extract 3 Abscissas (L_1, L_2, L_3) and 3 weights (w_1, w_2, w_3)
    - Determine statistical information about the PSD
      - volume based average floc size \((d_{43} = m_4/m_3)\), length based average floc size \((d_{10} = m_1/m_0)\), average floc density \((m_0)\), ...
QMOM/PBM Methodology: Aggregation

- Aggregation dynamics
  - Collision frequency function ($\beta_{ij}$)
    - Based on orthokinetic flocculation assuming turbulent shear (Saffman and Turner 1956)
      \[
      \beta_{ij} = \frac{1}{6.18} (L_i + L_j)^3 \left(\frac{\epsilon}{\nu}\right)^{0.5}
      \]
  - Collision efficiency function ($\alpha_{ij}$)
    - Accounts for unsuccessful particle collisions due to electrostatic repulsion or hydrodynamic retardation (Adler 1981)
      \[
      \alpha_{ij} = C_1 \left[ \left\{ \frac{(3 \pi \mu \epsilon/\nu)^{0.5} L_i^4 (L_i/L_j) (L_j/L_i + 1)^2}{(32 A d_0)} \right\} \right]^{-0.18}
      \]
QMOM/PBM Methodology: Breakup

- Breakup dynamics
  - Breakup frequency function \( k_{bsi} \)
    - Breakup of particles in the viscous dissipation sub-range (Kusters 1991)
      \[
      k_{bsi} = \left[ \frac{4}{15 \pi} \right] \left( \frac{\varepsilon_p}{\nu} \right)^{0.5} \exp\left[ -\frac{C_2}{L_i \varepsilon_p} \right]
      \]
  - Fragment distribution function \( F_i(k) \)
    - Formation of two fragments with mass ratio 1:4
      \[
      F_i(k) = L_i^k \left[ \left( \frac{4^{k/3}}{5^{k/3}} \right) + 1 \right] \quad \text{if} \quad L_i \geq L_i^{5^{1/3}}
      \]
      \[
      F_i(k) = 0 \quad \text{else}
      \]
QMOM/PBM Methodology: Marchisio et al. (2003)

Table 1
Aggregation kernels

<table>
<thead>
<tr>
<th>Kernel</th>
<th>$\beta(L, \lambda)$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Brownian</td>
<td>$\frac{(L + \lambda)^2}{L\lambda}$</td>
<td>0</td>
</tr>
<tr>
<td>Sum</td>
<td>$L^3 + \lambda^3$</td>
<td>3</td>
</tr>
<tr>
<td>Hydrodynamic</td>
<td>$(L + \lambda)^3$</td>
<td>3</td>
</tr>
<tr>
<td>Differential force</td>
<td>$(L + \lambda)^2</td>
<td>L^2 - \lambda^2</td>
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Table 2
Breakage kernels

<table>
<thead>
<tr>
<th>Kernel</th>
<th>$a(L)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant</td>
<td>1</td>
</tr>
<tr>
<td>Power law</td>
<td>$L^\alpha$</td>
</tr>
<tr>
<td>Exponential</td>
<td>$\exp(\delta L^3)$</td>
</tr>
</tbody>
</table>
QMOM/PBM Methodology: Marchisio et al. (2003)

| Mechanism                  | \( b(L|\lambda) \)                                      | \( \tilde{E}_i^{(k)} \)                  |
|----------------------------|--------------------------------------------------------|-----------------------------------------|
| Symmetric fragmentation    | \[
\begin{cases}
2 & \text{if } L = \frac{\lambda}{3 L_0^3} \\
0 & \text{otherwise}
\end{cases}
\] | \( 2(3-k)^{1/3} L_i^k \)                |
| Erosion                    | \[
\begin{cases}
1 & \text{if } L = 1 \\
1 & \text{if } L = (\lambda^3 - 1)^{1/3} \\
0 & \text{otherwise}
\end{cases}
\] | \( 1 + (L_i^3 - 1)^{k/3} \)             |
| Mass ratio 1:4             | \[
\begin{cases}
1 & \text{if } L = \lambda \left( \frac{1}{3} \right)^{1/3} \\
1 & \text{if } L = \lambda \left( \frac{4}{3} \right)^{1/3} \\
0 & \text{otherwise}
\end{cases}
\] | \( L_i^k \frac{4^{k/3} + 1}{3^{k/3}} \) |
| Parabolic distribution     | \[
\frac{3C L_i^2}{\lambda^3} + (1 - \frac{C}{2})\left[ \frac{72 L_i^6}{\lambda^6} - \frac{72 L_i^5 L_i^k}{\lambda^6} + \frac{18 L_i^2 L_i^{2k}}{\lambda^3} \right]
\] | \[
\frac{3C L_i^k}{3^{k/3}} + (1 - \frac{C}{2})\left[ \frac{72 L_i^k L_i^k}{3^{k/3}} - \frac{72 L_i^k}{8^{1/3} L_i^k} + \frac{18 L_i^{2k}}{3^{k/3} L_i^k} \right]
\] |
| Uniform                    | \[
\begin{cases}
6L_i^2 \lambda^3 & \text{if } 0 < L < \lambda \\
0 & \text{otherwise}
\end{cases}
\] | \( L_i^k \frac{6}{k+3} \)                |

*Note.* All the functions presented in the table are scaled with reference to \( L_0 = 1 \) which is the size of the primary particles.
Numerical Methods: The Flow Field (1)

1 / Solve the flow field

► The flow field is solved for each geometrical configuration: i.e. impeller type: axial (A310 Foil), radial (Rushton turbine), Taylor-Couette flow), tank geometry and volume, and average characteristic velocity gradient ($G_m = [\epsilon_{p\text{mean}}/\nu]^{0.5}$ in s$^{-1}$)

► A grid sensitivity analysis is performed to insure the validity (and cell number independency) of the flow field. A compromise has to be found between grid-insensitivity and total number of cells (and near wall refinement)

Keep in mind that if the flow field is solved quickly, the CFD/QMOM (6 equations to solve i.e. 1 for each moment) is, on the contrary, CPU demanding

► The flow field is used as initial condition for the CFD/QMOM model and PT/QMOM
Numerical Methods: The Flow Field (2)

2 / Example of flow fields ($G_m = 40s^{-1}$)

Spatial distribution of the normalized turbulent energy dissipation rate ($\varepsilon_p/\varepsilon_{p\text{mean}}$) for $G_m = 40s^{-1}$.
Numerical Methods: Set Initial Conditions

1 / Set initial conditions for QMOM/CFD model

- Initial particle size distribution set by the choice of 3 abscissas (dimensionless size indicator) and 3 weights (dimensionless number concentration indicator).

2 / Determine empirical constants with experimental data for \((G_m) = 40 \text{s}^{-1}\)

- \(C_1\) is determined with the slope of experimental \((d_{43})\) evolution during the initial linear growth period \(\Rightarrow C_1 = 24\) (A310) and 42 (Rushton).
- \(C_2\) is determined with the steady-state value of \((d_{43})\) at the end of the flocculation process \(\Rightarrow C_2 = 2.5\) (A310) and 9.3 (Rushton).

- Constants depend on various parameters (particle type, water and coagulant chemistry, temperature, …) but not on flow field characteristics.

3 / CFD/QMOM Approach \(\Rightarrow\) Transport Equation is solved for each moment.
Numerical Methods: The Flow Field: BC

- **BC for A310 fluid foil**

<table>
<thead>
<tr>
<th>Gm (s⁻¹)</th>
<th>VOLUFLOW</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>-1.734980E-03</td>
</tr>
<tr>
<td>70</td>
<td>-2.540000E-03</td>
</tr>
<tr>
<td>90</td>
<td>-3.010000E-03</td>
</tr>
<tr>
<td>150</td>
<td>-4.258000E-03</td>
</tr>
</tbody>
</table>

- **BC for Rushton turbine**

<table>
<thead>
<tr>
<th>Gm (s⁻¹)</th>
<th>VTIP</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>0.2748</td>
</tr>
<tr>
<td>70</td>
<td>0.4000</td>
</tr>
<tr>
<td>90</td>
<td>0.4736</td>
</tr>
<tr>
<td>150</td>
<td>0.6644</td>
</tr>
</tbody>
</table>

Values of the Boundary Conditions (BC) VOLUFLOW (A310) and VTIP (RUSHTON) to set in the Q1 file in order to obtain the appropriate value of the CVG (Gm). BC are valid for a given tank geometry, cell number, and impeller type. Values were adjusted empirically in order to obtain the correct CVG.
Numerical Methods: CFD/QMOM: Results for D43n

- Results for A310 fluid foil (30min)
- Results for Rushton turbine (30min)

\[(G_m) = 40\text{s}^{-1}\]

\[(G_m) = 90\text{s}^{-1}\]
Results: Mean Particle Size Evolution ($<d_{43n}>$)

1 / Evolution of the normalized spatially-averaged floc size

- Growth rate increases when ($G_m$) increases
- Floc size decreases when ($G_m$) increases due to higher breakup rate

\[ \text{Slope} = \Delta <d_{43n}> / \Delta \text{time} \]
**Results: Mean Particle Size Evolution ($d_{43n}$)**

2 / Transient evolution of $d_{43n}$

- **Growth region**: aggregation rate > breakup rate
- **Steady state region**: aggregation rate $\approx$ breakup rate
- For $(G_m) \geq 70\, \text{s}^{-1}$: peak region before decreasing to a lower steady-state mean particle size

- **CFD/QMOM model confirms experimental observations for mixing speeds $(G_m \geq 70\, \text{s}^{-1})$ that display a peak followed by a smaller steady state value**
**Results**: Spatial Distribution of $d_{43n}$

- **$G_m = 40s^{-1}$**
  - 1 minute
  - 5 minutes
  - 15 minutes

- **$G_m = 90s^{-1}$**

  ▶ Larger flocs are found in the center of the recirculation zone
Results: *Tank Average Moment Rate Equation* $(\Delta m_4)$

- $(G_m) = 40s^{-1}$:
  - $(\Delta m_4)$ increases during the linear growth phase while breakage rate is negligible
  - Breakage rate increases but $(\Delta m_4) \geq 0$
- $(G_m) = 150s^{-1}$
  - $(\Delta m_4) \leq 0$ when breakage rate exceeds aggregation rate

- A breakage rate that exceeds the aggregation rate $\Rightarrow$ peak region
Results: *Spatial Distribution of (Δm₄)*

- 85% of the tank volume promote aggregation while 15% promote floc breakup.
- Same ratio (85/15%) is observed but higher breakup rates with increasing $(G_m)$. 

![Graphs showing spatial distribution with different time intervals and $(G_m)$ values](image)
Questions

- Transient spatial variation of $d_{43n}$

(Gm) = 40-1/s

(Gm) = 90-1/s
Numerical Methods: Set Initial Conditions (1)

1 / Set initial conditions for PT/QMOM model
► A stand alone FORTRAN code is used to generate the initial location of flocs to be tracked. A sensitivity study was performed and showed that 1000 flocs were sufficient to insure no change in the floc size evolution with increasing number of particles.

2 / Example of path of one particle for 30min (as a function of impeller type)

![Graphs showing path of particles for different impellers](image-url)
Numerical Methods: Set Initial Conditions (2)

3 / PT/QMOM Approach

- The path of each particle is solved using PHOENICS (GENTRA option).
- The result file (GHIS) that includes location and time for each tracked particle) is used in a stand alone QMOM FORTRAN code (TRACKINGhis.for). The stand alone QMOM model uses for the aggregation-breakup dynamics the same constants (C1, C2) than in the CFD/QMOM model.
- **Tips:** The CPU time to compute GENTRA particle tracking is long (simulation of 30min of particle transport in the tank). Particle tracking (PT) is typically run for 200/250 particles at a time.

- **PT/QMOM vs CFD/QMOM:** The main advantage of the PT/QMOM approach over the CFD/QMOM approach is that flow field conditions (Gm, impeller type, tank size, …) are separated from flocculation dynamics (QMOM).

This approach (PT/QMOM) allows to investigate only “non flow field” conditions (particle type, water and coagulant chemistry, … i.e. reflected in the values of QMOM constants C1 and C2) and to explore alternative aggregation and breakup kernel formulations.
Numerical Methods: PT/QMOM: Std Alone QMOM

The stand alone FORTRAN program TRACKINGHIS_EPDT is used with PHOENICS PT results files (GHIS) to compute the floc size evolution using the QMOM. The program is organized as follows (only key elements are reported):

**PROGRAM TRACKINGhis**

*C This program uses the Quadratic Method of Moments for agglomeration/breakup processes. We use there a quadrature C approximation with 3 nodes. This program is for stand alone QMOM and devoted to be used with results files of PHOENICS C particle TRACKING (GHIS).

**C Variables definition**

| **C Step 1** | 
|---|---|
| a) Delete x,y,z coordinates in GHIS raw data file | REMOVE UNECESSARY DATA IN (GHIS) PT FILE |
| b) Delete redundant data in PT file | PREPARE DATA FOR QMOM |
| c) Transform files in equispaced time step files | |
| • The GHISEPDT file is used with the QMOM (1 data every TGAP for algorithm stability) | |
| • The GHISEPDT2 file is used for average Ep values (1 data every 1 sec) | |

| **C Step 2** | 
|---|---|
| Mean EP calculation at each time step DT | COMPUTE THE MEAN EP AT EACH TIME STEP FOR ALL (1000) PARTICLES (TANK) |
| Mean EP calculation for each particle all time long | COMPUTE THE MEAN EP FOR EACH PARTICLE (30MIN) |

| **C Step 3** | 
|---|---|
| D43 calculation with QMOM (Define here C1 and C2) | COMPUTE THE FLOC SIZE EVOLUTION (D43) FOR EACH PARTICLE (30MIN WITH DT=TGAP) |
| Mean D43 calculation | COMPUTE THE VOLUME AVERAGED FLOC SIZE (D43) AT EACH TIME STEP FOR ALL (1000) PARTICLES (TANK) |

END

C Turn key subroutines (ORTHOG and GAUCOF) from Press et al. (1992)
Numerical Methods: PT/QMOM: Results for D43n

Results PT/QMOM

A310 vs Rushton

Comparison PT/QMOM and CFD/QMOM

A310
(Gm) = 40s⁻¹

RUSHTON
(Gm) = 90s⁻¹
Summary: Framework

Step 1: Flow Field
- Solve CFD flow field for tank geometry, CVG, impeller type
- Flow field DINI File (EP, KE, U, V, W)

Step 2: Flocculation
- CFD/QMOM (Mi\textsubscript{\text{ini}}, C1, C2, …)
  - Result File (D43, Mi, ABi, Wi)
- Particle Tracking
  - GHIS File
  - Std Alone QMOM (C1, C2)
  - .DAT File (D43, Mi, ABi, Wi)

Step 3: Settling
- IPSA/QMOM (Settling) (Mi\textsubscript{\text{ini}}, R1\textsubscript{\text{ini}}, R2\textsubscript{\text{ini}}, …)
  - Result File (R1, R2)
- ASM (ABi, Wi, …) (Settling)
  - RST File ([PTi], FRSL, FRLO)
Example: Secondary Clarifier
Example (Secondary Clarifier)
Example (Secondary Clarifier)

- The Mixture Model/QMOM were used to solve this problem. Physical properties of the two phases according to the following table:

<table>
<thead>
<tr>
<th>Var</th>
<th>VALUE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_c$</td>
<td>1000 kg/m³</td>
<td>Liquid phase density</td>
</tr>
<tr>
<td>$\eta_c$</td>
<td>1·10⁻³ Pa·s</td>
<td>Liquid phase viscosity</td>
</tr>
<tr>
<td>$\rho_d$</td>
<td>1100 kg/m³</td>
<td>Solid phase density</td>
</tr>
<tr>
<td>$d_d$</td>
<td>2·10⁻⁴ m</td>
<td>Diameter of solid particles (initial conditions)</td>
</tr>
<tr>
<td>$g_z$</td>
<td>-9.82 m/s²</td>
<td>z-component of gravity vector</td>
</tr>
<tr>
<td>$\phi_{\text{max}}$</td>
<td>0.62</td>
<td>Solid phase maximum packing concentration</td>
</tr>
<tr>
<td>$v_{\text{in}}$</td>
<td>1.25 m/s</td>
<td>Inlet velocity</td>
</tr>
<tr>
<td>$v_{\text{out}}$</td>
<td>-0.05 m/s</td>
<td>Outlet velocity</td>
</tr>
<tr>
<td>$\phi_{\text{in}}$</td>
<td>0.003</td>
<td>Volume fraction of solid phase of incoming sludge</td>
</tr>
</tbody>
</table>
Example (Secondary Clarifier)

- Initial Distribution:

![Graph showing Initial Distribution with Abscissa (microns) and Weights, with d43 = 200 microns highlighted.]
Results (Secondary Clarifier)

- Velocity Contour

D43=200 microns (constant)

D43=550 microns (evolved)
Results (Secondary Clarifier)

- **Sludge Mass Contour**

  D43=200 microns (constant)

  D43=550 microns (evolved)
Results (Secondary Clarifier)

- Sludge Mass Contour

D43 = 200 microns (constant)

D43 = 550 microns (evolved)
Results (Secondary Clarifier)

- d43 Contour
Results (Secondary Clarifier)

- d43 Contour
Results (Secondary Clarifier)

- Sludge mass Contours (influence of floc porosity Kinnear (2002))

  D43=550 microns (evolved)

  Floc porosity

  D43=650 microns (evolved)
Thoughts on ASM/QMOM

• Current formulation is not rigidly linked to dispersed phase
• Does not completely capture the change in flocculation distribution above and below the solids blanket
• Simple approach to include particle interaction kinetics with two phase problem