

# Comparison between Direct Quadrature Method Of Moments and The Method Of Classes for Bubbly Flow

4 th OpenFOAM  
workshop  
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**Brahim Selma**, Rachid Bannari, Pierre Proulx  
Department of Chemical Engineering & Biotechnology  
Université de Sherbrooke (QC)

OpenFOAM



Département de génie chimique



# Outlines

- Background
- Objectives
- Tests cases:
  - Bubble column
  - Double-turbine stirred-tank reactor
- Conclusion and outlook

# Background

## WHY Population Balance Equation ???

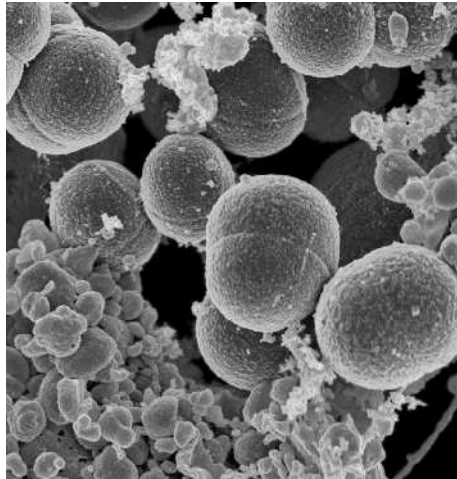
**1. Population Balance Equation PBE:** is encountered in several engineering disciplines. It is used to study bubbly flow, particle size distribution (PSD) of plasma, polymerization, fermentation,...etc.

**2. Direct applications of PBE:**

- Bubbly flows (ex. Bubble column; stirred-tank reactor; distillation column;...)
- Plasma (PSD; nanoparticles aggregation, growth, nucleation)
- Bioreactors, Air-lift reactors
- Engineering, Environment, Pollution

# Objectives...

How can we represent this population of  
bacteria !



# Objectives...

**On The Solution Of PBE Using Two Different Methods:**

- 1. The Method Of Classes (CM)**
- 2. The Direct Quadrature Method Of Moments (DQMOM)**

**WHICH TECHNIQUE IS THE BEST FOR SOLVING  
PBE???**

# The Population Balance Equation...

General PBE  $\longrightarrow$  
$$\frac{\partial}{\partial t}(\rho_G n_i) + \nabla \cdot (\rho_G u_{G,i} n_i) = \rho_g S_i$$

Term source  $\longrightarrow$  
$$S_i = (B_i^{coal} - D_i^{coal}) + (B_i^{br} - D_i^{br})$$

Two Techniques

**CM** (most commonly used)

**DQMOM** (New)

# The Method Of Classes

In **CM** the birth and death rates due to coalescence and break-up are as follow [1]:

Death rate due to coalescence

Birth rate due to coalescence

$$B_i^{coal} = \sum_{\substack{j \geq k \\ x_{i-1} \leq x_i + x_k \leq}} [1 - \frac{1}{2} \delta_{j,k}] \eta Q_{j,k} \alpha_{Gk} \frac{x_i}{x_j x_k}$$

$$D_i^{coal} = \alpha_{Gi} \sum_{k=1}^M Q_{i,k} \frac{\alpha_{Gk}}{x_k}$$

Death rate due to break-up

Birth rate due to break-up

$$B_i^{br} = \sum_{k=i}^M n_{i,k} \Gamma_k \alpha_{Gk} \frac{x_i}{x_k}$$

$$D_i^{br} = \Gamma_i \alpha_{Gi}$$

# The Direct Quadrature Method Of Moments

The **DQMOM** is inspired from the method of moments (MOM) firstly developed by McGraw (1997) in which the analytical solution is replaced by a quadrature approximation (numerical closure):

$$m^{(k)}(t) = \int_0^{+\infty} n(\xi; t) \xi^k d\xi \approx \sum_{i=1}^n L_i(t)^k w_i(t)$$

Here the abscissas ( $L$ ) and weights ( $w$ ) are **directly** determined using the following system:

$$\begin{cases} \frac{\partial}{\partial t} w_i + \nabla \cdot (\phi w_i) = a_i \\ \frac{\partial}{\partial t} L_i + \nabla \cdot (\phi L_i) = b_i \end{cases}$$

Non linear system solving for determining **a** and **b**

$$\rightarrow \sum_{i=1}^N [(1-k)L_i^k a_i + kL_i^{k-1} b_i] = S^{(k)} \quad k = 0, \dots, 2N - 1$$

# The Direct Quadrature Method Of Moments

In **DQMOM** the terms of birth and death rates are determined using the approach of Marchisio and al. [2]:

$$B_{coal}^{(k)} = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \omega_i \omega_j (L_i^3 + L_j^3)^{k/3} \beta_{ij}$$

$$B_{break}^{(k)} = \sum_{i=1}^N \bar{b}_i^{(k)} a_i^* \omega_i$$

$$D_{coal}^{(k)} = \sum_{i=1}^N \sum_{j=1}^N \omega_i \omega_j L_i^k \beta_{ij}$$

$$D_{break}^{(k)} = \sum_{i=1}^N \omega_i L_i^k a_i^*$$

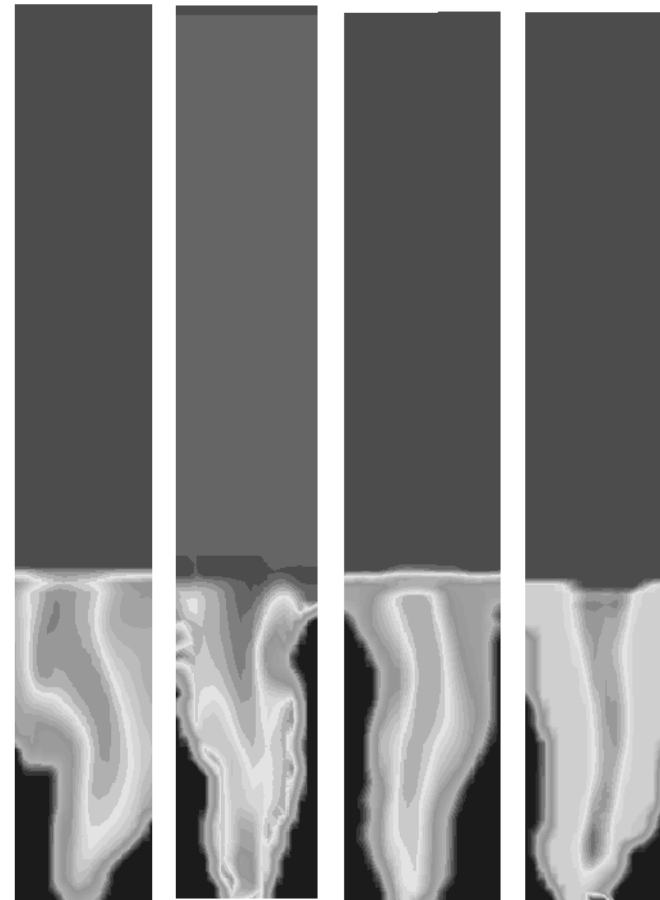
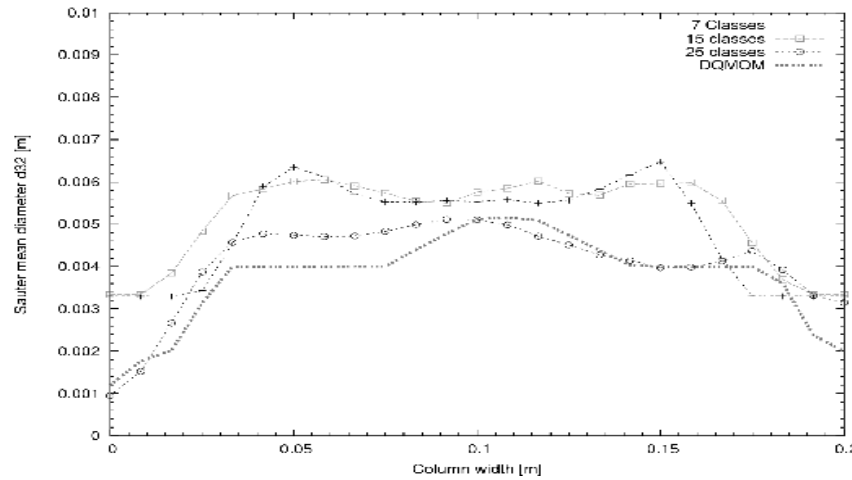
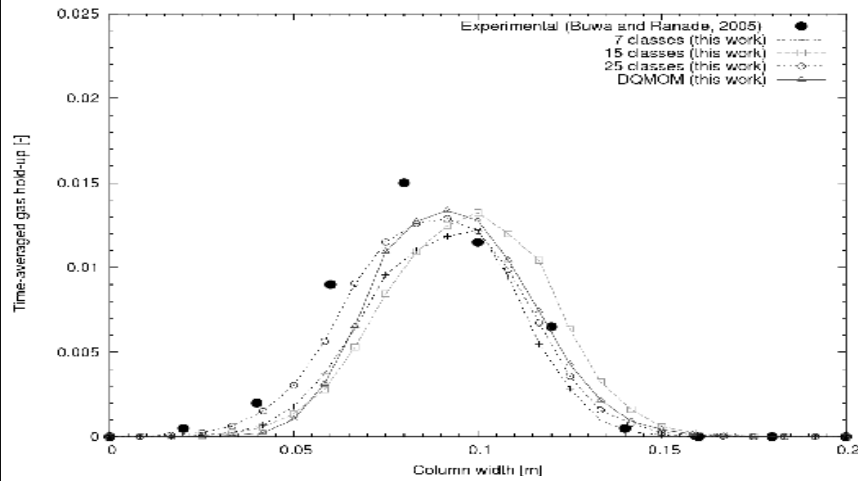
Coalescence rate  
between two classes I  
and j

$$\beta_{ij} = \beta(L_i, L_j), a_i^* = a(L_i), \text{ and } \bar{b}_i^{(k)} = \int_0^\infty L^k b(L/L_i) dL$$

Binary break-up

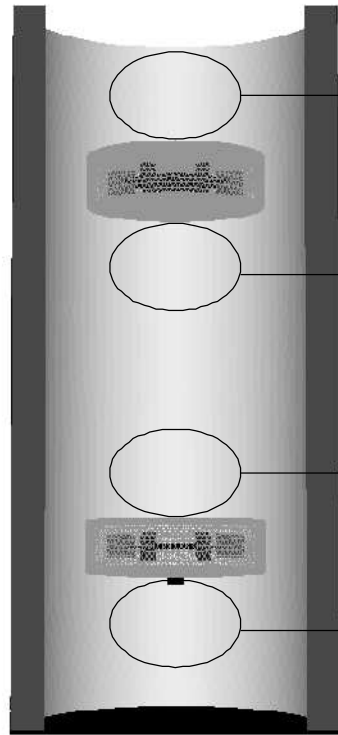
$$\bar{b}_i^{(k)} \approx 2^{(3-k)/3} L_i^k$$

# Case A: Bubble columns modelling using OpenFOAM

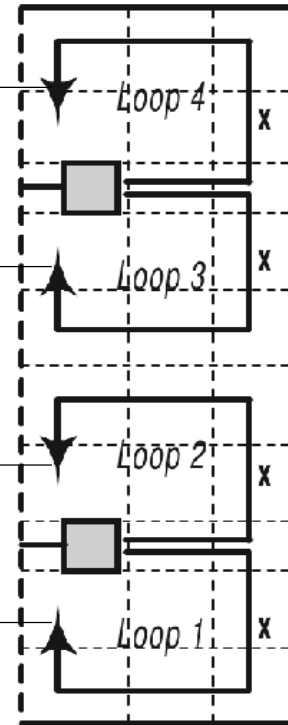


# Case B: Stirred-tank reactor

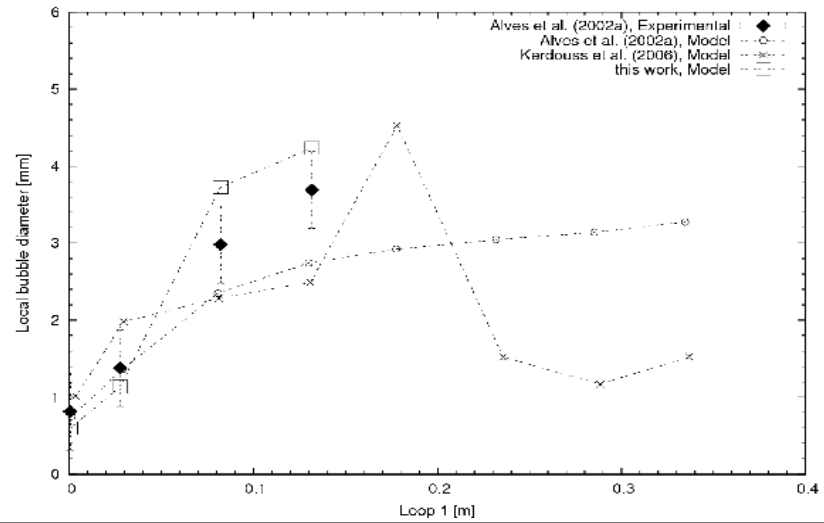
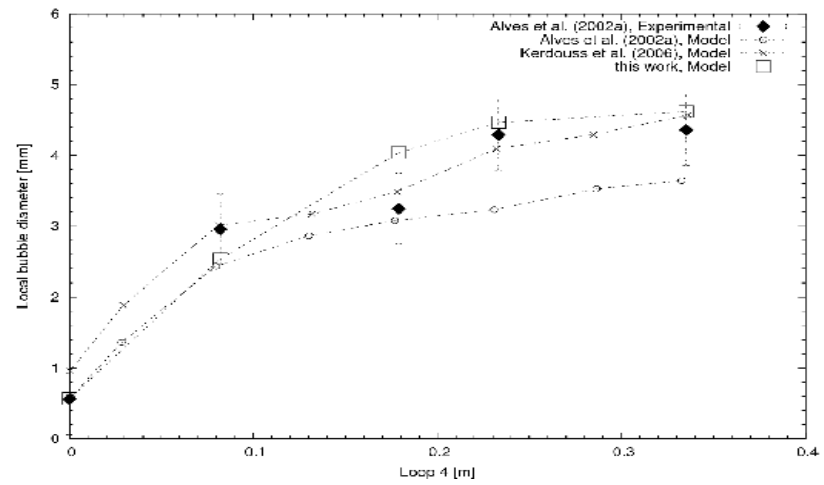
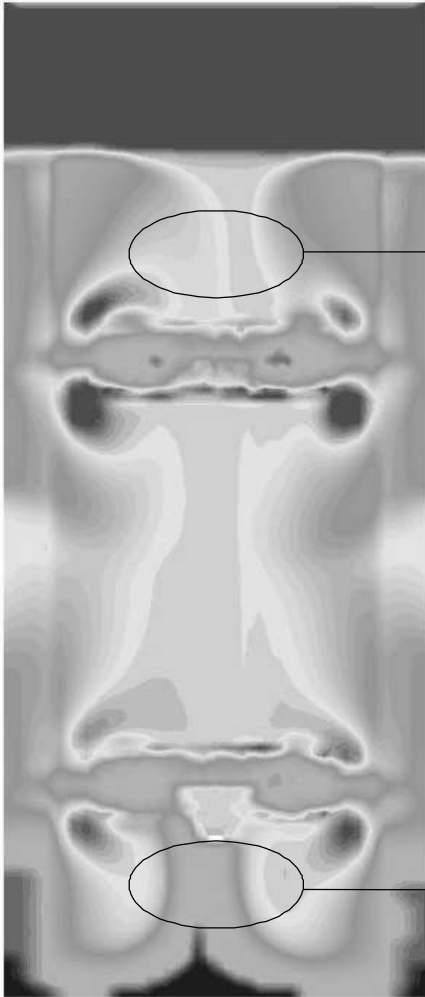
Present Model



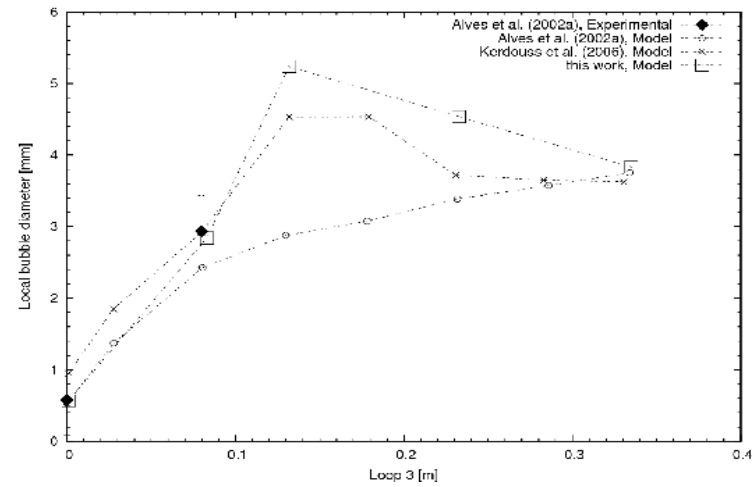
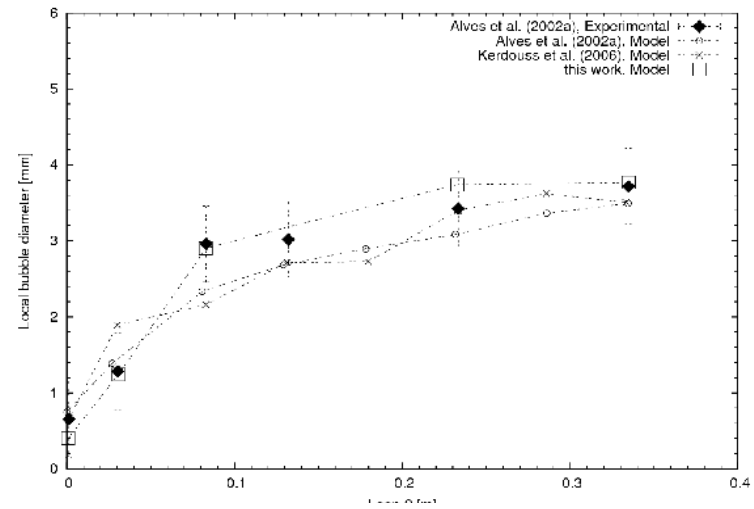
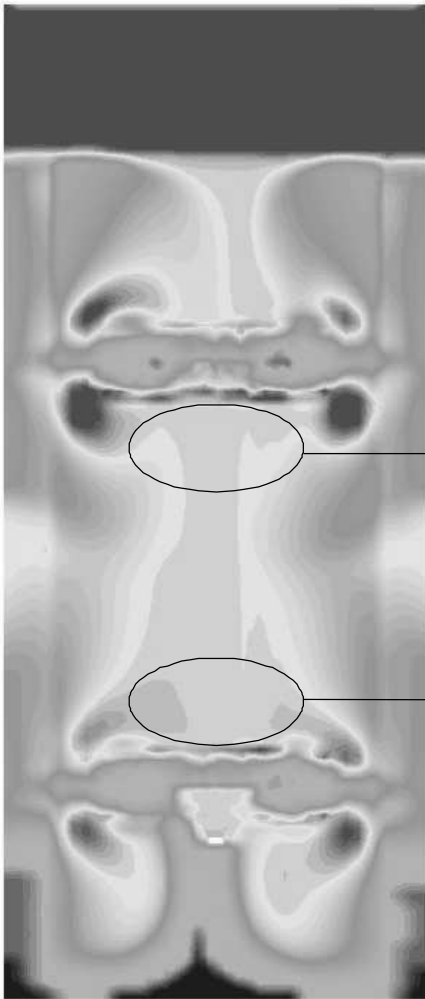
Experimental [2]



# Stirred-tank reactor modelling using OpenFOAM

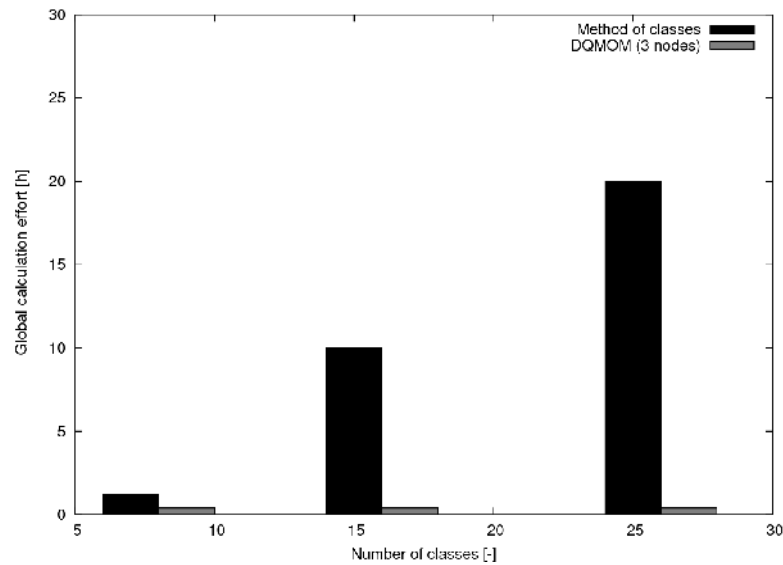


# Stirred-tank reactor modelling using OpenFOAM

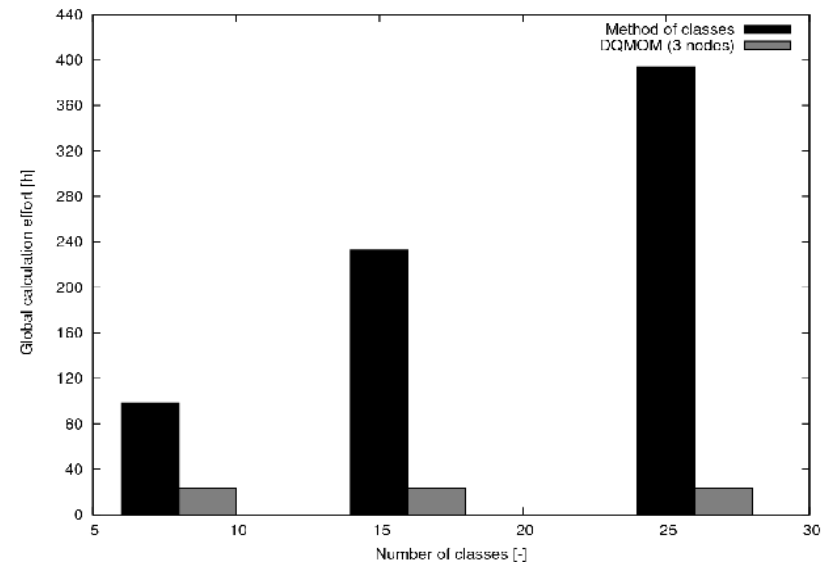


# Computational time requirement between **CM** and **DQMOM**

Case A: bubble column  
**6000** cells



Case B: stirred-tank reactor  
**255000** cells



# Conclusion and Outlook

## •Conclusion

- In the case A, the **DQMOM** gives a good results when compared to the experimental data and models published in the literature.
- For quantitative comparison the Sauter mean diameter **d<sub>32</sub>** is chosen for its wide application for determining the mass transfer coefficient.
- In the case B, different loops are used to compare the present model with available measurements from the literature, agreement is also good.
- Drastic reduction in the computational requirements is obtained when using the DQMOM method when compared with the method of classes.

## •Outlook

- The next generation for solving PBE is the **DQMOM**
- Performance should be made on a large variety of different models of bubbles coalescence and breakage
- We must take care for choosing the initial conditions of first order of moments

# Thanks

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