**Supplementary Data**

## Model development via single compartment validation

The evaluation on the reliability of the PD-QMOM algorithm in predicting gas-liquid dispersions was carried out by running the coalescence and break-up kernels simultaneously in a bubble column with settings adopted from Degaleesan (1997). The structure of the bubble column is cylindrical in shape with a diameter of 0.19 m. Gas is sparged into the column at a superficial gas velocity of 0.12 m/s through a perforated plate with 0.33 mm diameter holes. PD-QMOM was validated by employing a single compartment PBM; assuming a steady-state, well-mixed, and homogeneous system. The gas inflow and outflow is excluded as well. An overall gas hold-up of about 29% (initial water level at 0.96 m and aerated water level at 1.24 m) and mean turbulence dissipation rate roughly estimated to be equal to *ε* = 1.18 m2/s3 were obtained in their study (Degaleesan, 1997). The initial BSD was assumed to be lognormal with geometric mean diameter of 5 mm and standard deviation of 0.2. ODE integrations were conducted by setting both the relative and the absolute tolerances at 10-8. The results obtained were solved using *ode113* integrator in MATLAB. The maximum simulation time was set to *t* = 30 s since steady-state moment evolution can be achieved in less than a second as shown in Figure S1.

**Figure S1**

A sensitivity study was first carried out by solving the PBM equations to evaluate the effect on predicted mean bubble size using different number of quadrature approximation ranging from two to five. A comparison was also carried out between the predicted results and calculated correlations. Correlations use to estimate the mean bubble size are often related to liquid surface tension (), liquid density (), liquid viscosity () and gas superficial velocity (). Some correlations include the gas density () and gravity () as well, such as the one proposed by Wilkinson (1991):

|  |  |
| --- | --- |
|  | (S1) |

Another correlation for bubble size was proposed by Pohorecki et al. (2005):

|  |  |
| --- | --- |
|  | (S2) |

Table S1: Comparison of QMOM results obtained for different quadrature points, *n*, for *ε* = 1.18 m2/s3, lognormal distribution parameter (*dmean* = 5 mm, *σd* = 0.2).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *n* | 2 | 3 | 4 | 5 | Pohorecki et al. (2005) | Wilkinson (1991) |
| Initial *Li* (cm) | 0.393  0.588 | 0.352  0.500  0.710 | 0.324  0.448  0.605  0.836 | 0.303  0.411  0.542  0.714  0.969 |  |  |
| Initial *wi* (n/cm3) | 2.516  1.374 | 1.342  2.315  0.233 | 0.685  2.358  0.822  0.025 | 0.350  1.965  1.410  0.164  0.002 |  |  |
| *d32* (cm) | 0.410 | 0.413 | 0.412 | 0.412 | 0.36 | 0.44 |
| CPU time (s) | 4.20 | 16.30 | 46.87 | 102.86 |  |  |
| % excess time compare to *N* = 2 | 0.00% | 287.70% | 1014.66% | 2346.39% |  |  |
| % relative error compare to *N* = 5 | 0.54% | 0.24% | 0.01% | 0.00% |  |  |

Table S1 shows the predicted and calculated bubble Sauter mean diameter, *d*32, for the bubble column. The PBM predictions are in fair agreement with the values calculated from correlations by Wilkinson (1991) and Pohorecki et al. (2005). The variation in predicted bubble size was also found to be insignificant with increasing number of quadrature points. Marchisio et al. (2003) also found out that there was insignificant gain in QMOM prediction accuracy beyond three quadrature points in their study but the trend of decreasing overall error with higher number of quadrature approximation was reported. However, they too pointed out that higher number of quadrature approximation does not always reduce prediction error in certain aggregation and breakage problems (Marchisio et al., 2003). It is also interesting to note that, only minimal predictive accuracy was obtained with increasing number of quadrature points at the cost of greater computational effort; less than 0.6% gain in accuracy for more than 2000% of additional computational time using five quadrature points. Hence, it was not considered necessary to solve the QMOM with higher number of quadrature points (i.e. more than 3) because the gain in accuracy is almost insignificant.

The assessment on the algorithm response to higher turbulence dissipation rate (2.4 m2/s3), smaller initial bubble size (2.2 mm) and lower gas hold-up (0.11) was studied to test the algorithm for any possible dependencies on those three variables. All solutions were generated using three quadrature points and the results for these runs (i.e. case 1 to 8) were shown in Table S2.

Table S2: Comparison of QMOM result obtained at different *dmean* initial, *ɛ* and*αg* for three quadrature points.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Case | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Initial *Li* (cm) | 0.155  0.220  0.312 | 0.352  0.500  0.710 | 0.155  0.220  0.312 | 0.352  0.500  0.710 | 0.155  0.220  0.312 | 0.352  0.500  0.710 | 0.155  0.220  0.312 | 0.352  0.500  0.710 |
| Initial *wi* (n/cm3) | 15.752  27.182  2.731 | 1.342  2.315  0.233 | 15.752  27.182  2.731 | 1.342  2.315  0.233 | 8.879  15.321  1.539 | 0.756  1.305  0.131 | 8.879  15.321  1.539 | 0.756  1.305  0.131 |
| *ε* (m2/s3) | 1.18 | 1.18 | 2.4 | 2.4 | 1.18 | 1.18 | 2.4 | 2.4 |
| *αg* | 0.23 | 0.23 | 0.23 | 0.23 | 0.11 | 0.11 | 0.11 | 0.11 |
| *dmean* initial (cm) | 0.22 | 0.5 | 0.22 | 0.5 | 0.22 | 0.5 | 0.22 | 0.5 |
| *d32* (cm) | 0.41 | 0.41 | 0.30 | 0.30 | 0.37 | 0.37 | 0.26 | 0.26 |
| CPU time (s) | 16.54 | 16.30 | 26.15 | 25.68 | 12.96 | 13.13 | 21.23 | 21.21 |

As expected, higher turbulence dissipation rate promotes breakage to be the dominant mechanism in the system thus resulting to smaller mean bubble size. Theoretically, steady-state bubble size should be independent of any influence from initial bubble distribution and only dependent on turbulence dissipation rate and gas-hold up. The result obtained proves this theory as the final bubble size converged to a similar value despite having different initial bubble size (i.e. compare case 1 and 2 or case 3 and 4 or case 5 and 6 or case 7 and 8). Meanwhile, the effect of gas hold-up on the final bubble size can be observed when turbulent dissipation rate was set to constant (i.e. *ɛ* = 1.18 m2/s3 for cases 1, 2, 5, and 6). It shows that the final stable bubble size increases with increasing gas-hold up. This is due to increment in bubble-bubble collisions at higher gas hold-up, resulting to more coalescence events to take place. Breakage driven bubble-eddy collisions may also increase with increasing gas hold-up, however the rate is much slower than coalescence processes since the break-up kernel depends upon  from Eq. 14 in comparison with  in the coalescence kernel from Eq. 9. The combination of higher turbulence dissipation rate and lower gas hold-up produce even smaller bubbles as seen in case 7 and 8. This demonstrates that the present algorithm is capable of predicting qualitatively, the evolution of mean bubble size in gas-liquid dispersion, with respect to the variables.

A further comparison on the BSD was also evaluated between coalescence dominant mechanism and breakage dominant mechanism through the evolution of moments. By definition, the sum of QMOM weights is equivalent to the number of bubbles per unit volume. Assuming a spherical bubble, volume of gas,  from the abscissas and weights may be estimated from:

|  |  |
| --- | --- |
|  | (S3) |

where  is the total dispersion volume. The gas volume in the whole system may also be obtained from:

|  |  |
| --- | --- |
|  | (S4) |

The third moment,  is related to  by the following relation:

|  |  |
| --- | --- |
|  | (S5) |

Assuming an initial lognormal bubble distribution with mean bubble size of 2.2 mm and standard deviation of 0.2 mm, the initial BSD was obtained (refer supplementary data Figure 2A) using the following equation:

|  |  |
| --- | --- |
|  | (S6) |

where , *k*, *μ* and *σ* are the moments, order of moments, arithmetic mean and arithmetic standard deviation, respectively. The moments are then used to obtain a set of abscissas and weights using PD algorithm (refer supplementary data Figure 2B). However, the initial weights obtained from lognormal distribution were normalised so that *μ0* = *∑wi* = 1, and thus have to be adjusted to match the gas hold-up for both Eq. S4 and Eq. S5 as PBM calculations require *μ0* to be equal to the number of bubbles per unit volume of dispersion. After the adjustments were made, gas volume obtained from moments matched exactly with the calculated value as shown in Table S3. This adjustment method was applied for all PBM calculations in this work.

Table S3: Scaling the QMOM weights according to gas volume fraction.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *Li* | *wi* |  |  |  |  | *Vg, QMOM =* |
| (cm) | - | (cm3) | - | (n/cm3) | (cm3) | (cm3) |
| 0.15 | 0.34 | 0.005 | 45.66 | 15.75 | 7938.80 | 7938.80 |
| 0.22 | 0.60 |  |  | 27.18 |  |  |
| 0.31 | 0.06 |  |  | 2.73 |  |  |

Figure S1 illustrates the evolution of moments obtained from the PD-QMOM algorithm for cases 1 and 2 with varying initial bubble size. The turbulence dissipation rate and gas hold-up were constant for both cases at *ε* = 1.18 m2/s3 and *αg* = 0.23 respectively. The initial bubble size was set at 2.2 mm for Figure S1A and 5 mm for Figure S1B. The third moment which is related to the total bubble volume was conserved for both cases, coalescence and breakage problems correspondingly. In Figure 2A, the first three moments (i.e. is the total number of bubbles,  is the total bubble diameter and is the total bubble surface area) were observe to be decreasing because small initial bubble size tend to favour coalescence mechanism. The opposite can be observed in Figure S1B where the initial bubble size is larger, thus creating a condition favourable for breakage.

Results from the single compartment simulation reflect that QMOM algorithm is capable of predicting the bubble Sauter mean diameter in good agreement with published correlations for the air-water system. The developed PBM algorithm is capable of responding well to various settings, representing either a coalescence or break-up dominating system. Therefore, the present algorithm was used as a basis for the development of multi-compartment PBM.

**Figure S2**

**Figure S3**

**Figure S4  
Figure S5**

**Figure S6**

**List of Supplementary Data**

Figure S1: Example of initial bubble distribution for lognormal function with *dmean* = 2.2 mm, *σd* = 0.2 mm), (A) Bubble size distribution, (B) Weights and abscissas obtained using PD algorithm.

Figure S2: Computational grid showing tank wall and its internal for Laakkonen et al. (2007)’s geometry, (A) coarse, (B) intermediate, (C) fine.

Figure S3:Results on grid analysis at z = 0 with respect to the impeller and *r/R* = 0.37 (*N* = 513 rpm and *Qg* = 0.7 *VVM*), (A) Liquid tangential velocity, (B) Gas tangential velocity (Gimbun et al., 2009), (C) *ε* of the liquid phase, D) *k* of the liquid phase (Gimbun et al., 2009).

Figure S4: Prediction of turbulence kinetic energy, (A) Single phase, (B) Gas-liquid system (gas phase). Experimental data obtained from Deen (2001).

Figure S5: Comparison between the turbulent dissipation rate for single phase and gas-liquid stirred tank. Data points estimated using Wu and Patterson (1989) equation on dissipation rate,  and Deen (2001)’s measurement.