An algorithm for accurately solving population balance problems

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High accuracy in solving population balance equations was achieved in the present paper by using an algorithm as that follows, reduces the error resulting from discretization in the drop size domain, maintains optimum drop size integration range and the number of intervals used to describe the population, automaticaliy adjusts the step size in the time domain to account for varying the mean drop diameter, and identifies when quasi-steady state is approached.

السريان المتعدد الأطوار يظهر فى كثير من العمليات الهندسية مثل الكيميائية و البترول و التعدين و الصناعات الغذائية و الصناعات الدوائية. التفاعلات و عمليات انتقال الكتلة التى تظهر فى هذه الأنظمة تعتمد على توزيع جزيئات الطور المنتشر (قطرات- فقاعات- جزيئات صلبة)، و أيضا عمليات التكسر و الالتحام للقطرات و الفقاعات لها تأثير كبير على أداء المفاعلات الكيميائية. لوصف توزيع جزيئات الطور المنتشر فى الطور المستمر يستخدم نموذج الاتزان العددى. و من مزايا هذا النموذج أنه يحتوى على عمليات التكسر و الالتحام للقطرات و الفقاعات. توزيع الجزيئات الناتج من حل نموذج الاتزان العددى يستخدم لوصف الهيدروديناميكية و معدلات انتقال الكتلة بين الطورين. الغرض من هذا البحث هو تطوير طريقة الحل لنموذج الاتزان العددى لتحليل و تصميم المفاعلات الكيميائية المتعددة الأطوار فى الصناعة بطريقة واقعية. و تتلخص مشكلة استخدام نموذج الاتزان العددى فى قطاع الصناعة فى قدرة هذا النموذج الرياضى على اعطاء نتائج توافق النتائج المعملية، مستخدمين نماذج لوصف العوامل الهيدروديناميكية المؤثرة مثل معدل استنفاذ الطاقة، و ايضا نماذج لوصف عمليات التكسر والالتحام. و هذه النماذج غالبا لا تمثل ما يحدث فى الواقع العملى. فى البداية تم توضيح العوامل التى تؤثر فى دقة الحل العددى لنموذج الاتزان العددى. و هذه العوامل هى حجم الفترة الزمنية و فترة زيادة حجم القطرات و طريقة الحل المستخدمة و معدلات التكسر و الالتحام. و تم وضع طريقة تعتمد على تقليل الخطأ الناشئ من عملية التقسيم فى مجال حجم القطرات، و استخدام الحجم الأمثل لحجم القطرات فى حدود التكامل و العدد المثالى لحجم القطرات لوصف نموذج الإتزان العددى، و ايضا الضبط الأتوماتيكى لحجم الفترة الزمنية لأخذ التغير فى حجم القطرة المتوسط فى الاعتبار، بالاضافة الى تحديد الفترة التى يحدث عندها اتزان بين عملية التكسر و الالتحام للقطرات.

Keywords: Population balance model, Breakage and coalescence processes, Drop/Bubble size distribution, Multiphase systems, Mixing processes

1. Introduction

Population balances is a technique used for modeling and analyzing the behavior of dispersed systems. It was originally developed as a tool for describing biological systems and since 1964 was used to analyze and control processes involving solid particles, drops, bubbles and combinations thereof. The Population Balance Equation (PBE) can be used to describe multi-phase operations such as crystallization, grinding, inter-phase heat and mass transfer, multi-phase reactions, and flotation [1].

There is however some unhappiness with this approach, particularly within the industrial sector. This is mainly due to the ability to obtain "good" fit to experimental data using models that bear little resemblance to reality (e.g. spatial variation in local energy dissipation rates, binary daughter drops, collision models).

The overall objective of this project is to develop a user friendly Population Balance (PB) program that can be used to analyze/ design industrial multi-phase contactors in a more realistic fashion. Phase I aims to identify the factors affecting the accuracy of numerically solved PB problems. Based on the findings obtained, a user friendly algorithms capable of accurately solving PBE was developed.

2. Problem formulation

In a dispersed phase system, the material domain comprises a continuous phase and a

dispersed phase, the latter as a population of particles (drops, bubbles, or solid) in which the identities of individuals are continually destroyed and recreated by breakup and coalescence processes. Considering the control volume in fig. 1. The population balance model is based on an equation for the continuity of particle numbers in a dispersed phase and is developed from the general conservation equation.

Accumulation rate = Flux in (convection & diffusion) – Flux out + Net generation rate. (1)

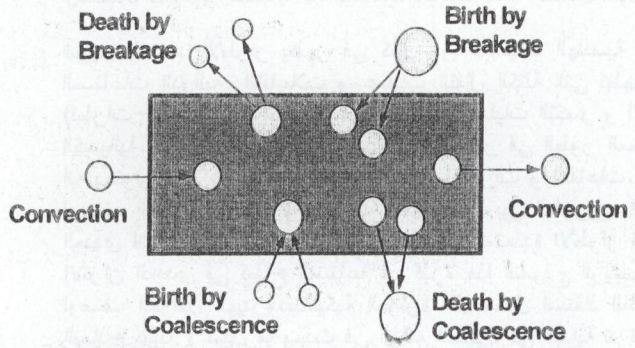

Fig. 1. Control volume,

Consider the distribution of entities $n(r, \xi_1, \xi_2,\ldots, \xi_m, t)$ or the population of particles of the dispersed phase at position r, where r represents the spatial coordinates or "external coordinates", t is the time, and ξ_i represents the i th other property of the entity. ξ_i is also called the internal coordinate and used to give a quantitative description of the state of an individual particle, such as its mass, concentration, temperature, age, volume, etc. In addition to time, there are (3+m) independent variables involved that can be thought of as a (3+m) dimensional space.

The PBE in its most general form [1]:

$$\frac{\partial n}{\partial t} + \nabla \bullet \left(\bar{V} n\right) - B + D = 0 \quad (2)$$

Where $\bar{V}$ is the coordinate velocity in phase space. For well mixed batch mixing tank, with no reaction or heat/mass transfer, the problem simplifies to the following two dimensional situation [2]:

$$\frac{d[N(t)f(a,t)]}{dt} = B_B(a,t) - D_B(a,t) - D_c(a,t) + B_C(a,t). \quad (3)$$

Where: N(t) is the total number of particles at time t, f(a,t) is the fraction of particles have diameter between a and a+Δa and $B_B(a,t)$, $D_B(a,t)$, $B_C(a,t)$, and $D_C(a,t)$ are the birth rate by breakage, death rate by breakage, birth rate by coalescence, and death rate by coalescence, of particles of diameter a at time t, respectively.

3. Breakage rate

Breakage results in both "death" as well as "birth" within a certain drop size range.

$$B_B(a,t) = \int_a^{a_{max}} \beta(a,a')\, \varsigma(a')\Omega(a')\, N(t)\, f(a',t)\, da', \quad (4)$$

$$D_B(a,t) = \Omega(a)\, N(t)\, f(a,t). \quad (5)$$

From eqs. (4) and (5), the breakage rate is affected by [3]:

i- breakage frequency Ω(a), which is function of energy dissipation rate per unit mass ε, surface tension σ, density of dispersed phase ρ_D, density of continuous phase ρ_C, viscosity of dispersed phase μ_D, and viscosity of continuous phase μ_C,

ii- number of daughter drops ς(a), where ς(a') may be (2,3,4,...), and

iii- size distribution of daughter drops β(a,a'), where β(a,a') is assumed (equi-sized, Normal, Gamma, Beta,...).

4. Coalescence rate

Coalescence results in both "death" as well as "birth" within a certain drop size range.

$$B_C(a,t) = \int_0^{a/2} \lambda(a-a', a')\, \omega(a-a', a')\, N(t)\, f(a-a',t)\, da', \quad (6)$$

$$D_C(a,t) = N(t)\, f(a,t) \int_0^{a_{max}-a} \lambda(a,a')\, \omega(a,a')\, N(t)\, f(a',t)\, da'. \quad (7)$$

Here $\lambda(a, a')$ is the coalescence efficiency between drops of size a and a', and $\omega(a, a')$ is the collision frequency between drops of size a and a'. From eqs. (6) and (7), the coalescence rate is affected by [3]:

i- collision frequency $\omega(a, a')$, which is function in energy dissipation rate per unit mass ε, density of dispersed phase ρ_D, density of continuous phase ρ_C, and diameters of colliding drops (a, a'), and

ii- coalescence efficiency $\lambda(a, a')$, which is defined as the fraction of collisions between drops of diameter a and a' that result in coalescence. It is function of contact time between drops and coalescence time which is the time required for drops to coalesce.

5. Net generation

It is the difference between overall "birth" and "death" that affects the overall rate of drop size change. Fig. 2 shows the net generation term from a monodispersion of (a=1000 μm).

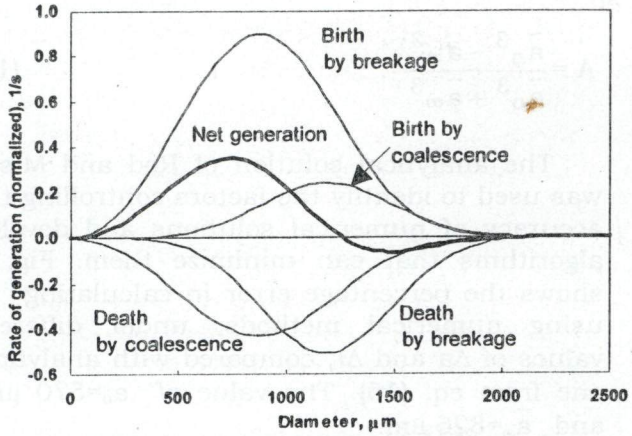

Fig. 2. Components of the net generation term.

6. Methods used to solve PBE

PB equations are usually complicated nonlinear integro-differential equations for which there is seldom an analytical solution available. The most commonly used solution methods are [4]:

i- statistical simulation (e.g. MontCarlo), and

ii- numerical integration.

Sovova [5] and Rod and Misek [6] derived exact solution for the PBE in a batch mixer, assuming simple power functions in drop size for breakage and coalescence. Generally, PBE requires numerical solution. Lee et al. [7] applied the population balance equation coupled with the proposed breakage kernel and the previously developed breakage model to the analysis of bubble size distribution for non-coalescing systems in a bench-scale airlift column. They solved the steady-state population balance equation using Simpson's integration technique. Niyogi et al. [8] solved the population balance equation numerically using adaptive fourth-order Runge-Kutta method. Chatzi et al. [9] described the steady-state drop size distribution in a batch stirred vessel by PBE. They solved PBE using composite Simpson's rule.

The numerical methods present considerable computational difficulties. The MontCarlo techniques are extremely flexible, powerful and free of convergence problems, but they require so much computer time that they are not practical for many purposes.

7. Errors involved in numerical methods

i- discretization errors (time and size domains),

ii- truncation errors (approximating exact mathematical procedures),

iii- round off errors (inexact representation of floating point numbers),

iv- propagated errors (errors from previous steps carried through to succeeding steps), and

v- when is quasi-steady state reached? the quasi-steady state means that the mean diameter of the drops stop changing with time any more, meanwhile breakage and coalescence processes still working.

8. Solution methods used in the new algorithm

i- Integration in size domain
- Trapezoid rule : $O(h^3 f'')$,
- Simpson's rule & $3/8^{th}$ rule,
- Simpson's extended rule : $O(1/n^4)$.

ii- Cubic Spline interpolation (to minimize discretization errors).

iii- Integration in time domain
- 4^{th} order Runge-Kutta method $O(h^5)$

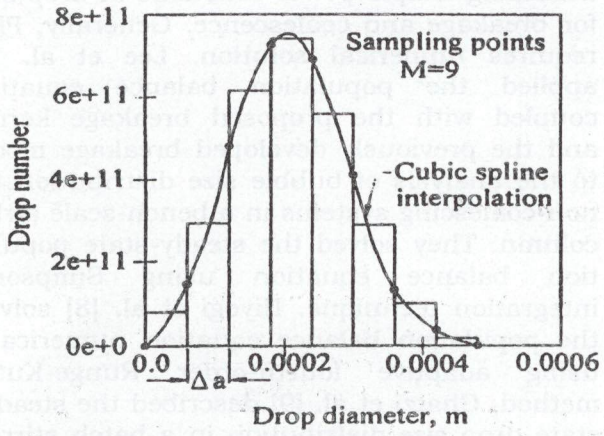

Fig. 3. Discretization of size domain.

9. The Rod and Misek analytical solution

Rod and Misek [6] obtained analytical solutions for the transient and equilibrium drop diameters by assuming simple power functions for breakage and coalescence processes, expressed by:

$$\Omega(a') = K_s\, a^{3(p+1)}\,, \tag{8}$$

$$\beta(a,a') = 3\, a^2/a'^3\,, \tag{9}$$

$$\varsigma(a') = 2\,, \tag{10}$$

$$\lambda(a\text{-}a',\, a')\ \omega(a\text{-}a',\, a') = K_c\,(a^3 + a'^3)^p\,. \tag{11}$$

Where K_s and K_c are the breakage and coalescence rate constants. The analytical solution of the steady-state PBE using the above models, leads to the steady-state drop number density:

$$f(a) = \frac{3a^2}{\bar{a}^3}\exp\left[-\left(\frac{a}{\bar{a}}\right)^3\right]. \tag{12}$$

Mean volume drop diameter $\bar{a}$, as the parameter of the distribution, is given by:

$$\bar{a} = \left(\frac{3}{\pi}\frac{K_c\phi}{K_s}\right)^{1/6}. \tag{13}$$

Where ϕ is the volume fraction of the dispersed phase. The transient distribution developing during the transition from one steady state, characterized by the mean volume diameter $\bar{a}_o$ to another steady state, characterized by the mean volume diameter $\bar{a}_\infty$, can be described by:

$$f(a,t) = \frac{3a^2}{[\bar{a}(t)]^3}\exp\left[-(a/\bar{a}(t))^3\right]. \tag{14}$$

The time variation of the value $\bar{a}$, depending on the exponent p, is described by differential equation,

$$\frac{d\bar{a}}{dt} = \frac{\Gamma(p+2)}{3}\,K_s\,\bar{a}^{3p-2}\,(\bar{a}_\infty^{\,6} - \bar{a}^{\,6}). \tag{15}$$

The solution of eq. (15), for p=0, has the form:

$$\bar{a}(t) = \bar{a}_\infty\left(\frac{1 + A\exp(-2K_s\bar{a}_\infty^{\,3}t}{1 - A\exp(-2K_s\bar{a}_\infty^{\,3}t)}\right)^{1/3}, \tag{16}$$

where;

$$A = \frac{\bar{a}_o^{\,3} - \bar{a}_\infty^{\,3}}{\bar{a}_o^{\,3} + \bar{a}_\infty^{\,3}}\,. \tag{17}$$

The analytical solution of Rod and Misek was used to identify the factors controlling the accuracy of numerical solutions and develop algorithms that can minimize them. Fig. 4 shows the percentage error in calculating $\bar{a}_\infty$ using numerical methods, under different values of Δa and Δt, compared with analytical one from eq. (16). The value of $\bar{a}_o$=570 μm, and $\bar{a}_\infty$=826 μm.

Fig. 5 shows the effect of the number of sampling points (M) on numerical solution to calculate $\bar{a}(t)$. The step time interval Δt= 1s, and the value of $\bar{a}_o$=1000 μm and $\bar{a}_\infty$=880 μm. As M increases, the error in determining the quasi-equilibrium drop size, $\bar{a}_\infty$=880, will decrease.

Fig. 6 shows the effect of the number of sampling points (M) on numerical solution to calculate $\bar{a}(t)$. The step time interval Δt= 1s, and the value of $\bar{a}_o$=775 μm and $\bar{a}_\infty$=875 μm. As M increases, the error in determining the

quasi-equilibrium drop size, $\bar{a}_\infty$=875, will decrease.

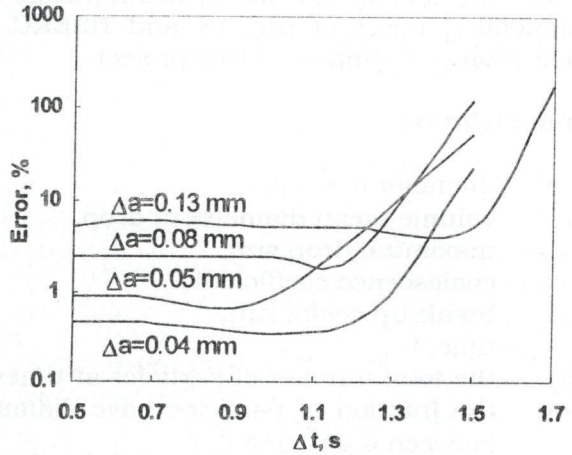

Fig. 4. Effect of discretization on solution error.

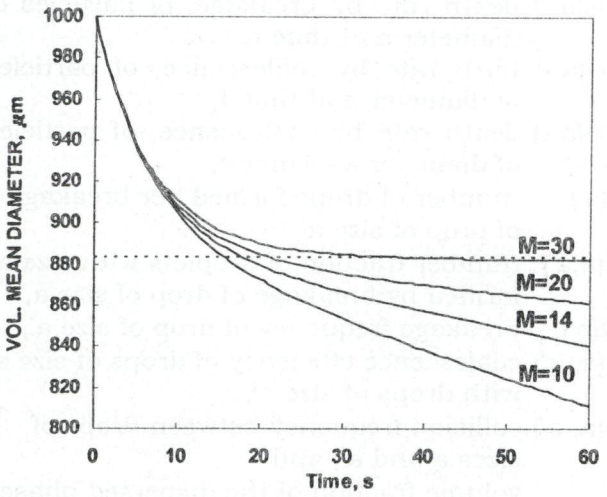

Fig. 5. Effect of M on quasi-equilibrium drop size (net breakage).

Fig. 7 shows the effect of M on the error and computing time of $\bar{a}_\infty$, compared with analytical solution. As M increases, the error decreases at the expense of increasing the computing time.

Fig. 8 shows the effect of a_{max} on the error and computing time, for both breakage and coalescence processes. Where a_{max} is assumed maximum drop size, where the drops will not exceed.

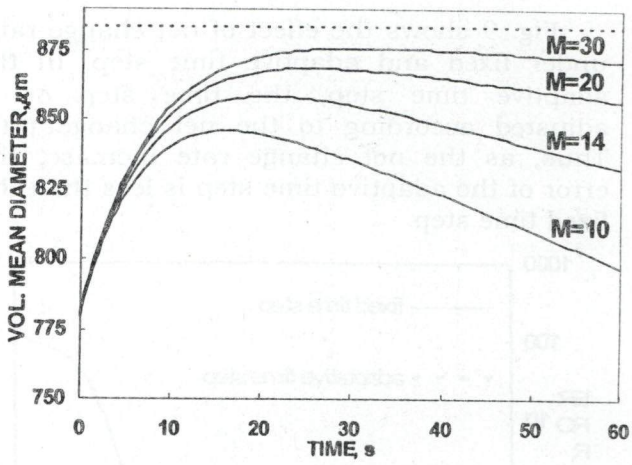

Fig. 6. Effect of M on quasi-equilibrium drop size (net coalescence).

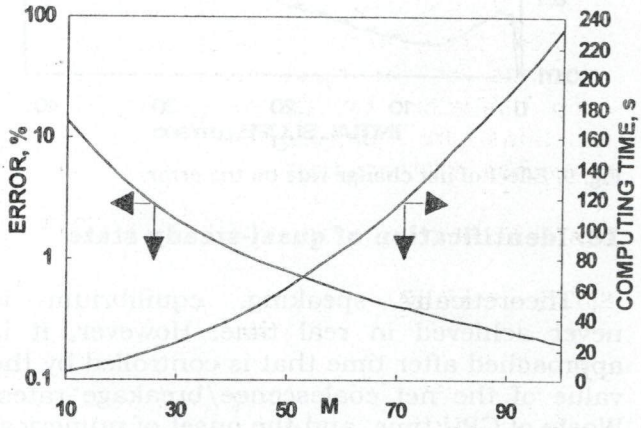

Fig. 7. Effect of M on error and computing time.

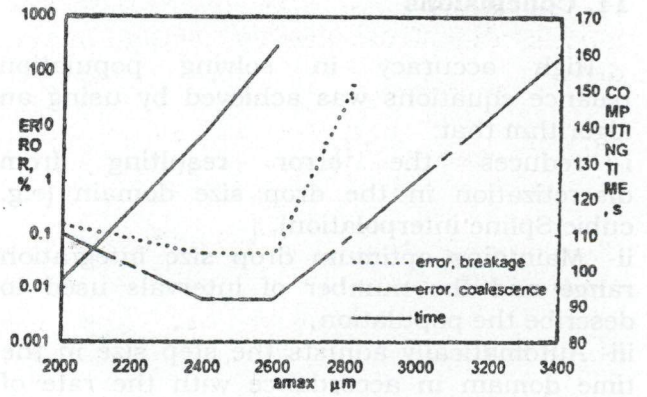

Fig. 8. Effect of a_{max} on error and computing time for breakage and coalescence processes.

Fig. 9 shows the effect of net change rate, under fixed and adaptive time step. In the adaptive time step, the time step Δt is adjusted according to the net change rate. Thus, as the net change rate increase, the error of the adaptive time step is less than the fixed time step.

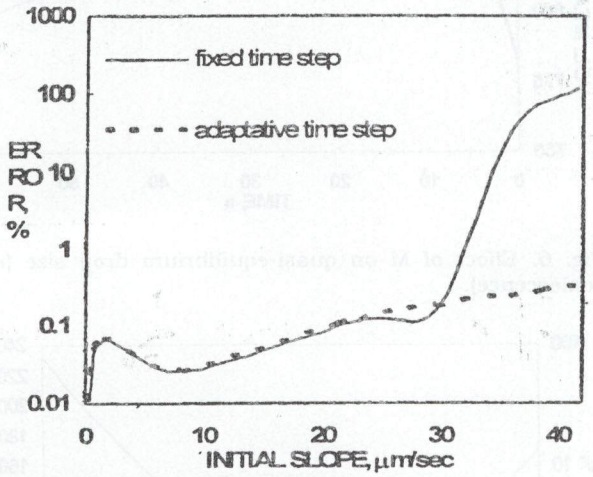

Fig. 9. Effect of net change rate on the error.

10. Identification of quasi-steady state

Theoretically speaking, equilibrium is never achieved in real time. However, it is approached after time that is controlled by the value of the net coalescence/breakage rates. Waste of CPU time, and the onset of numerical instabilities were observed to occur as the solution was continued beyond this point.

11. Conclusions

High accuracy in solving population balance equations was achieved by using an algorithm that:

i- reduces the error resulting from discretization in the drop size domain (e.g. cubic Spline interpolation),

ii- Maintains optimum drop size integration range and the number of intervals used to describe the population,

iii- Automatically adjusts the step size in the time domain in accordance with the rate of change of the mean drop diameter, and

iv- Identifies when quasi-steady state is approached.

Acknowledgement

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Nomenclature

a, a'	diameter of drop,
$\bar{a}$	volume mean diameter of drop,
a_{max}	maximum drop size,
Kc	coalescence coefficient,
Ks	break-up coefficient,
t	time,
N(t)	the total number of particles at time t,
f(a,t)	the fraction of particles have diameter between a and a+Δa,
$B_B(a,t)$	birth rate by breakage, of particles of diameter a at time t,
$D_B(a,t)$	death rate by breakage, of particles of diameter a at time t,
$B_C(a,t)$	birth rate by coalescence, of particles of diameter a at time t,
$D_C(a,t)$	death rate by coalescence, of particles of diameter a at time t,
$\varsigma(a')$	number of drops formed per breakage of drop of size a',
$\beta(a,a')$	number fraction of droplets with size a' formed by breakage of drop of size a,
$\Omega(a')$	breakage frequency of drop of size a',
$\lambda(a, a')$	coalescence efficiency of drops of size a with drops of size a',
$\omega(a, a')$	collision frequency between drops of sizes a and a', and
ϕ	volume fraction of the dispersed phase.

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