Modeling of Breakage Equations Using PBE Software

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Abstract –Particle breakage occurs in a variety of processing units in chemical processing ranging from crushers and grinders to breakage of particles in stirred vessels. Changes in the particle size distribution due to breakage are most often accounted for using population balance equations (PBEs). These PBEs are partial integral differential equations that are difficult to solve and for which there are few analytical solutions. This often makes solving these equations intractable for undergraduate students. The goal is to remove this barrier so that students can focus on the effects of breakage model parameters on the resulting particle size distributions. An initial version of a computer program has been developed for use in a particle and crystallization technology elective course in chemical engineering. The program uses MS Excel as an interface and allows the user to set the initial particle size distribution and the model parameters.

Keywords: Population Balance Equations, Software.

INTRODUCTION

In addition to standard lectures, the course will encourage active learning. Research shows [1-4] that students learn more when they are actively involved in the learning process. Wankat [4] states that teaching techniques such as computer simulations increase student learning because the students are actively involved and tend to spend more time on learning.

To facilitate the comprehension of PBE concepts, educational software will be developed for use in the PACT course. Since it is well known that the solution of breakage PBEs is problematic because they are partial integro-differential equations and that solution techniques vary depending on the models used [5], the use of a computer program is expected to benefit the students. The software's purpose is to facilitate instruction by allowing the students to concentrate on the concepts being taught rather than on solution techniques, to help make abstract concepts more tangible, and to integrate new research developments into the course. The software will enable the students to study the effects of the variables, which would aid the students in making design decisions.

At this time, the software is limited to only modeling particle breakage. A case study using this software will be presented.

Breakage Equation

A population balance equation (PBE) is commonly used to account for changes in particle size in a collection of particles. The particle size may be represented by a characteristic length, L, or by a volume, v. The PBE includes changes in the particle size distribution (PSD) due to various mechanisms including agglomeration, growth, nucleation, and breakage of particles. The number distribution of particles is typically represented by the number density function, where n(v) is the number density function based on the particle volume. The evolution of the number density function with time is given by the continuous PBE. A typical expression for the breakage equation is shown in the following equation where the first two terms on the right hand side account for the agglomeration, the next term accounts for growth and nucleation, and the last term accounts for breakage.

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$$\frac{\partial n(v)}{\partial t} = \frac{1}{2}\int_0^v a(v-w, w)\, n(v-w)\, n(w)\, dw - n(v)\int_0^\infty a(v, w)\, n(w)\, dw - \frac{\partial G_V(v)\, n(v)}{\partial v} + \int_v^\infty b(v, w)\, S(w)\, n(w)\, dw - S(v)\, n(v) \qquad (1)$$

The agglomeration kernel is a(v-w, w) where v and w are particle volumes; and the growth rate is G(v). In this paper only particle breakage is considered. This is easily handled in the PBE by setting the growth and agglomeration rates to zero. This will be referred to as the breakage equation since it only has one mechanism. In the breakage equation shown below, the first term on the right hand side is the birth term that accounts for particles larger than v breaking and forming child particles in the size range v + δv, and the last term is the death term.

$$\frac{\partial n(v)}{\partial t} = \int_v^\infty b(v, w)\, S(w)\, n(w)\, dw - S(v)\, n(v) \qquad (2)$$

The death term accounts particles of size v that break and fall into smaller size ranges. The function S(v) is the specific rate of breakage that accounts for the effect of particle size on the breakage rate. The birth term includes the breakage distribution function b(v, w) which is the probability of a child particle of volume v being formed due a parent particle of volume w breaking. In the breakage equation, there are many possible models for the breakage distribution function. The degree of difficulty in solving the equation often depends on the form of the breakage distribution function.

The solution method uses a discretization technique developed by Hill and Ng [6]. The discretized breakage equation is

$$\frac{d}{dt} N_i = \sum_{j=i+1}^{\infty} \beta_j\, b_{ij}\, S_j\, N_j - \delta_i S_i\, N_i \qquad (3)$$

where b_{ij} is the discretized number-based breakage function, no./no.; N_i is the number of particles in interval i, no./ m^3 of slurry or no./ kg of powder; S_i is the discretized volume-based specific rate of breakage, min^{-1}; and β_i and δ_i are the birth and death term factors, respectively. This technique guarantees that mass is conserved during particle breakage. The discretization allows easier solution as a set of ODEs, and allows flexibility in the selection of the breakage distribution function. Also, it allows the user to set the parameters for the breakage distribution functions as well as the breakage rate parameters, and the length of time that breakage occurs.

Breakage Distribution Functions

The breakage distribution function b(v, w) is the probability that a child particle of volume v is formed when a parent particle of volume w breaks. That is, it is the expected distribution of child particles for a parent particle of a given volume. A variety of empirical and theoretical expressions exist for the breakage distribution function. One empirical breakage distribution function is

$$b(v,w) = \frac{\phi\gamma}{3w}\,(v/w)^{\frac{\gamma}{3}-1} + \frac{(1 \quad \phi)\beta}{3w}\,(v/w)^{\frac{\beta}{3}-1} \qquad (4)$$

where ϕ, γ, and β are constants that depend on the material being broken [7]. The product function with a power law form has a theoretical basis [8] is as follows

$$b_v^{'}(v,w) = \frac{p\, v^m\, (w-v)^{m+(m+1)(p-2)}\, [m+(m+1)(p-1)]!}{w^{m+(m+1)(p-1)}\, m!\, [m+(m+1)(p-2)]!} \qquad (5)$$

where p is the number of child particles formed and m is a constant selected by the user.

IMPLEMENTATION

The software for performing the calculations uses an MS Excel interface. The input data is entered into the spreadsheet into the cells with a yellow background as shown in Figure 1. To run the simulation, the calculate button is selected. Clicking on the Calculate button causes a visual basic program to run. This visual basic program uses the input data from the flowsheet, sends the data to and calls a dll file that was originally written in Fortran, runs the Fortran subroutine, and returns selected results to the Excel spreadsheet. The Fortran subroutine solves the discretized PBEs using a Runga-Kutta method.

Input Parameters

Austin Parameters						Product Law Parameters		
Phi	0.36	Rho	3.217	g/cm^3		Sc	0	1/min
Gam	2.8	Sc	0.0000005	1/min		Alpha	0.34667	
Beta	3.5	Alpha	0.34667			p	5	# children
Delta	20	PrintTime	2	minutes		m	0	exponent
PhiV	0.5235988	MaxTime	10	minutes				
L(i)/L(i-1)	1.259921	L(1)	12.5	μm				

Figure 1. Example of the data input section of spreadsheet.

The software also allows the user to enter an initial size distribution as well as set the total time for particle breakage and time intervals where the breakage results are reported.

While it is well known that using computer software doesn't automatically improve student learning, it can be used effectively when there is no other known method for accomplishing the same goal. In this case, it allows students to solve the PBE in order to demonstrate the effects of the model parameters.

CASE STUDIES

Students may perform several case studies with the program. These can consist of studying the effects of a model's parameters, or investigating the differences between models.

Case I: Effects of parameters on an empirical breakage distribution function

One example of a homework problem would be to give the students an initial particle size distribution before particle breakage, as well as the breakage rate parameters. In addition, state that the Austin breakage distribution function, Eq. (4), would be used with the parameters $\phi = 0.36$, $\beta = 3.8$, and $\gamma = 2.5$. Ask the students to run the model for the base case and with at least three other values of γ. Have the students explain how changing the parameter γ affects the resulting distributions after 30 minutes of breakage.

One possible set of results for this problem is shown in Figure 2. The size of each size interval is shown as the major axis length in microns. The number fractions for the initial unbroken particles are shown for comparison purposes.

From examining Figure 2, students should recognize that more small particles are formed as γ is decreased, and that the number fractions of particles larger than 600 microns decrease as γ is decreased. Similar problems can be assigned where the parameters ϕ and β are investigated.

Case II: Effects of parameters on a theoretical breakage distribution function

Another student exercise would be to investigate effect of the parameter p in the breakage distribution function in Eq. (5). In this case the initial particle size is given with the breakage rate parameters, and the parameter m is set to a value of 2. The student are asked to run the simulation at a least 4 values of p including p = 3. They are also asked to explain how changing the number of child particles p affects the resulting distributions after 30 minutes of breakage.

Figure 3 is one example of the possible results. The graphs can differ depending on the chosen values of p. As in Case I, the size of each size interval is shown as the major axis length in microns and the number fractions for the initial unbroken particles are shown for comparison purposes.

The students should recognize that 1) the breakage distribution function causes a second peak to be formed between 200 and 300 microns, 2) the height of this second peak increases with p, and 3) the location of the peak shifts to lower particle sizes as p is increased. Alternatively, students could be asked to investigate the effects of the parameter m rather than p.

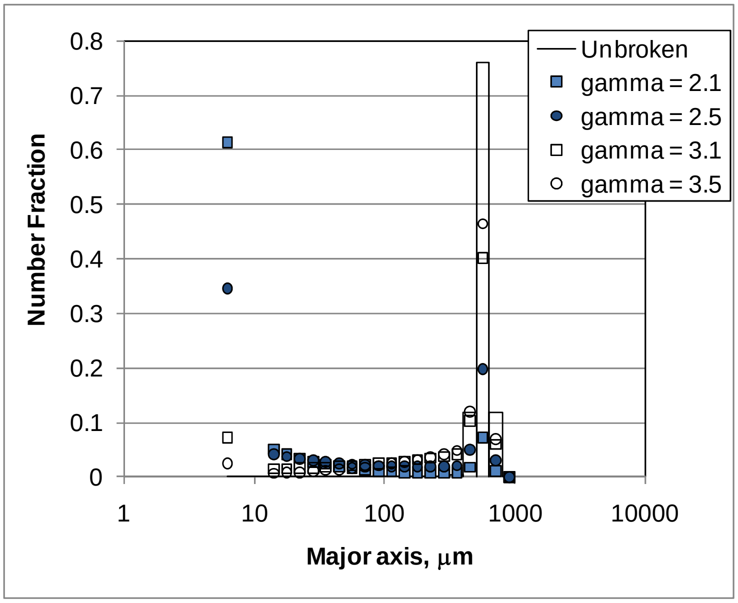

Figure 2. Effect of γ on the resulting size distribution using the empirical breakage distribution function.

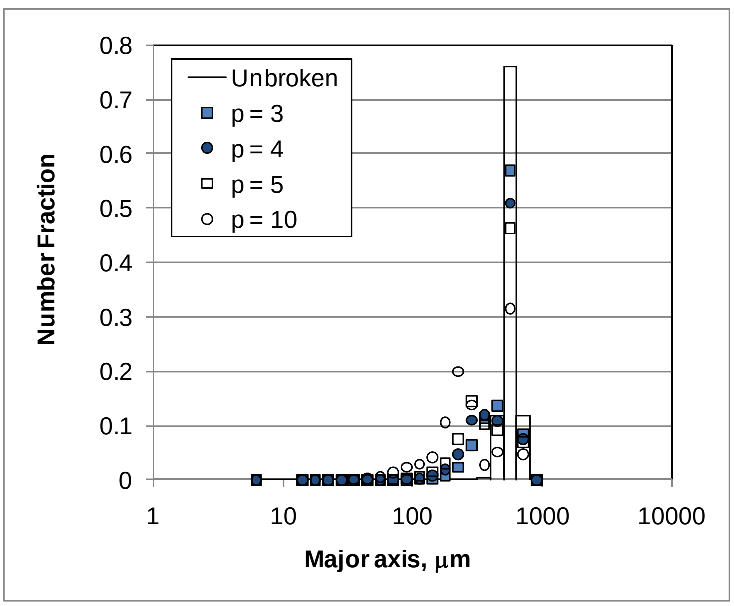

Figure 3. Effect of p on the resulting size distribution using the theoretical breakage distribution function.

Comparison of Cases I and II

A third exercise would be to ask the students to explain the differences between the results shown for Cases I and II. The goal would be to help the students understand the differences between the two breakage distribution functions. It is expected that the students would realize that the differences would partially depend on the parameter settings for each model. However, the students should also recognize that one difference between the two breakage functions is that the theoretical breakage function produces a secondary peak between 200 and 300 microns, while the empirical breakage function has a strong effect on the number fraction of particles in the smallest size interval.

Another exercise for helping students understand the differences between the two breakage distribution functions would be to provide them with an initial PSD and a final PSD and ask them which breakage distribution function is best able to describe the changes in the PSD. From studying the resulting PSDs in Cases I and II, they should be able to look at the shape of the resulting PSDs and qualitatively compare them to the given data to determine which function is a better match.

Additional Exercises

Other exercises are possible to investigate other aspects of the models. For example, the students can compare the results at various residence times to determine the effect of time on the PSD, investigate the effects of breakage rate parameters, and simulate the results of combining two breakage distribution functions.

BENEFITS

The benefits to the students and the instructor are that the program is flexible and that other exercises can be developed to demonstrate breakage concepts. The advantages to the students are that they 1) can investigate the effects of the model parameters without being encumbered with a solution technique, 2) do not need to know a programming language to use the program, 3) can study two different breakage functions independently, and 4) can study the combination of two different breakage distribution functions.

CONCLUDING REMARKS

The development of this program allows students to study the effects of various parameters on two different breakage distribution functions. Various case studies can be performed to demonstrate the effects of various parameters as well as the interactions between parameters. In addition, it allows the students to compare and/or combine two different breakage distribution functions. It also provides a tool for generating simulation results to compare with experimental data.

Future work includes expanding the program to more breakage models, and creating programs with other mechanisms such as agglomeration. It should be noted that many breakage distributions exist in the literature and there is no plan to include every model in this tool, but to provide the instructor and the student with some representative examples. This software has the flexibility to allow students to run simulations that demonstrate concepts in particle breakage, but avoids the difficulties of solving the equations.

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