DROP SIZE DISTRIBUTIONS BY POWER FUNCTIONS OF BREAKAGE AND COALESCENCE

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The frequencies of drop breakage and coalescence in a batch mixer are described by power functions of drop sizes. The shape of a steady state drop size distribution corresponding to the power functions is correlated with their exponents. The use of this correlation for direct determination of linear combination of power functions exponents from an experimental drop size distribution is demonstrated.

The breakage and coalescence of drops in a dispersion under turbulent regime are significant processes, which, however, do not permit an easy access in direct investigation. At present we lack their experimentally verified mathematical description. Besides the direct observation of these phenomena, other quantities and processes influenced by them may be investigated, *e.g.* the tracer spreading rate in the dispersed phase or the time variation of drop size distribution and its steady state. Comparing the respective measured values with those calculated from the mathematical model the most suitable relations for the breakage and coalescence rates may be identified.

The most often considered type of the dependence of breakage and coalescence frequency of the drop size are power functions[1-7]. Their significant advantage consists in their simplicity which in some cases makes even possible an analytical solution of the dispersion model. The purport of this study is to find connections between the parameters of power functions and the shape of the steady state drop size distribution in a model of a batch mixer.

THEORETICAL

Breakage and Coalescence Functions

Drop breakage and coalescence are described by means of four functions[8]: drop breakage frequency, volume distribution of daughter drops, average number of daughter drops from a single mother drop and coalescence frequency of drops of volumes v and v', which is the product of collision frequency and efficiency. Let the drop breakage frequency be

$$g(v) = C_1 v^{a} \quad (1)$$

and the drop coalescence frequency

$$\omega_1(v, v') = C_2(v + v')^{b}, \quad (2)$$

or

$$\omega_2(v, v') = C_2(vv')^{b/2}. \quad (3)$$

Let us suppose that during each breakage a pair of drops originates. The distribution of daughter drop volumes v' from the mother drop of volume v is given alternatively by the delta function

$$\beta_1(v, v') = \delta(v' - v/2) \quad (3)$$

which corresponds to the splitting of drops into halves; the normal distribution

$$\beta_2(v, v') = [1/(\sqrt{2\pi})\, s] \exp[-(v' - v/2)^2/2s^2], \quad (5)$$

where the standard deviation s is chosen so as to make the fraction of daughter drops overlapping the interval $(0; v)$ negligible; the uniform distribution of daughter drops

$$\beta_3(v, v') = 1/v, \quad v' \in (0; v). \quad (6)$$

From these expressions for g, ω and β six variants of the breakage and coalescence model arise (Table I).

Drop Population Balance

The balance of the number of drops of size v in a batch mixer for the binary breakage is[2]

$$\mathrm{d}nA(v)\,\mathrm{d}t = 0{\cdot}5 \int_0^{v} \omega(v', v - v')\, nA(v')nA(v - v')\,\mathrm{d}v' - g(v)\, nA(v) +$$

$$+ 2\int_v^{\infty} g(v')\,\beta(v', v)\, nA(v')\,\mathrm{d}v' - \int_v^{\infty} \omega(v, v' - v)\, nA(v)nA(v' - v)\,\mathrm{d}v'. \quad (7)$$

In steady state $\mathrm{d}\, nA(v)/\mathrm{d}t = 0$, and the solution of (7) for $a \neq b$ is

$$A(v) = Kv^{a-b-1} f(x), \quad (8)$$

where

$$K = 2C_1/nC_2\,, \tag{9}$$

$$x = K^{1/(a-b)}v\,. \tag{10}$$

The function $f(x)$ of the dimensionless variable fulfils the condition

$$\int_0^\infty A(v)\,dv = \int_0^\infty x^{a-b-1}\,f(x)\,dx = 1\,. \tag{11}$$

Simultaneously, it is the solution of an integral equation independent of the coefficients C_1, C_2 resulting by the substitution of g, ω, β into the population balance (7). Thus, for the coalescence frequency ω_1

$$0{\cdot}5\left[x^b\int_0^x x'^{a-b-1}(x-x')^{a-b-1}\,f(x')\,f(x-x')\,dx' - x^{2a-b-1}\,f(x)\right] + \\ + \int_x^\infty\left[x'^{2a-b-1}\beta(x',x)\,f(x') - x'^b x^{a-b-1}(x'-x)^{a-b-1}\,f(x)\,f(x'-x)\right]dx' = 0\,. \tag{12}$$

Particularly, for $a = b + 1$, $\omega = \omega_1$, $\beta = \beta_3$, Rod[9] has found the following analytical solution of the population balance:

$$f(x) = \exp(-x)\,,\quad A(v) = K\exp(-Kv)\,. \tag{13}$$

For the coalescence frequency ω_2, it holds

$$0{\cdot}5\left[\int_0^x x'^{a-b/2-1}(x-x')^{a-b/2-1}\,f(x')\,f(x-x')\,dx' - x^{2a-b-1}\,f(x)\right] +$$

TABLE I
Model variants

Coalescence frequency	Daughter drop distribution		
	β_1	β_2	β_3
ω_1	A	B	C
ω_2	D	E	F

$$+\int_x^\infty [x'^{2a-b-1}\beta(x',x)\,f(x') - x^{a-b/2-1}(x'-x)^{a-b/2-1}\,f(x)\,f(x'-x)]\,dx' = 0\,. \tag{14}$$

If $b = 2m$, $a = m + 1$, $\omega = \omega_2$, $\beta = \beta_3$ a problem, solved analytically by Bajpai and coworkers[7], arises. From Eqs (8)–(11), (14) it follows

$$f(x) = \exp\left[-\Gamma(1-m)^{1/(1-m)}\,x\right],$$
$$A(v) = Kv^{-m}\exp\left(-[K\,\Gamma(1-m)]^{1/(1-m)}\,v\right) \quad \text{for} \quad m < 1\,. \tag{15}$$

If $m \geqq 1$ or $a \leqq b$, the integral on the lhs of (11) diverges and the problem has no solution.

This fact may be generalized. The model of dispersion (7) with power functions (1)–(3) has a meaningful physical solution in the region $a > b$. With the decreasing difference of the exponents the steady state drop size decreases; in the limit $a \to b$ the solution of population balance is $A(v) = \delta(v)$, which means an infinite number of droplets of zero-size.

The mean drop volume may be calculated from (8):

$$\langle v\rangle = \int_0^\infty vA(v)\,dv = K^{-1/(a-b)}\int_0^\infty x^{a-b}\,f(x)\,dx\,. \tag{16}$$

Because

$$K = 2C_1\langle v\rangle/XC_2\,, \tag{17}$$

the mean volume as a function of hold-up is:

$$\langle v\rangle = (XC_2/2C_1)^{1/(a-b+1)}\left[\int_0^\infty x^{a-b}\,f(x)\,dx\right]^{(a-b)/(a-b+1)}. \tag{18}$$

Normalized Drop Size Distribution

Relating the drop size in the distribution (8) to a mean drop size for the given dispersion, a normalized dimensionless drop size distribution arises, independent of the coefficients C_1, C_2. As the coefficients C_1, C_2 change with the intensity of mixing and with the composition of liquid phases, while the exponents a, b are directly connected with the mechanism of breakage and coalescence and therefore remain constant in a wide range of experimental conditions, the normalized shape of distribution is especially suitable for investigation allowing conclusions of general validity. Following Chen and Middleman[10] the volume distribution as a function of the ratio of the drop diameter to the respective Sauter mean is used. From (*8*) it results

$$A_v(d/d_{32}) = 3/G\,(Fd/d_{32})^{3(a-b)+2}\, f[(Fd/d_{32})^3]\,, \tag{19}$$

where

$$F = \int_0^\infty x^{a-b}\, f(x)\, dx/G\,, \quad G = \int_0^\infty x^{a-b-1/3}\, f(x)\, dx\,. \tag{20}$$

The shape of the distribution is characterized by its moments. In the individual variants of the model the first moment, the standard deviation derived from the second moment, and the asymmetry derived from the third moment of the function (*19*) are investigated.

For the formulation of Bajpai and coworkers[7] and Rod[9] the moments may be derived directly from the analytically obtained distribution. The distribution of drops in Bajpai's problem is given by (*15*) and its normalization according to (*19*) gives

$$A_v(d/d_{32}) = 3/\Gamma(5/3 - m)\left[\frac{\Gamma(2-m)}{\Gamma(5/3-m)}\frac{d}{d_{32}}\right]^{5-3m} .\exp\left(-\left[\frac{\Gamma(2-m)}{\Gamma(5/3-m)}\frac{d}{d_{32}}\right]^3\right). \tag{21}$$

This normalized distribution is defined for $m < 5/3$. Its characteristics are

$$M_1 = \Gamma(5/3 - m)\,\Gamma(7/3 - m)/\Gamma(2 - m)^2\,, \tag{22}$$

$$\sigma = B^{0.5}\Gamma(5/3 - m)/\Gamma(2 - m)^2\,, \tag{23}$$

$$A_c = \{[(2 - m)\,\Gamma(2 - m)^3 - \Gamma(7/3 - m)^3]/B - 3\Gamma(7/3 - m)\}/B^{0.5}\,, \tag{24}$$

where B is

$$B = \Gamma(8/3 - m)\,\Gamma(2 - m) - \Gamma(7/3 - m)^2\,. \tag{25}$$

Numerical values of the characteristics in dependence on m, calculated from (*22*)–(*25*), are given in Table II. The first moment of the distribution varies with the parameter m very slowly. Almost in the whole range of m the asymmetry remains low. The mean square deviation is most sensitive to the m values, and therefore it is most suitable for the determination of m from the distribution shape.

The solution described by (*13*), which was investigated by Rod[9] coincides with Bajpai's problem, if $m = 0$. In the remaining cases the population balance (*7*) has been solved numerically by means of the method of finite differences with the discretization of drop volumes for 40 equidistant values. The procedure is described in another work[11]. For each of the six variants of the model the distributions for at least 20 combinations of exponent values were calculated. The exponents were chosen in the range $0 \leqq a \leqq 3{\cdot}5$; $-3 \leqq b \leqq 1$, while $a - b \geqq 1$. The numerical solutions of the balance had been normalized before determining their characteristics.

Correlation of Characteristics

The main calculation results are brought together in the correlations of the standard deviation of normalized solution with the exponents of breakage and coalescence functions. The standard deviation from Table II may be correlated with the parameter m by a simple relation

$$\sigma_c = 0{\cdot}35(5/3 - m)^{-0.53} \tag{26}$$

which is valid in the range $m \in \langle -3; 2/3 \rangle$ with an accuracy better than 1%. The relation may be expanded on the whole model F, a special case of which the Bajpai's problem may be regarded, if it is expressed in the dependence on the linear combination of exponents

$$z = a - 1{\cdot}1b\,. \tag{27}$$

TABLE II

Characteristics of drop size distribution

m	M_1	σ	A_c	σ_c	M_{1c}
−3	1·0249	0·1561	0·014	0·155	1·026
−8/3	1·0269	0·1621	0·016	0·161	1·028
−7/3	1·0293	0·1689	0·018	0·168	1·030
−2	1·0321	0·1766	0·020	0·176	1·033
−5/3	1·0355	0·1855	0·023	0·185	1·036
−4/3	1·0397	0·1958	0·027	0·196	1·041
−1	1·0450	0·2082	0·032	0·208	1·046
−2/3	1·0519	0·2231	0·038	0·224	1·053
−1/3	1·0613	0·2418	0·048	0·243	1·062
0	1·0748	0·2662	0·059	0·267	1·075
1/3	1·0957	0·2998	0·079	0·301	1·095
2/3	1·1321	0·3503	0·111	0·350	1·130
1	1·2092	0·4395	0·168	—	—
4/3	1·4610	0·6682	0·290	—	—
5/3	∞	∞	0·633	—	—

After rearrangement the standard deviation of the distribution is

$$\sigma_c = 0{\cdot}386(z + 1)^{-0.53}\,. \tag{28}$$

By comparing this correlation with the calculations the relative mean error of 2% has been found. The fit might have been increased introducing a more elaborate function than the linear combination of exponents (*27*), but the precision achieved fully complies with the purpose of the present study.

For the remaining models similar correlations given in the σ_c column of Table III have been found. Sub s_σ in Table III the mean relative deviations of the σ values calculated by solving the balance from those corresponding to the correlation are listed. The Table also contains the correlation of the first moment with the standard deviation of the distribution and its mean relative deviation from the correlated first moments s_M.

The asymmetry is not so unambiguously connected with the standard deviation of the distribution as its first moment. In models A, D it is positive in the whole range of the calculation, its value being $A_c = 0{\cdot}22 \pm 0{\cdot}13$, in the models B, E $A_c = 0{\cdot}13 \pm 0{\cdot}07$. In the models C, F for small values of differences of the exponents it is close to zero: $A_c = \pm 0{\cdot}05$ for $1 \leqq z \leqq 2$. For higher z values the fluctuation of the asymmetries calculated for different variants C, F increases, the A_c values values ranging from $-0{\cdot}3$ to 0.

Consequently, the six investigated models split into pairs A–D, B–E, C–F, with frequency ω, given by (*2*) or (*3*) in each pair. From Eq. (*2*) and (*3*) follows the fact that for $b = 0$ both models in each pair coincide. The calculation results show that for $b \neq 0$ the exchange of both coalescence functions causes only insignificant changes in the shape of the normalized distribution, the pairs having common correlations in the whole range of the calculations.

The models with different distributions of daughter drop sizes, however, are distinguished more clearly. The bisection of drops in the models A, D and the uniform volume distribution in the models C, F are the boundary instances, between

TABLE III

Correlation of characteristics

Model	z	σ_c	s_σ, %	M_{1c}	s_M, %
A, D	$a - 0{\cdot}75b$	$0{\cdot}345(z + 1)^{-0.55}$	1	$1 + 0{\cdot}99\sigma^2$	0·05
B, E	$a - 0{\cdot}8b$	$0{\cdot}350(z + 1)^{-0.54}$	1	$1 + \sigma^2$	0·05
C, F	$a - 1{\cdot}1b$	$0{\cdot}386(z + 1)^{-0.53}$	2	$1 + 1{\cdot}06\sigma^2$	0·1

which the normal distribution of the models B, E is situated. For the models differing in the function β the drop bisection leads to the narrowest drop size distribution with the smallest standard deviation.

Comparison with Data

Experimental drop size distributions were obtained by Chen and Middleman[10] by means of photographing the dispersion in batch mixer at a low hold-up of dispersed phase. The set of the results of 112 experiments differing in the chemical composition of the liquids, and in impeller frequency and size, was correlated by a single normalized distribution

$$A_{vc}(d/d_{32}) = [1/0{\cdot}23(\sqrt{2\pi})] \exp[-9{\cdot}2(d/d_{32} - 1{\cdot}06)^2] \qquad (29)$$

with the characteristics $M_1 = 1{\cdot}06$, $\sigma = 0{\cdot}23$, $A_c = 0$.

The models corresponding to this distribution have been determined according to Table III. After substituting $\sigma = 0{\cdot}23$ into the correlations M_{1c}, the results are for A, D $M_{1c} = 1{\cdot}052$, for B, E $M_{1c} = 1{\cdot}053$ and for C, F $M_{1c} = 1{\cdot}056$, which is nearest to 1·06. Also the requirement of zero symmetry is best fulfilled by the models C, F. Consequently the experimental data (*29*) shall be modelled by the variants C, F.

By the substitution of $\sigma_c = 0{\cdot}23$ into the correlation from Table III, $z = 1{\cdot}66$ is calculated. The model sought thus consists of the following functions:

$$g(v) = C_1 v^a ,$$
$$\omega(v, v') = C_2(v + v')^b \quad \text{or} \quad \omega(v, v') = C_2(vv')^{b/2} ,$$
$$\beta(v, v') = 1/v , \quad 0 < v' < v , \qquad (30)$$

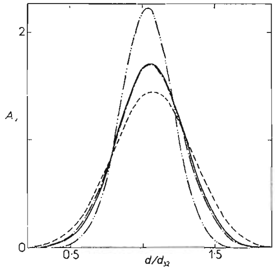

FIG. 1

Normalized distributions according to model *F*. ----- $a = 1$, $b = 0$, $J = 0{\cdot}058$; -·-·-·- $a = 1$, $b = -0{\cdot}6$, $J = 0{\cdot}003$; -··-··-·· $a = 1$, $b = -2$, $J = 0{\cdot}132$, ——— experimental distribution according to Chen and Middleman[10] with exponents

$$a - 1{\cdot}1b = 1{\cdot}66 . \tag{31}$$

From the range of the exponents, for which the validity of the correlation has been verified, follows $0 \leqq a \leqq 2{\cdot}76$.

The correctness of the result was checked by the calculation of drop size distribution in the points $(a = 0,\ b = -1{\cdot}51)$, $(a = 1,\ b = -0{\cdot}6)$ and $(a = 2,\ b = 0{\cdot}31)$ for the variants C, F. Characteristics of these distributions are, according to expectations, within the range $M_1 \in \langle 1{\cdot}055; 1{\cdot}057\rangle$, $\sigma \in \langle 0{\cdot}229; 0{\cdot}234\rangle$, $A_c \in \langle -0{\cdot}1; 0\rangle$. Quantitatively, the overall fit of the distribution with the experimental distribution *(29)* was evaluated by means of the criterion

$$J = 0{\cdot}5 \int_0^\infty \left| A_{ve}(d/d_{32}) - A_v(d/d_{32}) \right| d(d/d_{32}) \tag{32}$$

which may range from zero to one. A few examples of distributions with the respective J values are given in Fig. 1. The six distributions tested imply the range $0{\cdot}002 \leqq J \leqq 0{\cdot}010$ which demonstrates that the proposed models are good representations of the experimental distributions.

LIST OF SYMBOLS

a	breakage frequency exponent
$A(v)$	frequency distribution of drop sizes, L^{-3}
A_c	asymmetry of normalized distribution
$A_v(d/d_{32})$	normalized volumetric drop size distribution
$A_{ve}(d/d_{32})$	normalized experimental distribution
b	coalescence frequency exponent
C_1	breakage frequency coefficient, $L^{-3a} T^{-1}$
C_2	coalescence frequency coefficient, $L^{-3(b-1)} T^{-1}$
d	drop diameter, L
d_{32}	Sauter diameter, L
$f(x)$	function defined by Eqs *(11)*, *(12)* and *(14)*
$g(v)$	breakage frequency of drops of volume v, T^{-1}
J	criterion of distribution fit, defined by Eq. *(32)*
$K = 2C_1/nC_2$	parameter of drop size distribution, $L^{3(b-a)}$
$m = b/2$	exponent in problem of Bajpai and coworkers
M_1	first moment of normalized distribution
M_{1c}	correlated first moment of distribution
n	number of drops in unit volume of dispersion, L^{-3}
s_M	mean relative deviation of M_1 from M_{1c}
s_σ	mean relative deviation of σ from σ_c
t	time, T
v, v'	drop volume, L^3

$\langle v \rangle$	mean volume, L^3
x, x'	dimensionless drop size defined by Eq. (*10*)
X	hold-up of dispersed phase
z	linear combination of exponents
$\beta(v, v')$	daughter drop size distribution, L^{-3}
σ	standard deviation of normalized distribution
σ_c	correlated standard deviation of distribution
$\omega(v, v')$	coalescence frequency of drops of volumes v and v', $L^3 T^{-1}$

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