Preliminaries about Atomization

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Abstract

This document presents a review of the main theoretical and empirical models used to describe atomization phenomena, with a particular focus on secondary atomization of droplets. Atomization is analyzed through two main categories: primary atomization, characterized by Kelvin-Helmholtz and Rayleigh-Taylor instabilities at the liquid-gas interface, and secondary atomization, which describes the fragmentation of droplets under the action of aerodynamic forces. The models studied include the empirical correlations of Pilch and Erdman, based on Weber and Ohnesorge numbers to predict breakup times, the Reitz models (RD) using linear instability analysis, the hybrid KH-RT model combining Kelvin-Helmholtz and Rayleigh-Taylor mechanisms with consideration of viscous effects, the TAB and ETAB models based on the mass-spring-damper analogy, and finally the FAST model (Fractal-Atomization-Spray-Theory) describing the statistical evolution of size distributions via a stochastic approach. This synthesis provides the theoretical foundations necessary for numerical modeling of atomization in various applications.

1. Introduction to Atomization

The atomization phenomenon can be divided into two categories:

- Primary atomization, which refers to phenomena ranging from the formation of instabilities, the main ones being Kelvin-Helmholtz and Rayleigh-Taylor, at the interface between liquid and gas phases up to the ejection of liquid clusters.
- Secondary atomization, which describes the fragmentation of liquid clusters generated during primary atomization under the action of aerodynamic forces from the carrier flow. It is characterized by strong deformations. However, surface tension forces and liquid viscosity contribute to stabilizing the droplet.

Kelvin-Helmholtz instabilities appear in a shear layer of the same fluid or two fluids of different densities. An infinitesimal perturbation normal to the shear layer at the interface is then amplified via the rolling up of a vorticity sheet. Rayleigh-Taylor instability, on the other hand, results from the perturbation of a mixture with density stratification, more precisely, from the acceleration of a dense and light fluid.
In our case study, we will focus more on droplet fragmentation and therefore model the secondary atomization phenomenon. However, primary atomization should not be excluded as it can occur for large droplets. Now, for atomization, two characteristic numbers allow quantifying the types of breakup:

- Weber number: $We = \frac{\rho_g d(u-u_g)^2}{\sigma}$
- Ohnesorge number: $Oh = \frac{\sqrt{We}}{Re}$

Thus, we define the following breakup regimes:

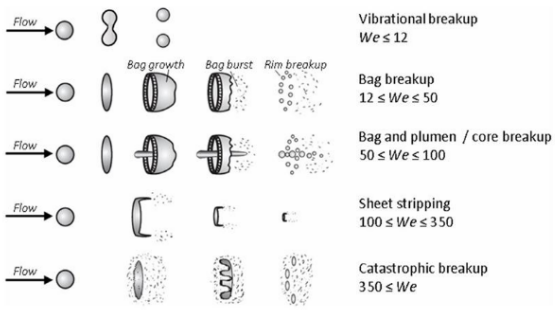

Figure 1: The breakup regimes

Therefore, after this brief introduction, we can present the different models that allow describing the atomization phenomenon.

2. Pilch and Erdman Correlations [5]

The correlations of Pilch and Erdman are based on correlations between the dimensionless Weber and Ohnesorge numbers with characteristic breakup times for droplets. The established correlations are rigorous and have remained, and still are, a reference in the study of liquid atomization. However, it is important to note that these correlations are empirical and often limited to negligible viscous effects when determining characteristic breakup times.

Thus, Pilch and Erdman present a fragmentation criterion, very useful and widely used in the literature today, based simply on the Weber number and the Ohnesorge number, therefore without neglecting viscous

effects. Then, we define a critical Weber number for fragmentation $\mathrm{We_{crit}}$, according to Brodkey's work:

$$\mathrm{We_{crit}} = 12 \cdot (1 + 1.077 \cdot \mathrm{Oh}^{1.6}) \tag{1}$$

Then, Pilch and Erdman distinguish two characteristic breakup times which are:

- Breakup initiation time: corresponds to the time required for a droplet to initiate the breakup processes. Before this time, the droplet is considered not to have started its fragmentation. It is defined according to the following formula:

$$T_{\mathrm{init}} = 1.9 \cdot \mathrm{We}^{-1/4} \cdot (1 + 2.2 \cdot \mathrm{Oh}^{1.6}) \tag{2}$$

- Total breakup time: corresponds to the total time a droplet will take to fragment until the end of breakup. This time includes the breakup initiation time. However, it is only defined in the non-viscous case with the following correlations:

$$T_{\mathrm{tot}} = \begin{cases} 6(\mathrm{We} - 12)^{-1/4} & \text{if } \mathrm{We_{crit}} \leq \mathrm{We} < 18 \\ 2.45(\mathrm{We} - 12)^{1/4} & \text{if } 18 \leq \mathrm{We} < 45 \\ 14.1(\mathrm{We} - 12)^{-1/4} & \text{if } 45 \leq \mathrm{We} < 2670 \\ 5.5 & \text{if } 2670 \leq \mathrm{We} \end{cases} \tag{3}$$

The breakup initiation times and total breakup times are dimensionless times. It is necessary to multiply them by a characteristic time given by Pilch as:

$$t_c = \frac{d}{|u - u_g| \cdot \left(\frac{\rho_g}{\rho_l}\right)^{1/2}} \tag{4}$$

where u is the droplet velocity and u_g is the gas velocity, d is the initial diameter of the droplet.
In our equations, we can therefore consider the two cases below, with r_{child} to be defined by ourselves:

1. We assume that there is total breakup instantaneously after the initiation of breakup, therefore after a time T_{init}. We will then observe discontinuities and discrete variations. Nevertheless, care must be taken when using discrete processes in CQMOM.

$$\frac{dr}{dt} = H(\mathrm{We} - \mathrm{We_{crit}}) \cdot (r_{\mathrm{child}} - r) \cdot f(\frac{t}{T_{init}}) \tag{5}$$

where H is the Heaviside function, and

$$f(x) = \begin{cases} 1 & \text{if } x \text{ integer,} \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

2. We assume that breakup begins at T_{init} and the droplet reaches total breakup at T_{tot}. The time between the beginning and end of breakup is therefore $T_{\mathrm{tot}} - T_{\mathrm{init}}$. The breakup process will then be considered continuous and linear. Thus:

$$\frac{dr}{dt} = H(\mathrm{We} - \mathrm{We_{crit}}) \cdot \frac{r_{\mathrm{child}} - r}{T_{\mathrm{tot}} - T_{\mathrm{init}}} \tag{7}$$

3. Reitz Model (with RD) [6] [2]

Here, droplet fragmentation is caused by instabilities that develop at the liquid-gas interface. Reitz focuses on the linear model of Kelvin-Helmholtz instabilities.

We then define the wavelength of instabilities Λ and the fastest growing instability or "fastest growing wave" Ω:

$$\Lambda = 9.02a \frac{(1 + 0.45Z^{0.5})(1 + 0.4T^{0.7})}{(1 + 0.87\mathrm{We_2}^{1.67})^{0.6}} \tag{8}$$

$$\Omega = \left[\frac{\sigma}{\rho_1 a^3}\right]^{0.5} \frac{(0.34 + 0.38\mathrm{We_2}^{1.5})}{(1 + Z)(1 + 1.4T^{0.6})} \tag{9}$$

with:

$$Z = \mathrm{Oh_1} = \frac{\mathrm{We_1}^{0.5}}{\mathrm{Re_1}} \tag{10}$$

$$T = Z \cdot \mathrm{We_2}^{0.5} \tag{11}$$

where index 1 designates the liquid, 2 the gas, and a is the radius of the parent droplet.

The radius of the child droplet r_{child} from a parent droplet of radius a is thus defined:

$$r_{\mathrm{child}} = \begin{cases} B_0\Lambda & \text{if } B_0\Lambda \leq a \\ \min\left\{\left(\frac{3\pi a^2 U_{\mathrm{rel}}}{2}\right)^{1/3}, \left(\frac{3a^2}{4}\right)^{1/3}\right\} & \text{if } B_0\Lambda > a \end{cases} \tag{12}$$

with $B_0 = 0.61$.

The second equation applies to droplets larger than the jet and it is assumed that the jet creates a droplet with a frequency of $\Omega/2\pi$. Here we will consider that the jet is assimilated to a droplet with diameter equal to the jet diameter.

We now define the limits of bag breakup and shear breakup:

$$\text{Bag Breakup :} \quad \mathrm{We_2} \geq 6 \tag{13}$$

$$\text{Shear Breakup :} \quad \frac{\mathrm{We_2}}{\sqrt{\mathrm{Re_2}}} \geq 0.5 \tag{14}$$

We therefore obtain the following evolution:

$$\frac{dr}{dt} = H(\mathrm{We_2} - 6)\left(1 - H\left(\frac{\mathrm{We_2}}{\sqrt{\mathrm{Re_2}}} - 0.5\right)\right)\frac{r_{\mathrm{child}} - r}{\tau_{\mathrm{bag}}} + H\left(\frac{\mathrm{We_2}}{\sqrt{\mathrm{Re_2}}} - 0.5\right)\frac{r_{\mathrm{child}} - r}{\tau_{\mathrm{shear}}} \tag{15}$$

with:

$$\tau = \begin{cases} \pi\left[\frac{\rho_1 a^3}{2\sigma}\right]^{0.5} & \text{bag regime} \\ \frac{B_1 a}{U_{\mathrm{rel}}}\left(\frac{\rho_1}{\rho_2}\right)^{0.5} & \text{shear regime} \end{cases} \tag{16}$$

where $B_1 = 1.8$ or $\sqrt{3}$ (O'Rourke) or 8 (Nicholls).

Now, it is worth noting that the characteristic times τ_{bag} and τ_{shear} presented here have not been determined by the linear analysis of Kelvin-Helmholtz instabilities, nor have the transition criteria between the bag regime and the shear regime. Therefore, we can use these times and

criteria for other situations. In reality, the basic Reitz and Diwakar (RD) model does not include linear instability analysis, which is actually only useful for determining r_{child}. The RD model states the characteristic times and transition criteria. Therefore, we will keep in mind that, if droplet fragmentation is not due to KH instabilities, we can simply adapt r_{child} and remain consistent with the RD model.

4. KH-RT Model [7]

The objective of this model is to combine the linear analysis of Kelvin-Helmholtz (KH) instabilities with the study of Rayleigh-Taylor (RT) instabilities. Therefore, such a model could, in theory, model both primary atomization mechanisms (mainly KH) and secondary atomization mechanisms (mainly RT). However, it should be noted that the model now becomes more complex and this may impact the speed of calculations for a simulation. Moreover, the model depends on constants that are determined empirically. Therefore, I invite the reader to be cautious about using such a model and in choosing these constants, which must remain consistent with the assumptions, physical conditions...

4.0.1 KH Instability

Can be considered for secondary atomization if the droplets are large enough, but we practically fall back into primary atomization.

$$r_{\text{child}} = B_0 \Lambda_{\text{KH}} \quad \text{where } B_0 = 0.61 \tag{17}$$

$$\Omega_{\text{KH}} = \left[\frac{\sigma}{\rho_1 a^3}\right]^{0.5} \frac{(0.34 + 0.38\text{We}_2^{1.5})}{(1+Z)(1+1.4T^{0.6})} \tag{18}$$

$$\Lambda_{\text{KH}} = 9.02a \frac{(1+0.45Z^{0.5})(1+0.4T^{0.7})}{(1+0.87\text{We}_2^{1.67})^{0.6}} \tag{19}$$

$$\tau_{\text{KH}} = \frac{3.726 B_1 a}{\Lambda_{\text{KH}} \Omega_{\text{KH}}} \quad \text{where } 10 \leq B_1 \leq 60 \tag{20}$$

4.0.2 RT Instability

Rather the one involved in secondary atomization.

$$\Omega_{\text{RT}} = \sqrt{\frac{2}{3\sqrt{3}\sigma} \frac{|g_t(\rho_l - \rho_g)|^{3/2}}{\rho_g + \rho_l}} \tag{21}$$

$$g_t = \frac{3 C_D \rho_g (u - u_g)^2}{4 \rho_l d_p} \tag{22}$$

Corresponding wave number:

$$K_{\text{RT}} = \sqrt{\frac{|g_t(\rho_l - \rho_g)|}{3\sigma}} \tag{23}$$

Corresponding wavelength:

$$\Lambda_{\text{RT}} = \frac{2\pi C_{\text{RT}}}{K_{\text{RT}}} \tag{24}$$

Corresponding characteristic quantities:

$$\tau_{\text{RT}} = \frac{C_\tau}{\Omega_{\text{RT}}} \quad \text{where } C_\tau = 9 \tag{25}$$

$$r_{\text{child}} = \frac{\pi C_{\text{RT}}}{K_{\text{RT}}} \quad \text{where } C_{\text{RT}} = 0.1 \tag{26}$$

A fragmentation criterion proposed in this article is to use the length in Levich theory and consider that there is breakup if the droplet diameter is greater than the Levich length. However, this is valid for non-viscous flows and very high Weber numbers. Numerically, we find that this criterion does not work in our case and we will therefore take the Weber criterion from Pilch.

The temporal evolution of the droplet radius is therefore:

$$\frac{dr}{dt} = H(\text{We}-\text{We}_{\text{crit}}) \left[\left(1 - H\left(r - \frac{\Lambda_{\text{RT}}}{2}\right)\right) \frac{r_{\text{child,KH}} - r}{\tau_{\text{KH}}} + H\left(r - \frac{\Lambda_{\text{RT}}}{2}\right) \frac{r_{\text{child,RT}} - r}{\tau_{\text{RT}}} \right] \tag{27}$$

4.1 Viscous RT Instability Case [1]

In our simulations, we notice that the Ohnesorge number is not negligible and therefore viscous effects must be taken into account. However, in the previous RT theory, viscous effects are neglected. These have the influence of damping instabilities at the liquid-gas interface. We will still limit ourselves to not too significant damping, which is a correct approximation in our case. When we fall into the case of KH instabilities, that is, for large droplets, the Ohnesorge becomes small again and we can neglect viscous effects again.

Ω_{RT} which we call here n satisfies the following equation:

$$n^2 + 2\nu k^2 n - \sigma^2 = 0 \tag{28}$$

where $k^2 \gg \sigma^2$ (also valid for $k^2 \sim \sigma^2$), k is the wave number (K_{RT}) of the instability, $\nu = \mu/\rho$ kinematic viscosity and:

$$\sigma^2 = \frac{|(\rho_l - \rho_g) g_t|}{(\rho_l + \rho_g) k} - \frac{\sigma_l k^3}{\rho_l + \rho_g} \tag{29}$$

We will subsequently neglect the term $\left(-\frac{\sigma_l k^3}{\rho_l + \rho_g}\right)$.

Hence:

$$n = \sqrt{\nu^2 k^4 + \sigma^2} - \nu k^2 \tag{30}$$

We thus obtain the wavelength and wave number corresponding to the maximum of n:

$$\Lambda_m = \frac{2\pi}{k_m} = 4\pi \left(\frac{\nu^2}{g'}\right)^{1/3} \tag{31}$$

$$g' = \frac{|(\rho_l - \rho_g) g_t|}{\rho_l + \rho_g} \tag{32}$$

$$\tag{33}$$

Then, we can define our characteristic quantities:

$$\tau_{\text{RT,visq}} = \frac{C_\tau}{n_m} \text{ where } n_m = \sqrt{\nu^2 k_m^4 + \sigma^2} - \nu k_m^2 \tag{34}$$

$$r_{\text{child,RT,visq}} = C\frac{\Lambda_m}{2} \quad \text{where } C \text{ constant to be determined} \tag{35}$$

Thus, the temporal evolution of the droplet radius is:

$$\frac{dr}{dt} = H(\text{We}-\text{We}_{\text{crit}}) \left[\left(1 - H\left(r - \frac{\Lambda_m}{2}\right)\right) \frac{r_{\text{child,KH}} - r}{\tau_{\text{KH}}} + H\left(r - \frac{\Lambda_m}{2}\right) \frac{r_{\text{child,RT,visq}} - r}{\tau_{\text{RT,visq}}} \right] \tag{36}$$

5. TAB Model [3]

The TAB model is based on the analogy between the deformation of a droplet oscillating in a flow and the behavior of a mass-spring-damper system subjected to an external force. When a droplet is subjected to a gas flow, it undergoes progressive aerodynamic deformation that can lead to its breakup.

This dynamics is described by the following differential equation:

$$m_d \frac{d^2x}{dt^2} = -b\frac{dy}{dt} - kx + f \tag{37}$$

with the following parameters:

- $x(t)$: displacement of the droplet equator from its equilibrium position (m)
- m_d: droplet mass (kg)
- b: damping coefficient related to liquid viscosity $(\frac{Ns}{m})$
- k: stiffness coefficient related to surface tension $(\frac{N}{m})$
- f: external force due to aerodynamic shear (N)

By replacing the terms with the model parameters and introducing the dimensionless deformation $y = \frac{x}{C_b r_d}$, we obtain:

$$\frac{d^2y}{dt^2} = \frac{C_f}{C_R}\frac{\rho_g}{\rho_d r_d^3}|u_{rel}|^2 - C_k\frac{\sigma}{\rho_d r_d^3}y - C_b\frac{\mu_d}{\rho_d r_d^2}\frac{dy}{dt} \tag{38}$$

Where:

- $y(t)$: dimensionless deformation
- C_f, C_R, C_k, C_b: empirical coefficients (external force, surface tension, viscosity)
- σ: surface tension $(\frac{N}{m})$
- ρ_d: liquid density $(\frac{kg}{m^3})$
- r_d: parent droplet radius (m)
- u_{rel}: relative velocity between droplet and gas $(\frac{m}{s})$
- ρ_g: gas density $(\frac{kg}{m^3})$
- μ_d: liquid viscosity $(\frac{kg}{ms})$

Breakup occurs when y reaches a critical value, typically $y = 1$.

However, to be able to use this model, it is crucial to position oneself in the correct breakup regime. The vibrational breakup regime, $We < 12$, is preferred because the oscillations experienced are significant and the dominant forces of the system are those related to surface tension and aerodynamic forces.

Finally, to complete the model, we define the child droplet radius which is calculated with the Sauter mean radius r_{32} (or diameter d_{32}):

$$r_{32} = \frac{r_d}{\left(1 + \frac{8K}{20} + \frac{\rho_d r_d^3}{\sigma}\dot{y}^2 \cdot \frac{6K-5}{120}\right)} \tag{39}$$

Where:

- r_d: initial droplet radius before breakup (m)
- r_{32}: Sauter mean radius after breakup (m)
- $\dot{y}$: rate of change of deformation (dimensionless)
- K: empirical coefficient related to oscillation mode energy (typically $K = 10/3$)

Finally, I would like to point out to the reader the importance of knowing information about droplet deformation or the volume/surface ratio. Therefore, when applying a method of moments, it may be wise to add a third parameter in the droplet state space. The radius and velocity of the droplet alone will no longer be sufficient.

5.1 ETAB Model [9]

The purpose of the ETAB model is, as its name indicates, to extend the validity domain of the TAB model to more regimes. Thus, it is also valid for the bag regime. However, this model is not valid for more violent regimes, that is, starting from the shear regimes.

In the ETAB breakup model, the rate of change of the droplet diameter is computed from:

$$\frac{r}{a} = e^{-K_{br}t} \tag{40}$$

where a and r are the radii of the parent and product drops, respectively. The breakup constant K_{br} depends on the breakup regime according to the Weber number as follows:

$$K_{br} = \begin{cases} k_1\,\omega & \text{if } We \le We_t, \\ k_2\,\omega\sqrt{We} & \text{if } We > We_t. \end{cases} \tag{41}$$

Here, k_1 and k_2 are constants, ω is the drop oscillation angular velocity, and $We_t = 80$ is the transitional Weber number.

The deformation of the drop surface is computed as:

$$y(t) = \frac{We}{12} + e^{-\frac{t}{t_d}} \left[\left(y(0) - \frac{We}{12} \right) \cos(\omega t) + \left(\frac{\dot{y}(0)}{\omega} + \frac{y(0) - We/12}{\omega t_d} \right) \sin(\omega t) \right] \quad (42)$$

Breakup occurs if the normalized drop distortion $y(t)$ exceeds the critical value 1. Note that $y = 2x/a$, where x is the actual drop displacement of the equator.

After breakup, the product droplets are initially supplied with a velocity component perpendicular to the path of the parent drop:

$$v_\perp = A\dot{x}, \quad (43)$$

where $\dot{x}$ is the radial velocity of the drop surface. The constant A is determined from the energy conservation criterion:

$$A^2 = \frac{5C_D}{4} + 18(1 - a/r_{32})We. \quad (44)$$

Here, C_D is the aerodynamic drag coefficient and r_{32} is the Sauter mean radius (SMR). In the original TAB model, $A = 1$, whereas in ETAB $A \approx 0.7$ for typical high-pressure injection.

To account for droplet surface stripping near the nozzle exit, the size distribution is given by:

$$g(r) = \frac{n+4}{r_0} \left(\frac{r}{r_0} \right)^{n+3}, \quad (45)$$

where r_0 is the nozzle radius and $n = 0.5$ has been determined computationally to fit experimental data.

This gives a mass distribution where most of the injected fuel mass is in the large droplets.

Constant	Explanation	Used	Default
C_α	Initial jet breakup angle	4.5	1.56
C_λ	Jet breakup length	5.5	5.5
k_1	Bag breakup regime	0.2222	0.2222
k_2	Stripping breakup regime	0.2222	0.2222
n	Exponent of size distribution	0.5	0.5

Table 1: ETAB model constants

6. FAST Model for Atomization [10]

The **FAST** model (Fractal–Atomization–Spray–Theory), proposed by Gorokhovski and Saveliev, is based on the Kolmogorov scenario (1941) applied to droplet fragmentation at *high Weber numbers*. It considers the breakup process as a succession of independent random events, leading to a self-similar distribution of droplet sizes.

We introduce the distribution function $F(r,t)$ representing the number of droplets of radius r at time t. The population balance is written as:

$$\frac{\partial F(r,t)}{\partial t} = \left(q_0 \hat{I}_+ - 1 \right) \nu_0 F(r,t), \quad (46)$$

where:

- q_0: average number of fragments produced by a breakup,
- ν_0: average breakup frequency,
- $\hat{I}_+$: fragmentation operator defined by

$$\hat{I}_+ F = \int_0^1 F\left(\frac{r}{a}\right) q(a) \frac{da}{a}, \quad (47)$$

with $q(a)$ the probability density of radius sharing (a fraction of parent radius).

We define the l-th moment by:

$$\langle r^l \rangle(t) = \int_0^\infty r^l F(r,t)\, dr. \quad (48)$$

By multiplying (46) by r^l and integrating, we obtain:

$$\frac{d}{dt}\langle r^l \rangle = \nu_0 \left(q_0 \langle a^l \rangle - 1 \right) \langle r^l \rangle, \quad (49)$$

where $\langle a^l \rangle = \int_0^1 a^l q(a)\, da$.

Mass conservation imposes:

$$\langle a^3 \rangle = \frac{1}{q_0}. \quad (50)$$

Putting l=0 leads to the equation for the droplet number density n:

$$\frac{\partial n}{\partial t} = \nu_0 (q_0 - 1) \cdot n \quad (51)$$

And so, we define the normalized distribution function $f(r,t) = \frac{F(r,t)}{n}$ and the frequency of production of new droplets $\nu = \nu_0 q_0$.

Using the Lyapunov theorem and the scale invariance hypothesis, the asymptotic solution of (46) tends towards a log-normal law:

$$f(r,t) \xrightarrow[t\to\infty]{} \frac{1}{r\sqrt{2\pi \langle (\ln a)^2 \rangle \nu t}} \times \exp\left[-\frac{(\ln(r/R)^2 + \langle \ln a \rangle \nu t)^2}{2\langle (\ln a)^2 \rangle \nu t} \right] \left(\frac{R}{r} \right)^{1 - \frac{\langle \ln a \rangle}{\langle (\ln a)^2 \rangle}} \quad (52)$$

which evolves towards a power law:

$$f(r,t) \xrightarrow[t\to\infty]{} \frac{1}{r^{1-\theta}}, \qquad \theta = \frac{\langle \ln a \rangle}{\langle (\ln a)^2 \rangle}. \quad (53)$$

Thus, the FAST model describes the droplet size distribution as an evolution from a log-normal law to a power law, characteristic of atomization regimes. I invite the reader to read the associated article for more details and rigor, as the study does not stop at the solution mentioned.

7. Useful study on Population Balance Equation for Atomization [8]

7.1 The Classical Population Balance Framework

At the core of the book lies the **Population Balance Equation (PBE)**, which tracks the evolution of the number density function $f(\mathbf{x}, t)$ of particles with internal state vector $\mathbf{x}$:

$$\frac{\partial f(\mathbf{x},t)}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{R}(\mathbf{x},t)\, f(\mathbf{x},t)) = B(\mathbf{x},t) - D(\mathbf{x},t), \quad (54)$$

where:

- $\mathbf{x}$: particle state vector (e.g., size, age, composition),
- $\mathbf{R}(\mathbf{x}, t)$: rate of change of the particle state (growth or shrinkage),
- $B(\mathbf{x}, t)$: birth rate of particles of state $\mathbf{x}$,
- $D(\mathbf{x}, t)$: death rate of particles of state $\mathbf{x}$.

7.2 Breakage Term in the PBE

The net birth rate due to breakage processes, $h(x, t)$, is expressed as the difference between a *source* term $h^+(x, t)$ and a *sink* term $h^-(x, t)$:

$$h(x,t) = h^+(x,t) - h^-(x,t) = B(x,t) - D(x,t). \quad (55)$$

The sink term represents the loss of particles of size x due to their own fragmentation:

$$h^-(x,t) = b(x)\, f(x,t), \quad (56)$$

where $b(x)$ is the *specific breakage rate*, i.e. the fraction of particles of size x breaking per unit time.

The source term accounts for the birth of new particles of size x resulting from the breakage of larger particles x':

$$h^+(x,t) = \int_x^\infty b(x')\, v(x')\, P(x|x')\, f(x',t)\, dx', \quad (57)$$

where:

- $v(x')$: average number of fragments produced from a particle of size x',
- $P(x|x')$: daughter distribution function giving the probability density that a particle of size x' produces a fragment of size x,
- $b(x')$: breakage frequency of particles of size x'.

Thus, the breakage contribution to the population balance is:

$$h(x,t) = B(x,t) - D(x,t)$$
$$= \int_x^\infty b(x')\, v(x')\, P(x|x')\, f(x',t)\, dx' - b(x)\, f(x,t). \quad (58)$$

An important constraint for physical consistency is the **mass conservation condition**:

$$\int_0^{x'} x\, P(x|x')\, dx = x', \quad (59)$$

ensuring that the total mass of fragments equals the mass of the parent particle.

7.3 Relevance to Atomization Studies

In the context of liquid atomization, this framework provides a rigorous way to model the dynamics of droplet size distributions. In particular, the detailed formulation of **breakage kernels** is crucial for predicting secondary atomization phenomena. The book's comprehensive treatment of birth and death functions thus directly informs the modeling strategy used in this work.

References

[1] Plesset, M. S., & Whipple, C. G. (1973). Viscous effects in Rayleigh–Taylor instability. *Physics of Fluids*, 17(1), 1–8.

[2] Nicholls, J. A. (1969). Two phase detonation as related to rocket motor combustion instability. NASA Contractor Report CR-72532, University of Michigan.

[3] O'Rourke, P. J., & Amsden, A. A. (1986). The TAB method for numerical calculation of spray droplet breakup. Los Alamos National Laboratory Report LA-UR-87-2105.

[4] Reitz, R. D., & Diwakar, R. (1986). Effect of drop breakup on fuel sprays. *SAE Transactions*, 95(3), 218–227.

[5] Pilch, M., Erdman, C. A., & Reynolds, A. B. (1981). Acceleration induced fragmentation of liquid drops. NUREG/CR-2247, U.S. Nuclear Regulatory Commission.

[6] Reitz, R. D. (1987). Modeling atomization processes in high-pressure vaporizing sprays. *Atomization and Spray Technology*, 3, 309–337.

[7] Beale, J. C., & Reitz, R. D. (1999). Modeling spray atomization with the Kelvin–Helmholtz/Rayleigh–Taylor hybrid model. *Atomization and Sprays*, submitted February 1999.

[8] Ramkrishna, D. (2000). *Population Balances: Theory and Applications to Particulate Systems in Engineering*. Academic Press, San Diego.

[9] Kaario, O., Tanner, F., Larmi, M., & other co-authors. (2002). Non-evaporating liquid spray simulations with the ETAB and WAVE droplet breakup models. *Atomization and Sprays*, 12(1), 1–15.

[10] Gorokhovski, M., & Saveliev, V. L. (2003). Analyses of Kolmogorov's model of breakup and its application into Lagrangian computation of liquid sprays under air-blast atomization. *Physics of Fluids*, 15(1), 184–192.