Deformation and Secondary Atomization of Droplets in Technical Two-Phase Flows
Outline

- Introduction
- Basics
- Empirical description
- Normal Mode Analysis
- Nonlinear deformation analysis
- Potential Theory Breakup model
- Motion of deformed droplets
- Validation of deformation models
- Modeling of droplet breakup
- Validation of breakup models
- Summary
Air assisted pressure swirl atomizer

Liquid: Tetradecane

$D_0 = 60 \mu m$

We$_0 \approx 15$
Low relative velocities

- Shape oscillations
- Forced deformations

Image source: Wiegand (1987)

Moderate to high relative velocities (top to bottom)

- Bag breakup
- Bag-plume breakup
- Plume-sheet breakup
- Sheet-thinning breakup

Image source & terminology: Guildenbecher (2009)
Forces acting \textit{on} and \textit{in} the droplet

- Surface tension
- Inertial forces
- Aerodynamic forces
- Viscous forces
<table>
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<tr>
<th>Moderate velocities</th>
<th>High velocities</th>
<th>Extremly high velocities</th>
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<tr>
<td>Transverse deformation by aerodynamic pressure distribution</td>
<td>Superposed separation of liquid by aerodynamic shear forces</td>
<td>Superposed hydrodynamic instability of front surface</td>
</tr>
</tbody>
</table>
Non-dimensional numbers

\[
\text{We} = \frac{\rho v_{\text{rel}}^2 D_0}{\sigma} \quad \text{Weber number}
\]

\[
\text{Re}_{\text{def}} = \frac{v_{\text{rel}} D_0}{\mu_d} \sqrt{\frac{\rho}{\rho_d}} \quad \text{Reynolds number of deformational flow}
\]

\[
\text{On} = \frac{\mu_d}{\sqrt{\rho_d D_0 \sigma_d}} \quad \text{Ohnesorge number} \left( = \frac{\sqrt{\text{We}}}{\text{Re}_{\text{def}}} \right)
\]

Characteristic times

\[
t^* = \sqrt{\frac{\rho_d}{\rho} \frac{D_0}{v_{\text{rel}}}} \quad \text{Pressure distribution} \leftrightarrow \text{Inertia forces}
\]

\[
t^*_\sigma = \sqrt{\frac{D_0^3 \rho_d}{\sigma}} \quad \text{Surface tension} \leftrightarrow \text{Inertia forces}
\]

\[
t^*_\mu = \frac{\mu_d}{\rho v_{\text{rel}}^2} \quad \text{Pressure distribution} \leftrightarrow \text{Dissipation}
\]

\[
t^*_v = \frac{D_0}{v_{\text{rel}}} \quad \text{Flow around droplet}
\]
Droplet in shock tube flow
Droplet in free fall
Droplet in premix module
Droplet in rocket engine preflow

\[ W_e = \frac{t}{t_{\sigma}} \]
## Classification of numerical models

<table>
<thead>
<tr>
<th>Model Type</th>
<th>Description</th>
<th>Advantages</th>
<th>Disadvantages</th>
<th>Applicability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical description</td>
<td>Correlations and similarity laws for description of droplet deformation.</td>
<td>+ Arbitrary deformations</td>
<td>− Limited to specific loading scenarios</td>
<td>Limited use for modeling</td>
</tr>
<tr>
<td>Simple mechanistic models</td>
<td>Deformation kinematics reduced to single degree of freedom: Droplet shapes approximated by spheroids.</td>
<td>+ Specific small &amp; large deformations</td>
<td>− Fitting of empirical constants required</td>
<td>Suitable for modeling</td>
</tr>
<tr>
<td>Normal mode analysis</td>
<td>Modal discretization of aerodynamic pressure distribution, kinematics and dynamics of deformation.</td>
<td>+ Small but arbitrary deformations</td>
<td>− Neglects nonlinear effects</td>
<td>Suitable for modeling</td>
</tr>
<tr>
<td>Direct numerical simulation</td>
<td>Spatial and temporal discretization of the Navier-Stokes equations in both phases.</td>
<td>+ Arbitrary deformation</td>
<td>− Extremely high computational effort</td>
<td>Can not be used for modeling</td>
</tr>
</tbody>
</table>
Empirical description

Load-based classification: On-We diagram

- Shear breakup
- Transitional breakup
- Bag-plume breakup
- Bag breakup
- Shape oscillations
- Deformation < 5%
- Deformation 5-10%
- Deformation 10-20%
- Deformation > 20%

Krzeczkowski (1980)
Hsiang & Faeth (1995)

\[ \rho_d / \rho = 580 - 12000 \]
\[ Re_0 = 240 - 16000 \]
Empirical description

Load-based classification: We-WeRe$^{-0.5}$ diagram


1. Bag breakup
2. Bag-plume breakup
3. Transitional breakup
4. Shear breakup

Pressure ranges:
- $p \approx 0.1\,\text{MPa}$
- $p \ll 0.1\,\text{MPa}$
- $p > 0.1\,\text{MPa}$
Empirical description

Temporal stages

Data source: Krzeczkowski (1980), Dai & Faeth (2001)
Root-normal distribution:
\[ f(x) = \frac{1}{2\sigma \sqrt{2\pi} x} \exp \left[ -\frac{1}{2} \left( \frac{\sqrt{x} - \mu}{\sigma} \right)^2 \right] \]
with \[ \frac{D_{0.5}}{D_{32}} = 1.2, \quad \mu = 1.0, \quad \sigma = 0.22. \]
Sauter diameter: \( \frac{D_{32}}{D_0} = 6.2 \text{ On}^{0.5} \text{ We}^{-0.25} = \text{Re}_{def}^{-0.5} \), On < 0.1, We_0 < 10^3.

Empirical description

Secondary droplet properties - differentiated by origin

Data source: Dai & Faeth (2001)
Decomposition of an arbitrary axisymmetric droplet shape into orthogonal deformation modes
Linearized Navier-Stokes equations

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 v_r \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (v_\theta \sin \theta) = 0
\]

\[
\rho_d \frac{\partial v_r}{\partial t} = -\frac{\partial p}{\partial r} + \mu_d \left[ \nabla^2 v_r - \frac{2}{r^2} v_r - \frac{2}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (v_\theta \sin \theta) \right] + \rho_d a \cos \theta
\]

\[
\rho_d \frac{\partial v_\theta}{\partial t} = -\frac{\partial p}{r \partial \theta} + \mu_d \left[ \nabla^2 v_\theta + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} - \frac{1}{r^2 \sin \theta} v_\theta \right] - \rho_d a \sin \theta
\]

Series expansion \((v = \nabla \psi)\)

\[
p_s - p_\infty = \frac{\rho v_{rel}^2}{2} \sum_{n=0}^{\infty} C_n P_n(\cos \theta)
\]

\[
p = \frac{\rho v_{rel}^2}{2} \sum_{n=0}^{\infty} \beta_n \left( \frac{r}{R} \right)^n P_n(\cos \theta)
\]

\[
\delta_r = R \sum_{n=0}^{\infty} \alpha_n \left( \frac{r}{R} \right)^{n-1} P_n(\cos \theta)
\]

Deformation equations \((n \geq 2)\) formulated on nondimensional time scale \(T_\sigma = t/t_{\sigma}^*\)

\[
\frac{d^2 \alpha_n}{dT_\sigma^2} + 8n(n-1)O_n \frac{d\alpha_n}{dT_\sigma} + 8n(n-1)(n+2)\alpha_n = -2nC_n\text{We} \quad (\text{Hinze 1948})
\]

\[
\frac{d^2 \alpha_n}{dT_\sigma^2} + 8(2n+1)(n-1)O_n \frac{d\alpha_n}{dT_\sigma} + 8n(n-1)(n+2)\alpha_n = -2nC_n\text{We} \quad (\text{Isshiki 1959})
\]

\(\sim\) Viscous term different in both theories !
Normal Mode Analysis

Pressure distribution on spherical surface

\[ p_s - p_\infty = \frac{\rho v_{rel}^2}{2} \]

- \( Re=50 \), Tomboulides und Orszag (2001)
- \( Re=100 \), Tomboulides und Orszag (2001)
- \( Re=500 \), Bagchi et al. (2001)
- \( Re=10^4 \), Constantinescu und Squires (2000)
- \( Re=1.62 \cdot 10^5 \), Achenbach (1972)

potential flow
Modal representation of pressure boundary condition

- Transition lamin.-turb.
- Wake unsteady
- Wake asymmetric
- Flow separation
- Rigid sphere, in uniform flow
Water droplet in vertical air flow (Pruppacher et al. 1970)

<table>
<thead>
<tr>
<th>$D_0$ [mm]</th>
<th>8.00</th>
<th>7.35</th>
<th>5.80</th>
<th>5.30</th>
<th>3.45</th>
<th>2.70</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_{rel}$ [m/s]</td>
<td>9.20</td>
<td>9.20</td>
<td>9.17</td>
<td>9.13</td>
<td>8.46</td>
<td>7.70</td>
</tr>
<tr>
<td>We</td>
<td>11.1</td>
<td>10.2</td>
<td>8.0</td>
<td>7.3</td>
<td>4.1</td>
<td>2.6</td>
</tr>
<tr>
<td>Re</td>
<td>4723</td>
<td>4340</td>
<td>3413</td>
<td>3105</td>
<td>1873</td>
<td>1334</td>
</tr>
</tbody>
</table>
Water droplet in horizontal shock tube flow: $D_0 = 1\text{mm}$, $\text{On} = 3.38 \cdot 10^{-3}$

<table>
<thead>
<tr>
<th>We:</th>
<th>1</th>
<th>5</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Re_{def}$</td>
<td>296</td>
<td>662</td>
<td>1025</td>
</tr>
<tr>
<td>Re:</td>
<td>491</td>
<td>1099</td>
<td>1701</td>
</tr>
<tr>
<td>$v_{rel}$</td>
<td>7.7 m/s</td>
<td>17.2 m/s</td>
<td>26.68 m/s</td>
</tr>
</tbody>
</table>
Linear analysis: First order theory \(\implies\) Forces and displacements at undeformed droplet

Nonlinear analysis: Second order theory \(\implies\) Forces and displacements dependent on deformation

Nonlinear phenomena:

- Mode coupling, excitation of higher modes
- Oscillation dynamics depends on amplitude (frequency and period)
- Nonlinear resonance effects
- Hydrodynamic instabilities
Dynamic equilibrium of mechanical energy contributions

\[
\frac{\rho_d}{2} \frac{d}{dt} \int_V v^2 dV + \sigma \frac{dS}{dt} = -\oint_S p_s v \cdot n dS - \int_V \Phi dV \quad \implies \quad F(y, \dot{y}, \ddot{y}) = 0
\]
Potential energy of surface: polynomial approximation

\[
\sigma \frac{dS}{dt} = \sigma \frac{dS}{dy} \frac{dy}{dt}, \quad \frac{1}{S_0} \frac{dS}{dy} = \begin{cases} 
9.98y^3 - 30.34y^2 + 33.94y - 13.58, & 0.5 < y < 1, \\
0.67y^3 - 4.01y^2 + 9.21y - 5.67, & 1 \leq y < 2.3.
\end{cases}
\]

Kinetic energy: viscous potential flow

\[
\frac{\rho_d}{2} \frac{d}{dt} \int_V v^2 dV = \frac{8}{5} \rho_d R^5 \left[ \frac{1}{3} \left( 1 + \frac{2}{y^6} \right) \frac{d^2y}{dt^2} - \frac{2}{y^3} \left( \frac{dy}{dt} \right)^2 \right] \frac{dy}{dt}
\]

Viscous dissipation: viscous potential flow

\[
\int_V \Phi dV = 12 \mu_d \int_V \left( \frac{\partial v_2}{\partial x_2} \right)^2 dV = 16\pi R^3 \mu_d \left( \frac{1}{y} \frac{dy}{dt} \right)^2
\]
Velocity potential on surface: stationary external flow

\[ \psi_s = \frac{2}{2 - \gamma_0} v_{rel} x_3 , \quad \gamma_0 = \begin{cases} \frac{2}{e^2} \left( \frac{\text{artanh } e}{e} - 1 \right), & y < 1, \\ \frac{2}{e^2} \left( 1 - \sqrt{1 - e^2} \frac{\text{arcsin } e}{e} \right), & y > 1. \end{cases} \]

Pressure distribution on surface

\[ \frac{p_s - p_\infty}{\rho/2v^2_{rel}} = 1 - \Delta \bar{p}_{\text{max}} \left( \frac{\partial x_3}{\partial s} \right)^2, \quad \left( \frac{\partial x_3}{\partial s} \right)^2 = \frac{1 - \xi^2}{1 - (1 - y^6)\xi^2}, \quad \begin{cases} s: \text{ Surface coordinate} \\ \xi: \text{ Non-dimensional axial coordinate} \end{cases} \]

Total work performed by aerodynamic pressure forces

\[ \oint_S p_s v \cdot n dS = -\frac{\rho v^2_{rel}}{2} 2\pi R^3 \Delta \bar{p}_{\text{max}} \frac{\lambda_0 dy}{y dt}, \quad \lambda_0 = \int_{-1}^{+1} \frac{1 - 4\xi^2 + 3\xi^4}{1 - (1 - y^6)\xi^2} d\xi = \begin{cases} \frac{2}{e^4} \left( 3 - e^2 \frac{\text{artanh } e}{e} - 3 \right), & y < 1 \\ \frac{2}{e^4} \left[ 3 - 2e^2 \frac{\text{arcsin } e}{e} - 3 \right], & y > 1 \end{cases} \]
Potential Theory Breakup model
Nonlinearity of aerodynamic load term

\[ C_2 = \frac{2}{3} \Delta p_{\text{max}} \], potential theory

\[ C_2 = \frac{2}{3} \Delta p_{\text{max}} \], CFD-simulation

\[ C_2 \lambda_0/y \], with \( C_2 \) from CFD-simulation

\[ C_2 \lambda_0/y \], polynomial approximation

\[ \lambda_0 \text{, exact} \]
\[ \lambda_0/y \text{, exact} \]

\[ \lambda_0, \lambda_0/y, C_2 \lambda_0/y \]
Taylor Analogy Breakup (TAB) model

\[
\frac{d^2 y}{d T_\sigma^2} + 40 \text{On} \frac{d y}{d T_\sigma} + 64 (y - 1) = 2C_2 \text{ We}
\]

Potential Theory Breakup (PTB) model

\[
\frac{1}{3} \left(1 + \frac{2}{y^6}\right) \frac{d^2 y}{d T_\sigma^2} - \frac{2}{y^7} \left(\frac{d y}{d T_\sigma}\right)^2 + 40 \text{On} \frac{1}{y^2} \frac{d y}{d T_\sigma} + 20 \frac{1}{S_0} \frac{d S}{d y} = \frac{15}{4} \frac{C_2 \lambda_0}{y} \text{ We}
\]
Equation of motion

\[ m_d \frac{d u_d}{d t} = \frac{\pi D^2}{8} \rho c_D \nu_{rel} \nu_{rel} + m_d g \]

Exposed cross section of droplet

\[ \pi D^2 = \pi D_0^2 y^2 \]

Aerodynamic drag coefficient

\[ c_D = f c_{D, sphere} + (1 - f) c_{D, disc} \]

\[ c_{D, sphere} = 0.36 + 5.48 \text{Re}^{-0.573} + \frac{24}{\text{Re}}, \quad \text{Re} \lesssim 10^4 \]

\[ c_{D, disc} = 1.1 + \frac{64}{\pi \text{Re}} \]

\[ f = 1 - E^2 \]
Wiegand (1987), experiment

Normal Mode Analysis
Motion of deformed droplets
Computed motion and deformation

Wiegand (1987)
Versuch 17-3W
Effect of viscous damping on free shape oscillations

Aspect ratio: \[ E = \frac{1 + \alpha_2}{1 - \frac{1}{2} \alpha_2}, \quad \text{Nomal Mode Analysis} \]
\[ E = \frac{1}{\gamma^3}, \quad \text{Spheroid-based models} \]
Validation of deformation models

Effect of increasing amplitude on free shape oscillations

NL T A B 3 model:

\[ \frac{\omega}{\omega_0} = \begin{cases} 0.0089 & \text{On} = 0.0089 \\ 0.0139 & \text{On} = 0.0139 \\ 0.0406 & \text{On} = 0.0406 \\ 0.0631 & \text{On} = 0.0631 \end{cases} \]

Frequency shift

Asymmetry of oscillation period
Validation of deformation models

Stationary deformation of droplets in free fall

\[ E_\infty = \frac{C_2}{3} \]

\[ u_d,\infty, c_{D, sphere} \]

\[ c_D(Re, We) \]

\[ \nu_{rel} \text{ prescribed} \]

\[ \text{coupled with droplet deformation} \]
Validation of deformation models

Maximum transverse distortion of droplets in shock tube flow

Slide 35
Validation of deformation models

Deformation of droplet in shock tube flow

- VOF method
- NM model

$\frac{S}{S_0}$ as a function of time $t$.

- NM model
- TAB model
- Output times

$\text{We} = 4.92, 9.83$
Validation of deformation models

Droplet falling through horizontal jet flow at $\text{We}_0 = 0.5$

Trajectories in laminar core flow

Trajectory data NLTAB3 model
Validation of deformation models

Droplet falling through horizontal jet flow at $\text{We}_0 = 3.3$

Trajectories in laminar core flow

Trajectory data NLTAB3 model
Validation of deformation models

Droplet falling through horizontal jet flow at $We_0 = 11.8$

Trajectories in laminar core flow

Trajectory data NLTAB3 model
Modeling of droplet breakup

Breakup criterion based on critical deformation

Leppinen et al. (1996), \( \text{We}_0 = 2 \), LLT-C
Kim (1977), \( \text{We}_0 = 12.6 \)
Dai & Faeth (2001), \( \text{We}_0 = 15 \)
Dai & Faeth (2001), \( \text{We}_0 = 20 \)
i, \( \text{NLTAB3} \)
i, empirical
\( y_{\max}, \text{PTB} \)
\( y_{\max}, \text{NLTAB3} \)
\( y_{\max}, \text{TAB} \)

\[ \frac{dy}{dT} = 0 \]

\[ \frac{dy}{dT} = 3.2 \]
Modeling of droplet breakup

Simulation of the On-We diagram

- Shear breakup: $W_e|_{y=1.8} = 69$
- Multimode breakup: $W_e|_{y=1.8} = 30$
- Stability limit: $y_{max} = 1.8$
- Critical damping: $c_D = c_D(Re)$

PTB, $c_D = c_D(Re)$
PTB, $c_D = c_D(Re,A)$
Hsiang & Faeth (1992), Exp.

PTB, $c_D = c_D(Re)$
We present a graphical representation of the modeling framework for droplet breakup. The diagram illustrates the relationship between the Weber number ($W_e$) and the deformation parameter ($\mu$), categorizing models into three types: Empirical models, Dynamic boundary layer models, and Dynamic deformation models. The graph shows how these models are distributed across different values of $W_e$ and $\mu$.
Validation of droplet breakup
Size distribution computed from differentiated model

We_0 = 15 (bag breakup)

We_0 = 125 (shear breakup)

- Air & Ethanol
- \( We = 68.5, \, On = 0.0076, \, Re = 4362 \)
- Software: OpenFOAM & Ladrop
- Dispersion model switched off
- Experimental data: Guildenbecher (2009)
Validation of droplet breakup

Comparison of load- and deformation-based simulations

breakup for $\text{We} > \text{We}_{0,c}$

breakup for $y > y_{\text{max}}$
Analytical models for description of linear and nonlinear deformation dynamics

Simple mechanistic approach for coupling of droplet deformation and motion

Empirical stability criteria, classification and kinematics of breakup process

Systematic validation and assessment of models based on fundamental test cases

Future: Test modelling framework within practical Euler-Lagrange simulations