Secondary Atomization Modeling by Fragmentation CQMOM vs Monte Carlo Comparison

Method of Moments with Fragmentation Source Term

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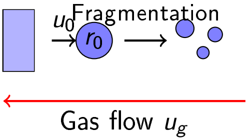
Presentation Outline

Context: Secondary Atomization

Problem Statement:

- Fuel injection
- Droplet fragmentation under aerodynamic effects
- Prediction of temporal evolution of droplet distribution



Objectives:

- Model a fragmentation model
- Solve using method of moments, specifically with CQMOM
- Validate simulation with Monte Carlo approach

Injection Configuration

Geometric Parameters:

- Nozzle diameter: $d_0 = 2$ mm
- Initial radius: $r_0 = 1$ mm
- Injection velocity: $u_0 = 100$ m/s
- Gas velocity: $u_g = -20$ m/s

Thermodynamic Conditions:

- Temperature: $T = 1200$ K
- Pressure: $P = 5$ bar
- High pressure configuration

Physical Properties:

Property	Gas	Liquid
Density (kg/m³)	5.16	800
Viscosity (Pa·s)	1.9×10^{-5}	1.5×10^{-3}

Surface tension: $\sigma_l = 25$ mN/m

Initial distribution:

- $\mu = [r_0, u_0]$
- Standard deviation 10% on radius and 5% on velocity
- 100 initial particles, max 25000

Characteristic Dimensionless Numbers

Definitions:

$$\mathrm{We} = \frac{\rho_g |u_r|^2 (2r)}{\sigma_l} \quad (1)$$

$$\mathrm{Re} = \frac{\rho_g |u_r| (2r)}{\mu_g} \quad (2)$$

$$\mathrm{Oh} = \frac{\sqrt{\mathrm{We}}}{\mathrm{Re}} \quad (3)$$

where $u_r = u - u_g$ is the relative velocity.

Fragmentation criterion:

$$\mathrm{We} > \mathrm{We}_{crit} = 12(1 + 1.077\mathrm{Oh}^{1.6})$$

Initial values:

- $\mathrm{We} = 1673.1$
- $\mathrm{Re} = 19.9$
- $\mathrm{Oh} = 2.0530$
- $\mathrm{We}_{crit} = 26.4$

Conclusion

$\mathrm{We} \gg \mathrm{We}_{crit}$
$\Rightarrow$ **Fragmentation expected**

Droplet Transport Equations

Radius evolution: $\frac{dr}{dt}$

- Reitz-Diwakar (RD) model with fragmentation
- Two modes: bag-mode and shear-mode
- Characteristic times:

$$\tau_{bag} = \pi \sqrt{\frac{\rho_l r^3}{2\sigma_l}} \tag{4}$$

$$\tau_{shear} = 1.8 \cdot r \sqrt{\frac{\rho_l}{\rho_g}} \cdot \frac{1}{|u_r|} \tag{5}$$

Velocity evolution: $\frac{du}{dt}$

$$\frac{du}{dt} = \frac{3}{8} C_D \frac{\rho_g}{\rho_l} \frac{1}{r} |u_g - u| (u_g - u) \tag{6}$$

where C_D is the drag coefficient as a function of Reynolds number.

Analytical Formulas of the drdt Model

Child radius:

$$r_{child} = 0.681 \cdot r \tag{7}$$

Final model:

$$\frac{dr}{dt} = H(\mathrm{We} - \mathrm{We}_{crit})(r_{child} - r)\left(\frac{H(\mathrm{We} - 6)(1 - H(\xi - 0.5))}{\tau_{bag}} + \frac{H(\xi - 0.5)}{\tau_{shear}}\right) \tag{8}$$

with $\xi = \mathrm{We}/\sqrt{\mathrm{Re}}$

Stochastic Fragmentation

Monte Carlo approach for fragmentation:

1. **Fragmentation detection for a single droplet:**
   - Frequency criterion: Fragmentation is allowed at frequency $\frac{1}{\tau_{bag}}$ or $\frac{1}{\tau_{shear}}$ for each droplet.
   - Volumetric criterion: $\sum V_{current} \leq V_{initial}$
   - Number criterion: $N_{droplets} \leq 200$ for a single initial droplet
   - Weber criterion: $\mathrm{We} > \mathrm{We}_{crit}$
2. **Number of daughter droplets:**
   - Truncated log-normal law
   - Privileged fragmentation into 2 or 3 droplets: $\mu = 2, \sigma = 1$
   - Domain: $[1, 5]$ daughter droplets
3. **Daughter droplet sizes:**
   - Log-normal distribution of volumes: $\mu = V_{initial}/(N_{daughters} + 1), \sigma = \mu/12$
   - Strict mass conservation
   - Constraint: $\sum V_{daughter} < 0.95 \cdot V_{initial}$ to ensure current droplet has defined volume
4. **Reset and loop:**
   - For an isolated droplet, we preserve information about number of daughter droplets and their respective sizes until fragmentation
   - When fragmentation occurs according to criterion, we recalculate for our initial droplet and all daughter droplets their number of child droplets with respective sizes
   - We loop this process, which will be stopped by the fragmentation criterion.

CQMOM Method with Source Term

Moment evolution:

$$\frac{\partial M_{ij}}{\partial t} = \underbrace{\sum_k w_k f_k^{(i,j)}}_{\text{Transport}} + \underbrace{S_{ij}}_{\text{Fragmentation source}} \tag{9}$$

Fragmentation source term:

- Based on CQMOM quadrature: $\{w_k, r_k, u_k\}$
- Birth and death rates at nodes
- Integration over log-normal distribution of products

$$S_{ij} = \sum_k w_k \left[\underbrace{B_{ij}(r_k, u_k; t)}_{\text{Birth}} - \underbrace{D(r_k, u_k; t)}_{\text{Death}} \right] \tag{10}$$

Analytical Formulas of Source Term

Fragmentation source term:

$$S_{ij} = \sum_k w_k \left[\underbrace{B_{ij}(r_k, u_k; t)}_{\text{Birth}} - \underbrace{D_{ij}(r_k, u_k; t)}_{\text{Death}} \right] \tag{11}$$

Birth term:

$$B_{ij}(r_k, u_k; t) = N_{frag} \cdot \Gamma(r_k, u_k; t) \cdot I_{ij}(r_k, u_k) \tag{12}$$

$$I_{ij}(u_k) = u_k^j \cdot \left(\frac{3}{4\pi}\right)^{i/3} e^{\frac{i\mu_{ln}}{3} + \frac{1}{2}\left(\frac{i\sigma_{ln}}{3}\right)^2} \tag{13}$$

Log-normal distribution: $\mu_{ln} = \ln\left(\frac{V_{mean}^2}{\sqrt{\sigma_V^2 + V_{mean}^2}}\right)$, $\sigma_{ln} = \sqrt{\ln\left(1 + \frac{\sigma_V^2}{V_{mean}^2}\right)}$

with $V_{mean} = \frac{V_k}{N_{frag}+1}$, $\sigma_V = \frac{V_k}{(N_{frag}+1)\times 12}$, $V_k = \frac{4}{3}\pi r_k^3$.

Fragmentation rate:

$$\Gamma(r_k, u_k; t) = H(\mathrm{We} - \mathrm{We}_{crit}) \left(\frac{H(\mathrm{We} - 6)(1 - H(\xi - 0.5))}{\tau_{bag}} + \frac{H(\xi - 0.5)}{\tau_{shear}} \right) \tag{14}$$

Parameter: $N_{frag} \approx 3.4$ (average value of number of droplets generated)

Death term: $D_{ij}(r_k, u_k; t) = r_k^i \cdot u_k^j \cdot \Gamma(r_k, u_k; t)$

Simulation Parameters

Numerical configuration:

- Time step: $\Delta t = 0.5\mu s$
- Total duration: 3 ms
- Initial particles: 100
- Max particles: 25000
- Method: DOP853 (Runge-Kutta)

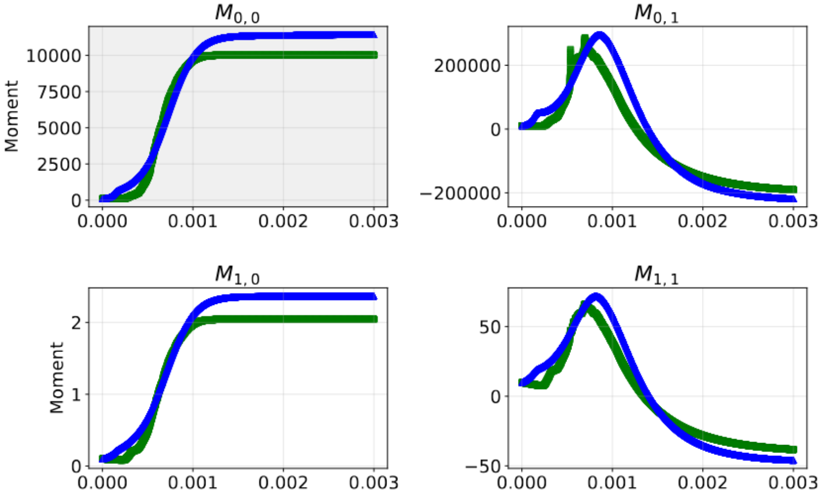
Computed moments:

- M_{00}: number of droplets
- M_{10}: Sum of average sizes
- M_{01}: Sum of average velocities
- M_{11}: mixed moment

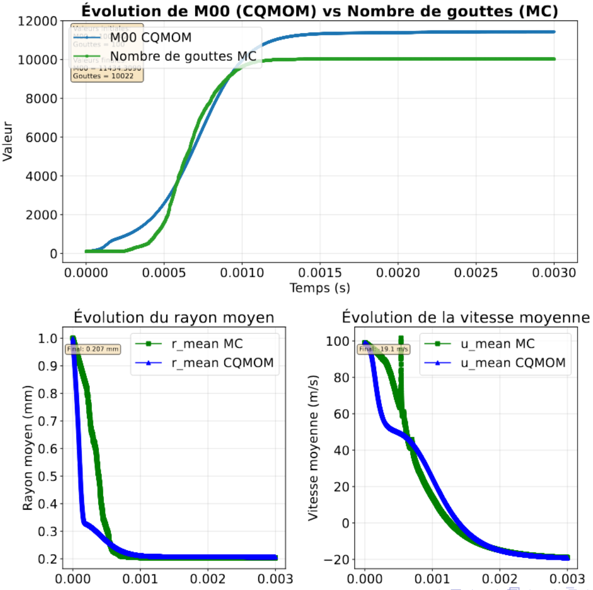
Compared methods:

- Monte Carlo (reference)
- CQMOM with source term

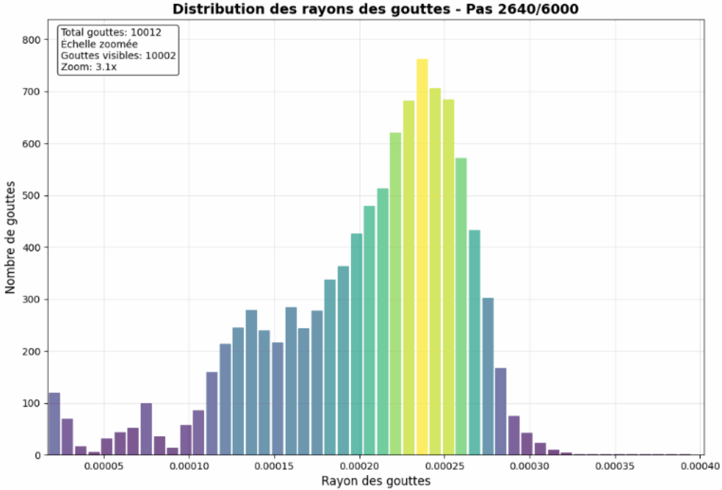
Results: Moment Comparison



Results: Evolution of Characteristic Quantities



Results: Final Radius Distribution.



Results Summary

Approach successes:

- ✓ Successful implementation of CQMOM source term
- ✓ Monte Carlo validation
- ✓ Physically realistic fragmentation
- ✓ Mass conservation respected
- ✓ Coherent evolution of moments

Identified limitations:

- No coalescence
- No evaporation
- Simplified daughter velocity distribution

Main conclusion

The CQMOM method with fragmentation source term allows efficient modeling of secondary atomization while maintaining reasonable numerical cost compared to complete Monte Carlo approaches.

Thank you for your attention!

Questions?