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Noureddine Lebaz, Nida Sheibat-Othman. Population balance models combined to CFD simulations for breakage prediction of emulsion droplets in SMX+ static mixers. 6th Conference on Population Balance Modelling, May 2018, Ghent, Belgium. hal-01966547

HAL Id: hal-01966547

<https://hal.science/hal-01966547>

Submitted on 9 Nov 2023

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Population balance modelling combined to CFD simulations for breakage prediction in SMX+ static mixers

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Highlights:

- The emulsification process is the basis of a wide range of industrial applications
- In-line static mixers achieve high mixing performances in short residence times with low energy consumption
- Steady-state correlations are widely used for the prediction of droplets mean diameter in static mixers, however:
 - The mean diameter is not completely representative of an emulsion with wide size distribution
 - Hydrodynamic equilibrium is usually assumed in these correlations, which is not always true
- A population balance model is proposed in this work in order to predict the full droplet size distribution

Theoretical framework:

- PBE accounting for a breakage process:

$$\frac{\partial n(v, t)}{\partial t} = \int_v^\infty \beta(v, v') g(v') n(v', t) dv' - g(v) n(v, t)$$

Breakage frequency : proposed by Alopaeus et al., 2002

$$g(v) = C_1 \varepsilon^{1/3} \operatorname{erfc} \left[\sqrt{C_2 \frac{\sigma}{\rho_c \varepsilon^{2/3} v^{5/9}} + C_3 \frac{\mu_d}{\sqrt{\rho_c \rho_d} \varepsilon^{1/3} v^{4/9}}} \right]$$

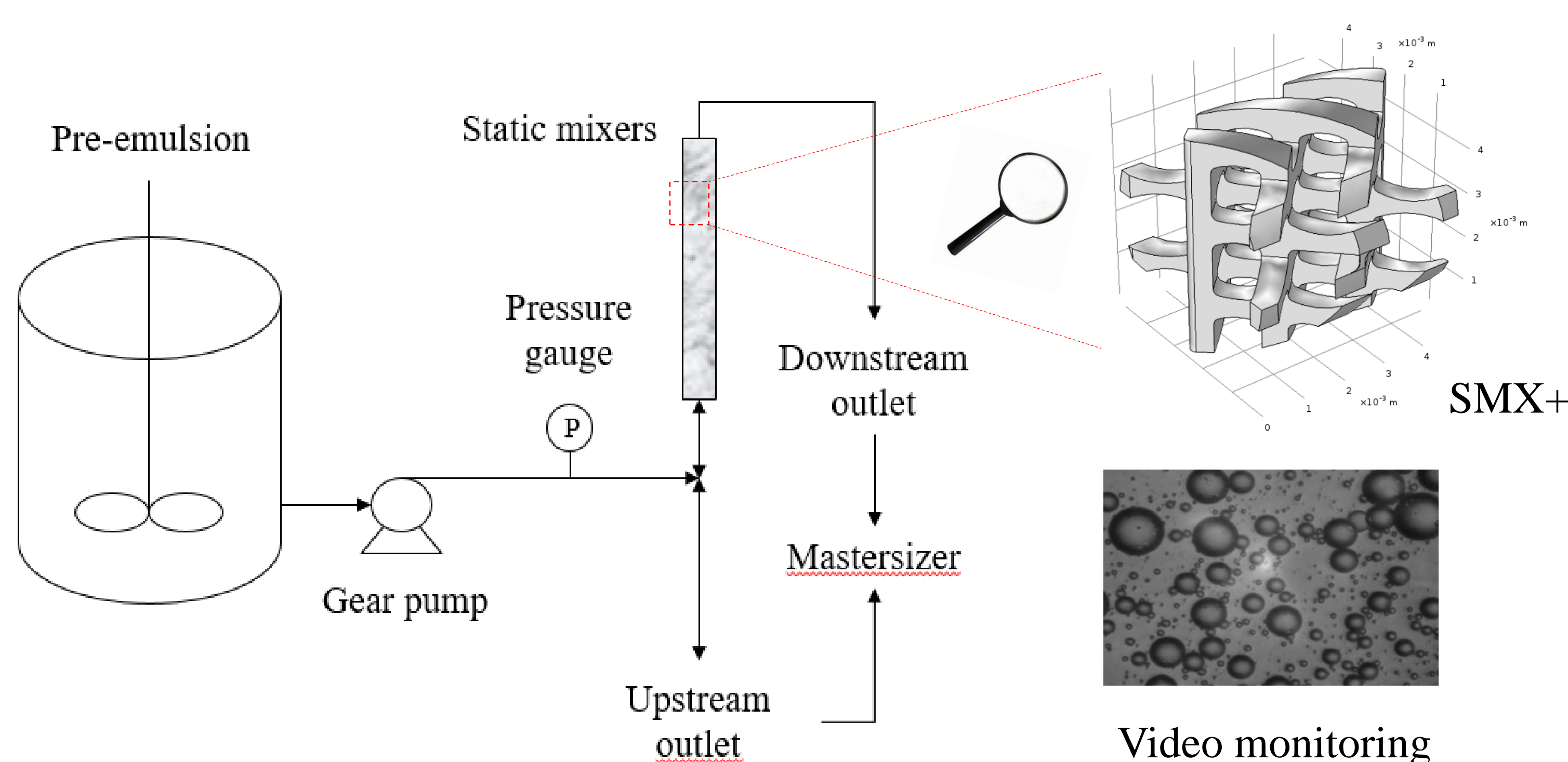
Daughter distribution function : Beta function with binary breakage

$$\beta(v, v') = 30 \frac{m}{v'} \left(\frac{v}{v'} \right)^2 \left(1 - \left(\frac{v}{v'} \right) \right)^2$$

- CFD simulations with COMSOL Multiphysics® are carried out to predict the energy dissipation rate : ε
- A finite volume scheme is adopted to solve numerically the PBE
 - The parameters of the breakage frequency are determined using the MATLAB® Optimization Toolbox

Experimental procedure:

- Oil-in-water pre-emulsions are prepared using Silicon oils with different viscosities
- Tween® 20 is used as emulsifier
- Monitoring of the DSD is done before and after the SMX+



The effects of the **number** of SMX+ elements, the **viscosity**, the **fraction** of the dispersed phase and the **energy dissipation rate** are investigated .

Conclusions:

- A population balance model accounting for droplet breakage in SMX+ static mixers is proposed and validated
- CFD simulations are performed in order to accurately assess the energy dissipation rate to be used in the PBE-based model
- The PBE-based model demonstrates a predictive capability under different operating conditions as validated by experimental data

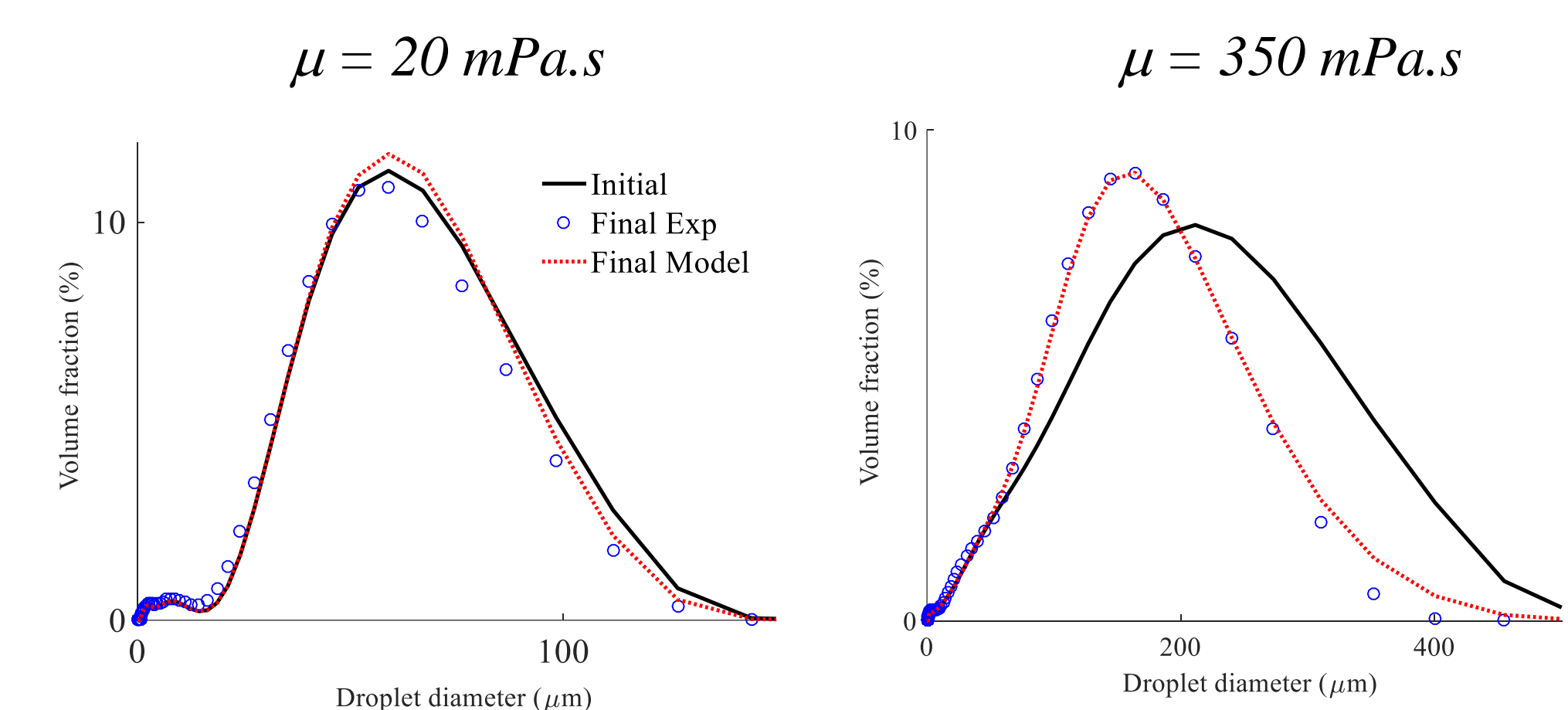
Results:

Parameter identification:

Breakage parameters :

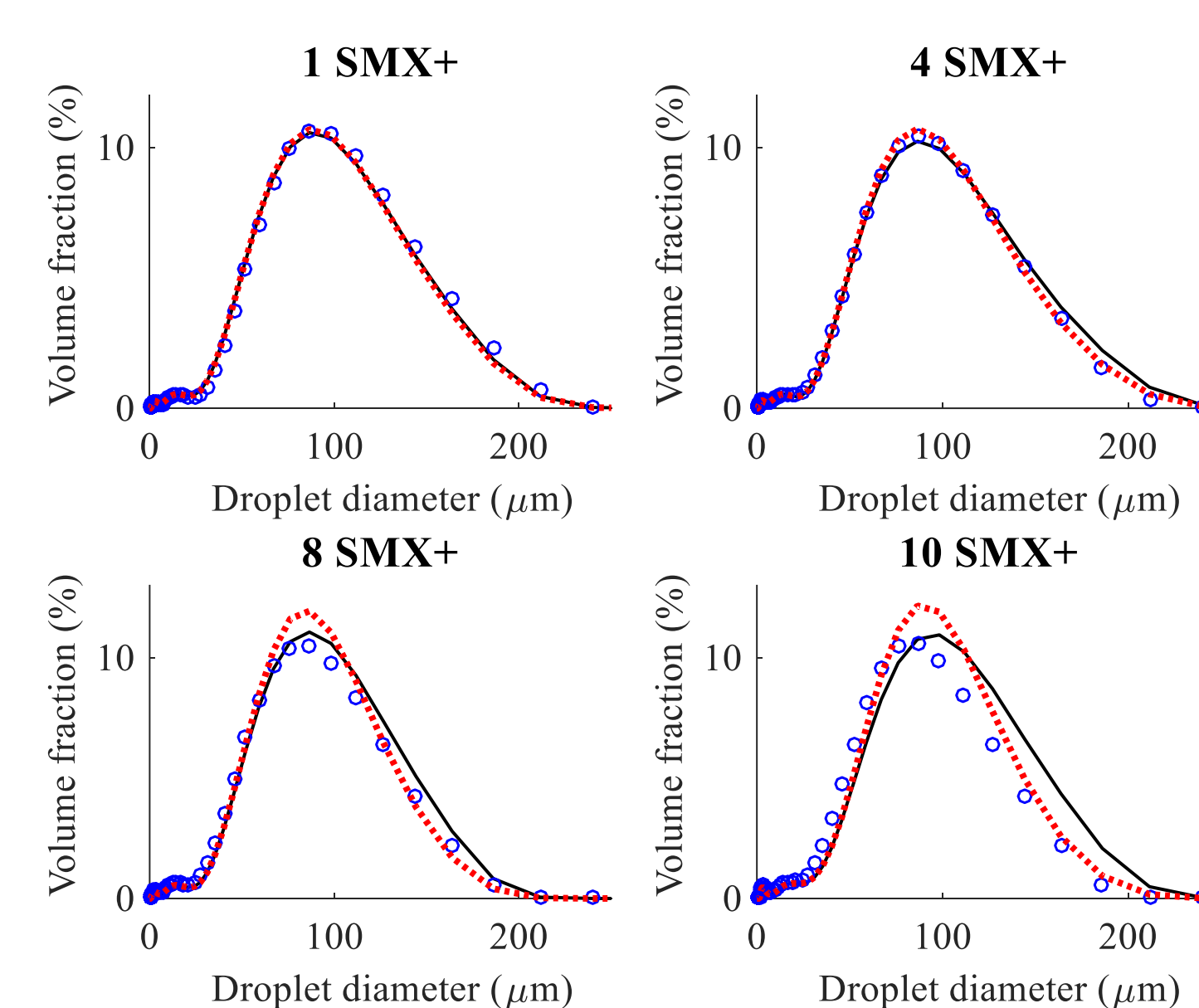
| C_1 | C_2 | C_3 |
|-------|-------|---------|
| 16.46 | 0.26 | 2.3e-14 |

- $\varepsilon = 63 \text{ m}^2/\text{s}^3$
- 10 SMX+
- $\Phi = 1 \%$



Prediction:

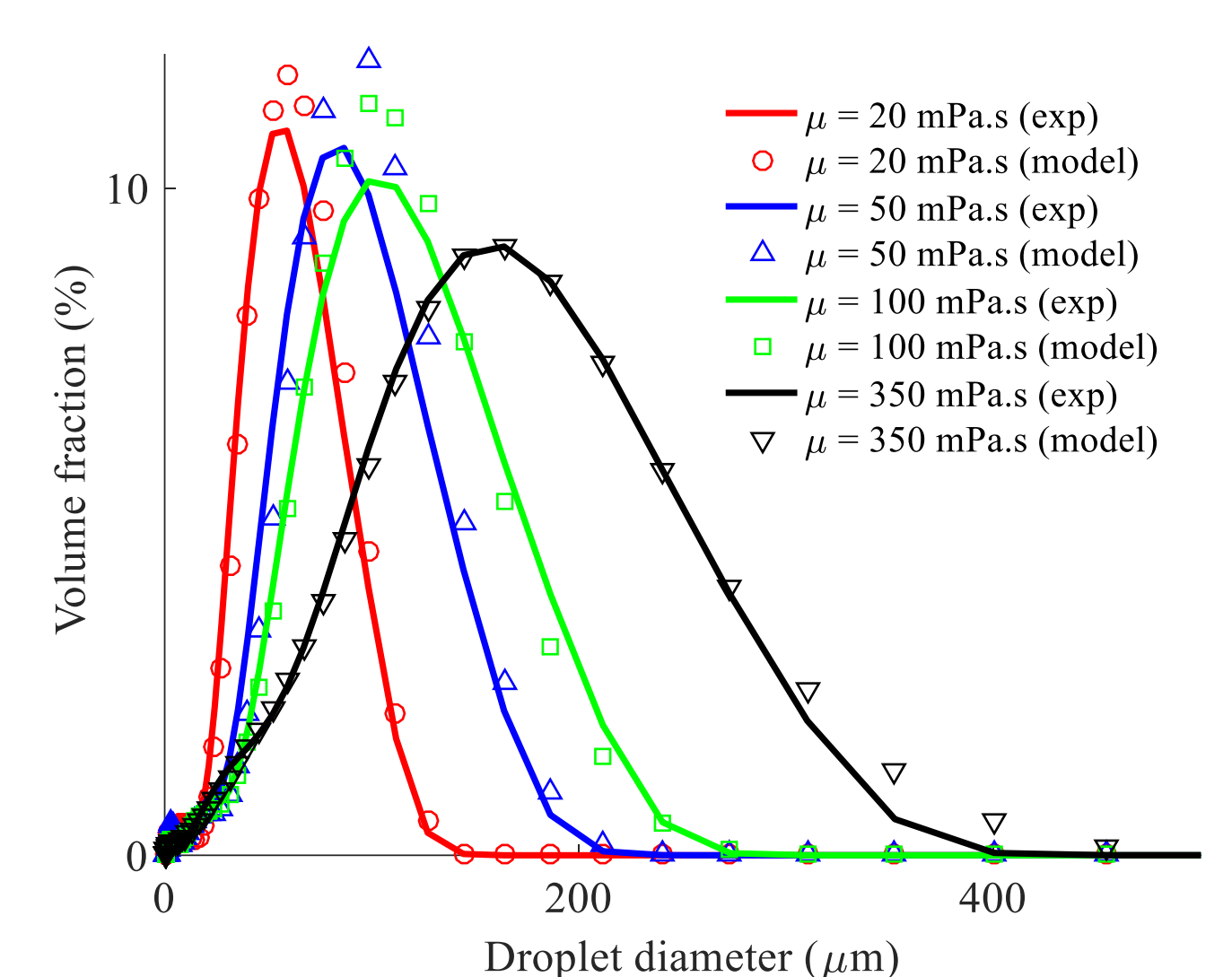
Number of SMX+



- $\varepsilon = 63 \text{ m}^2/\text{s}^3$
- $\mu = 50 \text{ mPa.s}$
- $\Phi = 1 \%$

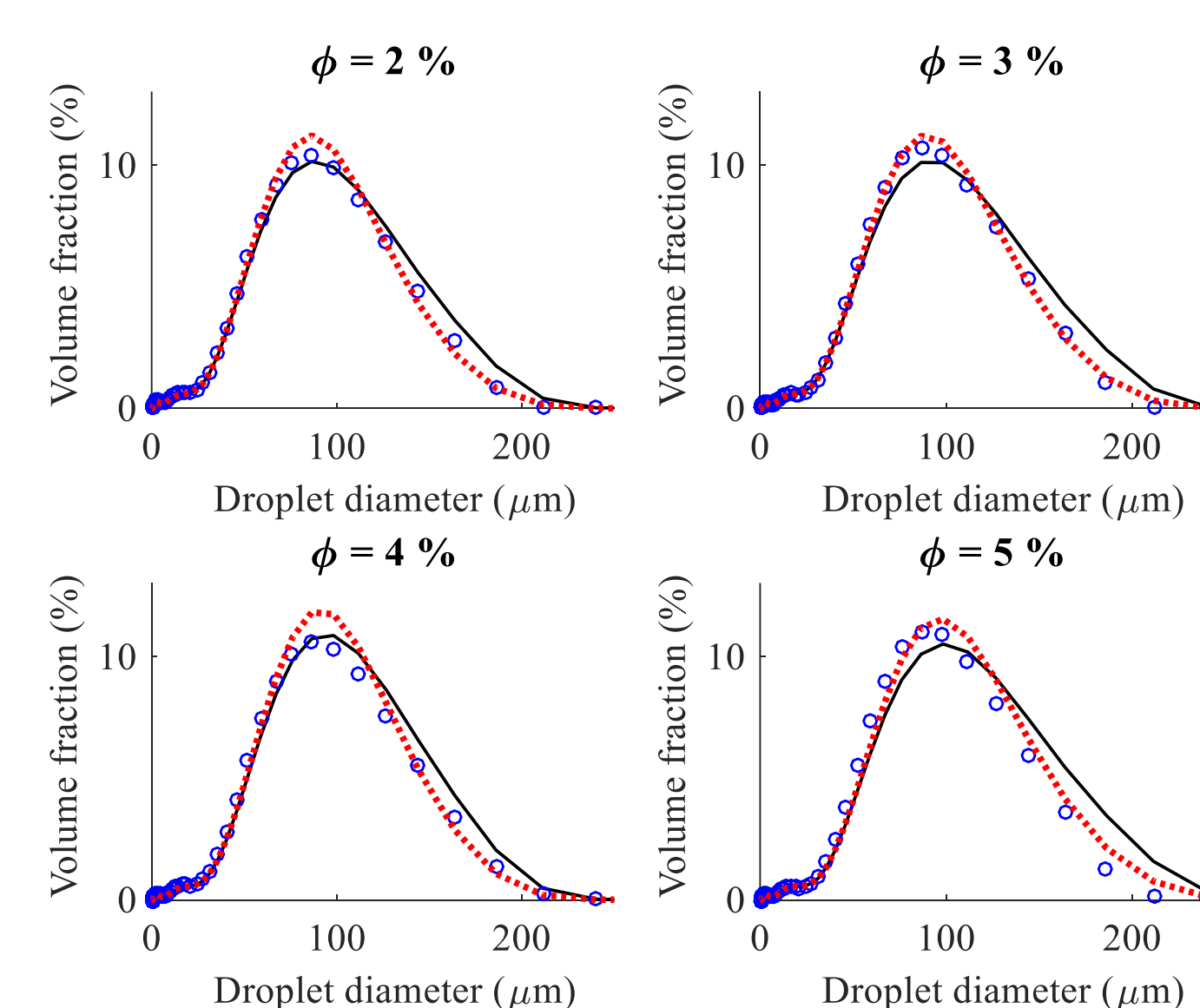
— Initial
○ Final Exp
... Final Model

Viscosity of the dispersed phase: μ



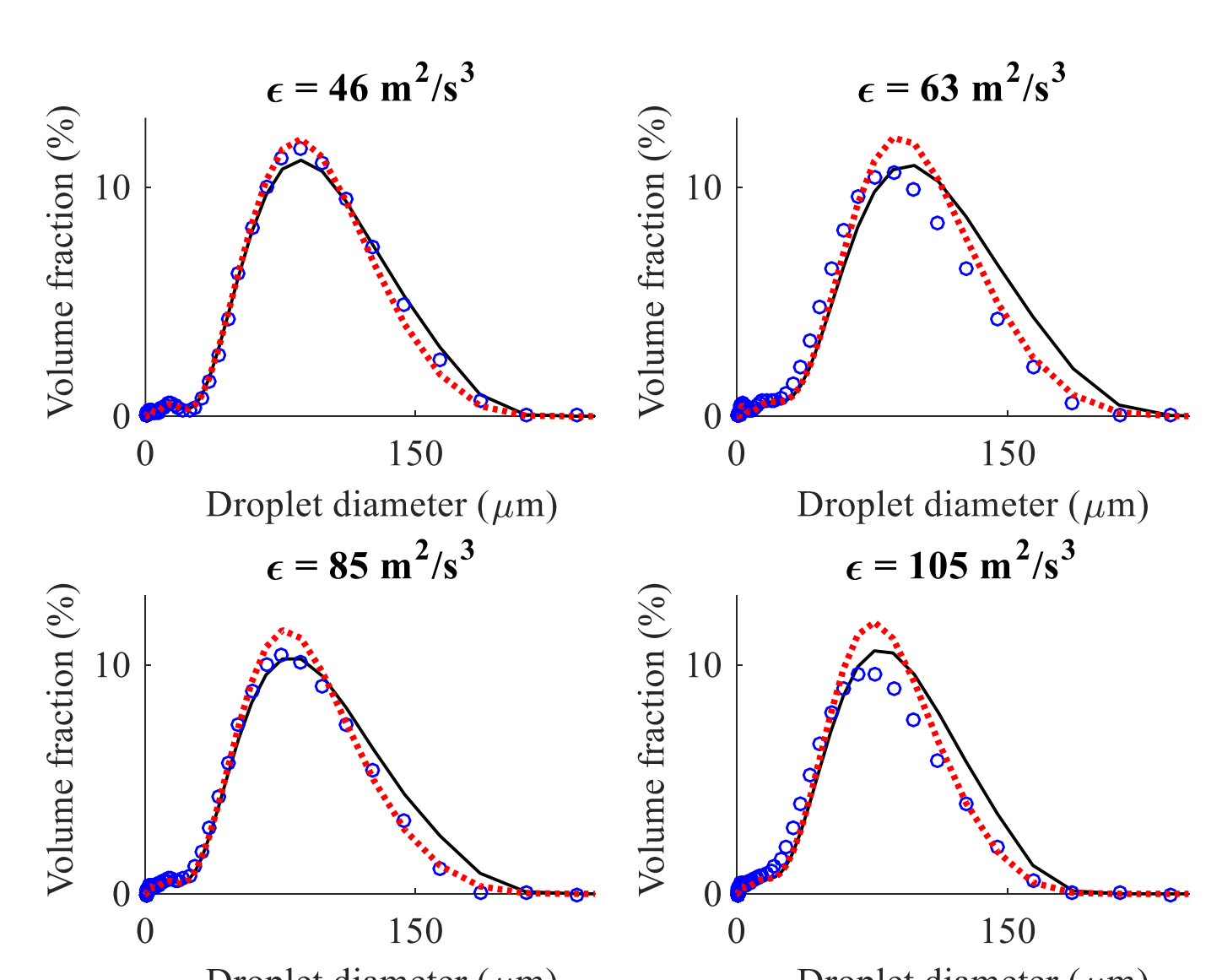
- $\varepsilon = 63 \text{ m}^2/\text{s}^3$
- 10 SMX+
- $\Phi = 1 \%$

Dispersed phase fraction: Φ



- $\varepsilon = 63 \text{ m}^2/\text{s}^3$
- $\mu = 50 \text{ mPa.s}$
- 10 SMX+

Energy dissipation rate : ε



- 10 SMX+
- $\mu = 50 \text{ mPa.s}$
- $\Phi = 1 \%$