Computations and Experiments on the Evaporation of Multi-Component Droplets

Kick-Off Meeting CONEX Project

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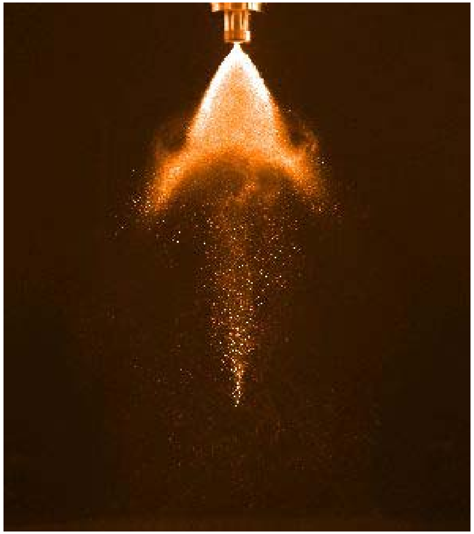
Outline of the Presentation

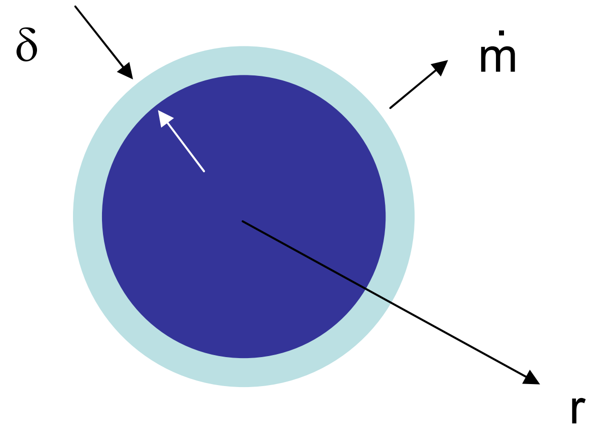
- Motivation
- Droplet evaporation modelling at high transfer rates
- Model development for multi-component liquids
- Experiments on multi-component droplet evaporation
- Model validation
- Conclusions

Motivation

- Many liquids in technical processes are multi-component mixtures
- Evaporation rates depend on volatility and therefore on liquid mixture composition
- Analysis of evaporation behaviour important for both chemical and mechanical engineering applications, including
  - spray combustion
  - spray absorption
  - spray cooling
  - spray drying
  - spray extraction



Modelling liquid droplet evaporation



- Formulation of the problem
  Evaporating droplet in gaseous environment, modelled with film theory

- Assumptions in modelling droplet evaporation
  - Droplet shape spherical
  - Solubility of air in liquid negligible
  - Mass diffusion by temperature and pressure gradients negligible
  - Gas phase in a quasi-steady state
  - No influences of chemical reactions
  - No heat transfer due to radiation
  - Infinite-conductivity and rapid-mixing models possible for modelling the liquid phase temperature and mixture component distributions

Droplet evaporation at high transfer rates

- Abramzon and Sirignano model for pure liquid drop evaporation
- Mass flux n_F of vapour in radial direction is $$n_F = Y_F(n_F + n_g) - \rho \mathcal{D}_{F,g} \frac{dY_F}{dr}$$

ρ	density of the gas
$\mathcal{D}_{F,g}$	binary diffusion coefficient of fuel vapor in gas
Y_F	mass fraction of fuel in the gas phase
n_A	mass flux of gas

- Gas insoluble in the liquid; therefore $$n_F(1 - Y_F) = -\rho \mathcal{D}_{F,g} \frac{dY_F}{dr} \qquad (*)$$
- For steady transport of mass $$n_F(4\pi r^2) = n_{F,S}(4\pi a^2) = \dot{m}$$
- Film theory for describing heat and mass transfer rates
- Radius of droplet including film for heat or mass transfer ($r_f = \delta + a$; δ - film thickness, different for heat and mass transfer) given by

$$r_{f,M} = a \frac{Sh^*}{(Sh^* - 2)}, \qquad r_{f,T} = a \frac{Nu^*}{(Nu^* - 2)}$$

Modelling pure liquid droplet evaporation

Integrating equation (*) between r=a and $r_{f,M}$ yields the evaporation rate

$$\dot{m} = 2\pi a (\overline{\rho}\,\overline{\mathcal{D}})_g Sh^* \ln(1+B_M) \quad \text{where} \quad B_M = \frac{Y_{F,s} - Y_{F,\infty}}{1 - Y_{F,s}}$$

Balance of the total enthalpy flux balance across a control surface, integrated between r = a and $r_{f,T}$

$$\dot{m} = 2\pi a \frac{\overline{k}_g}{\overline{c}_{P_F}} Nu^* \ln\left[1 + \frac{\overline{c}_{P,F}(T - T_S)}{L(T_S) + Q_L/\dot{m}}\right]$$

$L(T_S)$ – latent heat of vaporization at the droplet surface temperature T

Equating the evaporation rates yields heat transfer rate into the droplet

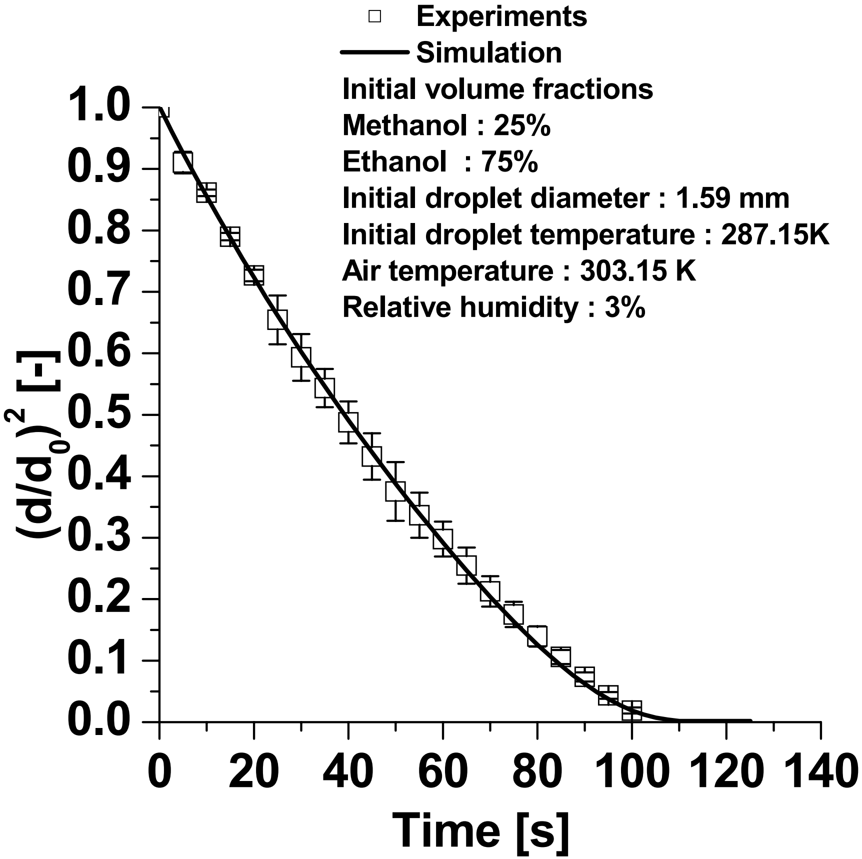
$$Q_L = \dot{m}\left[\frac{\overline{c}_{P,F}(T_\infty - T_S)}{B_T} - L(T_S)\right] \qquad B_T = (1+B_M)^{\phi} - 1 \qquad \phi = \frac{c_{p,F}}{c_{p,g}} \cdot \frac{Sh^*}{Nu^*} \cdot \frac{1}{\overline{Le}}$$

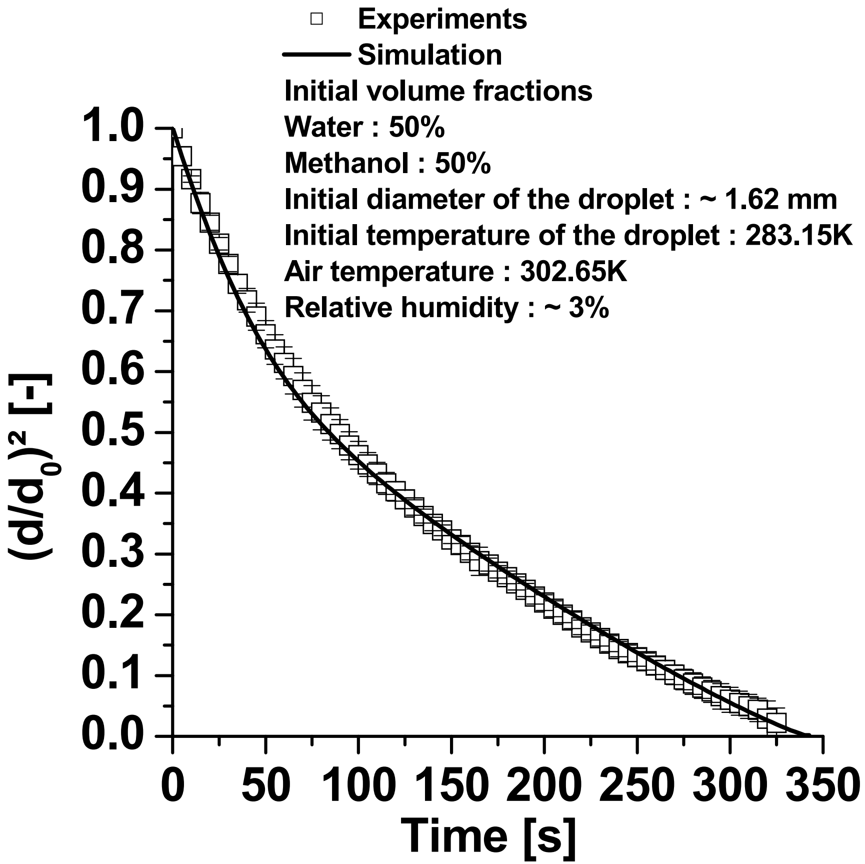
Rate of droplet heating reads

$$\frac{dT}{dt} = Q_L \Big/ \left[\frac{4}{3}\pi a^3 \rho_L c_{P,L}\right]$$

Extension to binary liquid mixtures

- Kastner (2001) extended the above model to binary mixture droplet evaporation
- Results for Methanol-Ethanol mixture (25% and 75% vol., resp.) and water-Methanol (50% vol. each): data from experiments and simulation





Generalised model development - I

Total evaporation rate $\dot{m} = \sum_{i=1}^{n} \dot{m}_i = \sum_{i=1}^{n} [2\pi a_{p,i} (\overline{\rho}\,\overline{\mathcal{D}})_{i,g}\ Sh_i^*\ ln(1 + B_{M,i})$

$\dot{m}$	Total evaporation rate of the droplet
ρ_g	Density of the gaseous phase
$\mathcal{D}_{i,g}$	Binary diffusion coefficient of component i in the gas
$a_{p,i}$	Volume-equivalent partial radius of component i
Sh_i^*	Modified Sherwood number of component i
$B_{M,i}$	Spalding mass transfer number of component i

Sh^* and $B_{M,i}$ computed for each component as

$$B_{M,i} = \frac{Y_{i,s} - Y_{i,\infty}}{1 - Y_{i,s}} \qquad Sh_i^* = 2 + \frac{Sh_0 - 2}{F(B_{M,i})} \qquad F(B_{M,i}) = (1 + B_{M,i})^{0.7} \frac{\ln(1 + B_{M,i})}{B_{M,i}}$$

$Y_{i,s}$ = mass fraction of component *i* at the droplet surface

$Y_{i,\infty}$ = mass fraction of component *i* far from the droplet surface

$F(B_{M,i})$ = universal function found by numerics and experiments

Generalised model development - II

- Liquid treated as a real mixture, gas phase as ideal
- The mole fraction x_i of a component i in the vapour layer given by

$$x_i = \gamma_i \, x_{L,i} \frac{p_{vap,i}}{p_m} \Rightarrow Y_i = \frac{x_i M_i}{\sum_j x_j M_j} \Rightarrow B_{M,i} = \frac{Y_{i,s} - Y_{i,\infty}}{1 - Y_{i,s}} \Rightarrow Sh_i^* = 2 + \frac{Sh_0 - 2}{F(B_{M,i})}$$

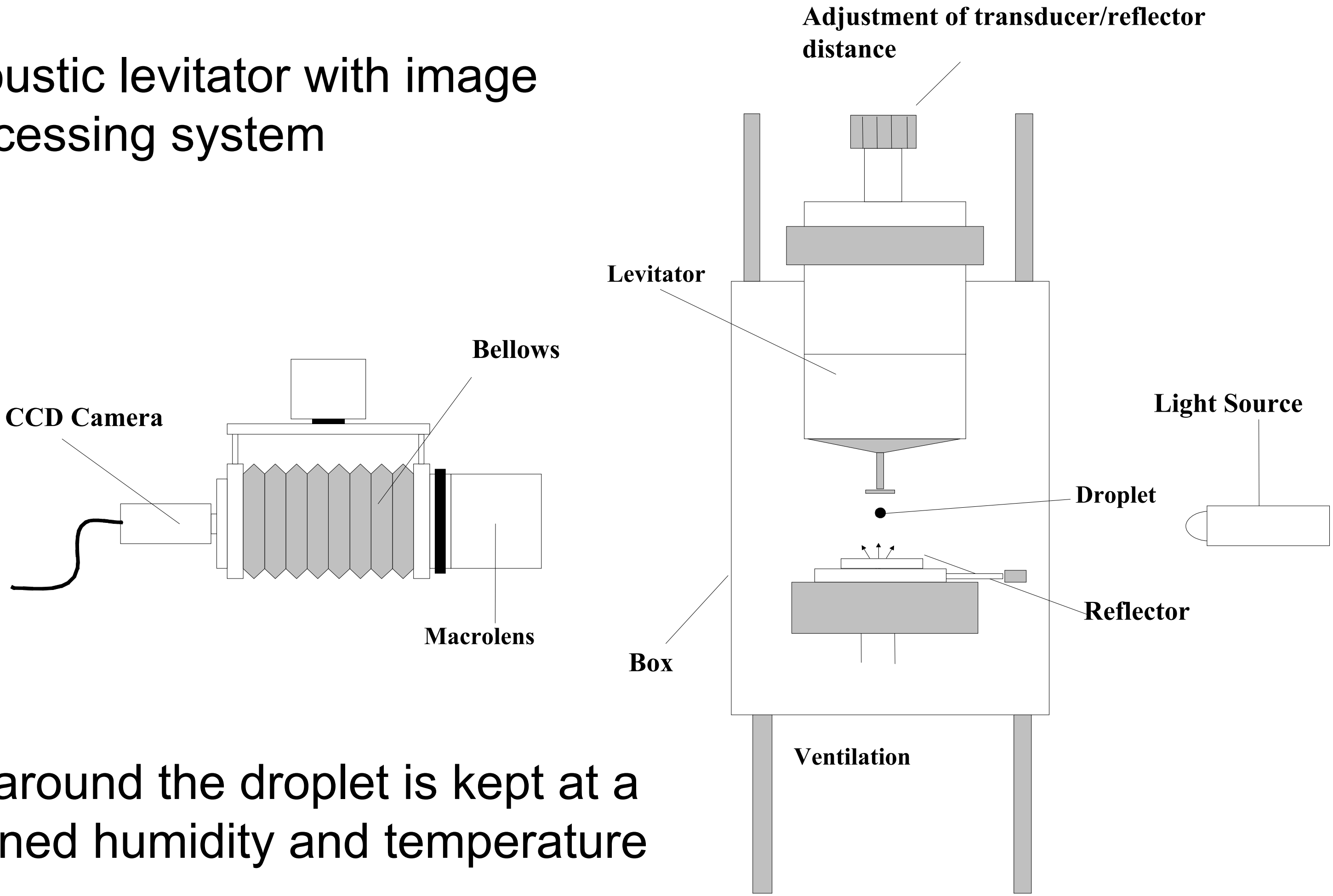
where

γ_i	activity coefficient of component i in the mixture
$x_{L,i}$	mole fraction of component i in the liquid phase
p_m	pressure of gas mixture in the environment of the droplet
$p_{vap,i}$	saturation vapour pressure of pure component i,

- Activity coefficients for binary liquids obtained by Wilsons coefficients
- The activity coefficients for multi-component liquid mixtures are obtained using the UNIFAC method (Prausnitz et al.)

Experimental Set-up

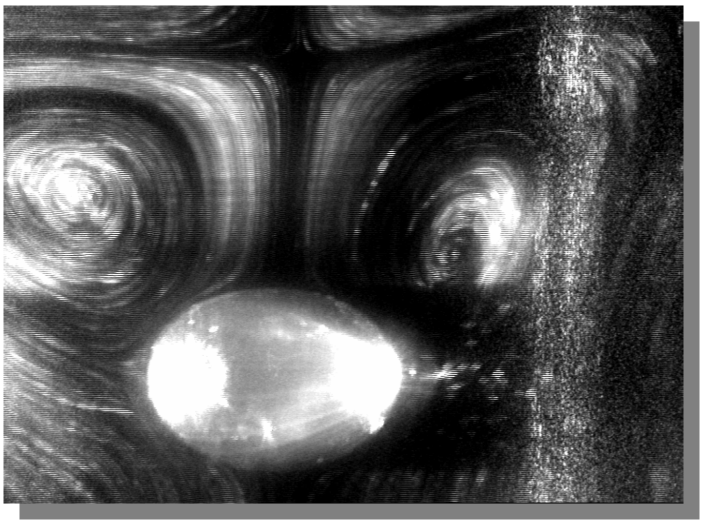
Acoustic levitator with image processing system



Air around the droplet is kept at a defined humidity and temperature

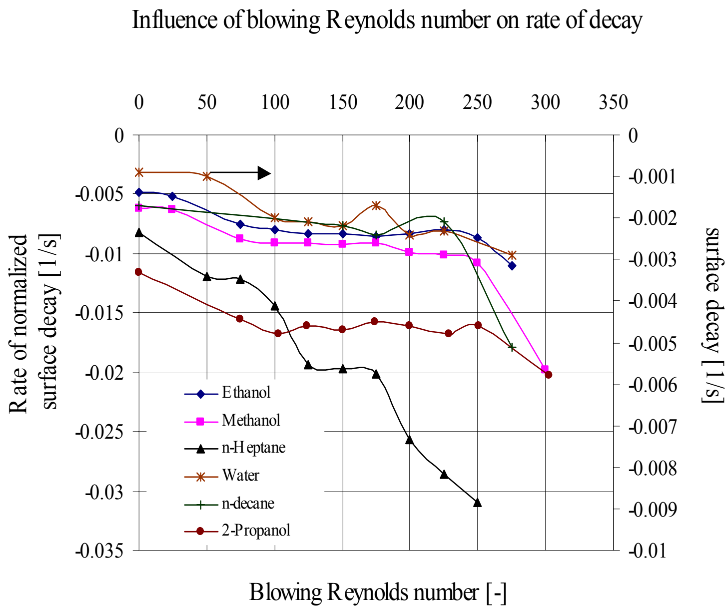
Characteristics of acoustic levitation

- Periodic boundary-layer flows – as described by Schlichting in context with oscillating cylinder in fluid at rest – result in secondary flow, also called ***acoustic streaming***
- Toroidal vortices above and below the droplet
- Vortices enhance and hinder evaporation of the droplet

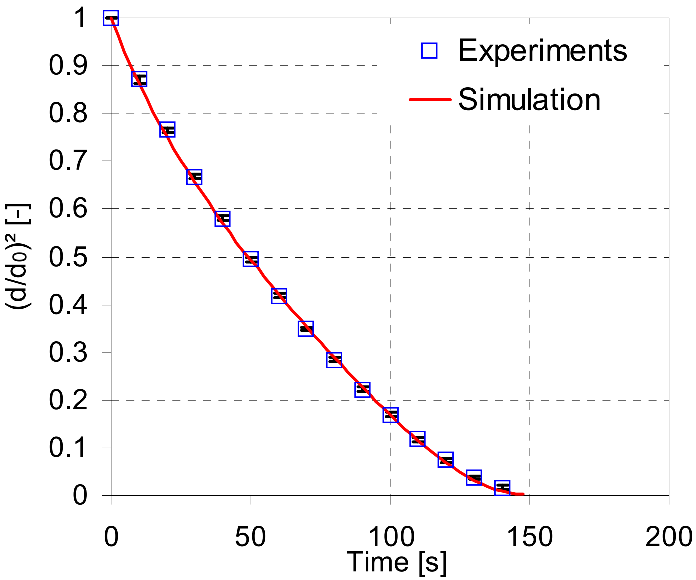


Photograph of an acoustically levitated 1.5µl Methanol droplet

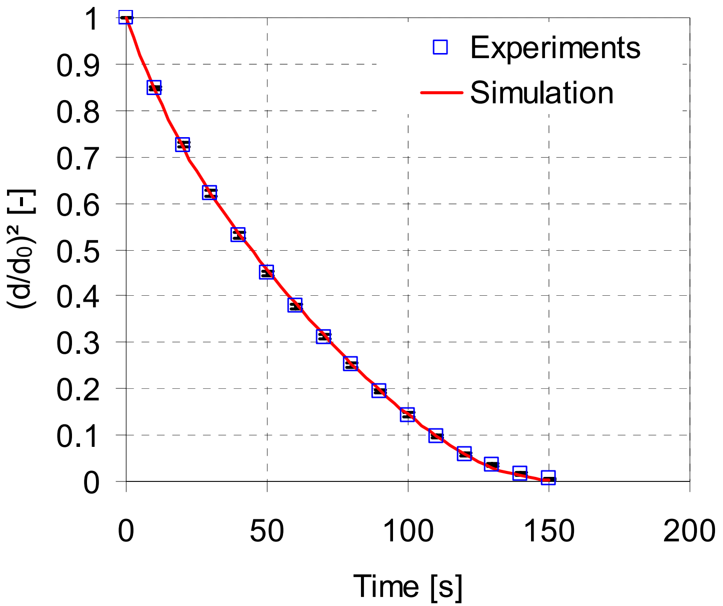
Ventilation removes vapour from the vortices



Evaporation of three-component liquid droplets

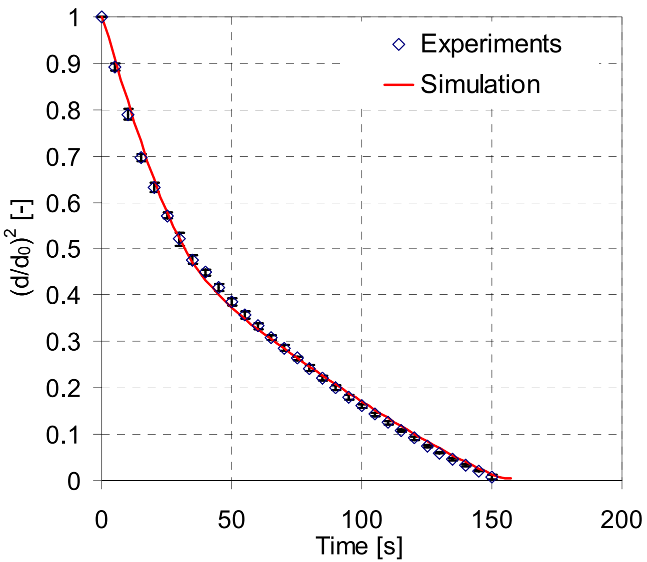


1.70 mm diameter droplets, containing 15% Methanol, 70% Ethanol, and 15% n-Heptane;
R.H. = 5%; T_d = 283.65K; T_s = 303.15K

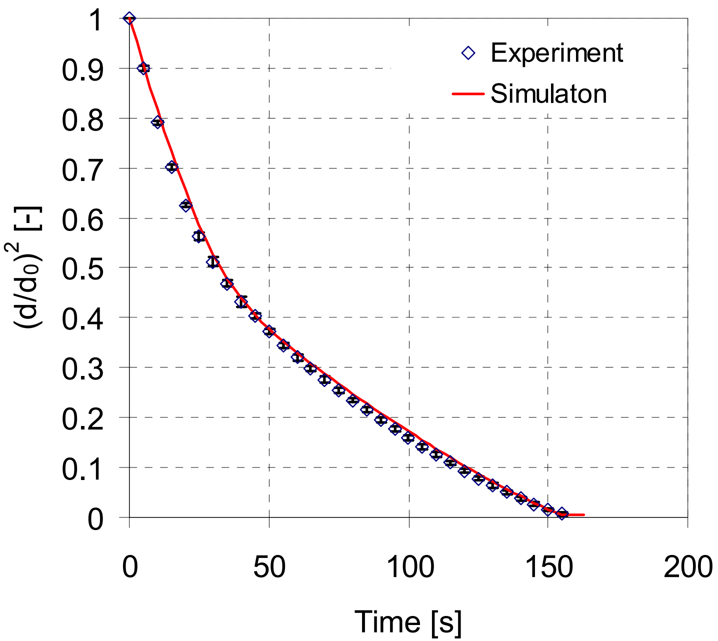


1.69 mm diameter droplets, containing 40% Methanol and 40% Ethanol, and 20% n-Heptane
R.H. = 5%; T_d = 280.65K; T_s = 303.15K

Evaporation of four-component liquid droplets

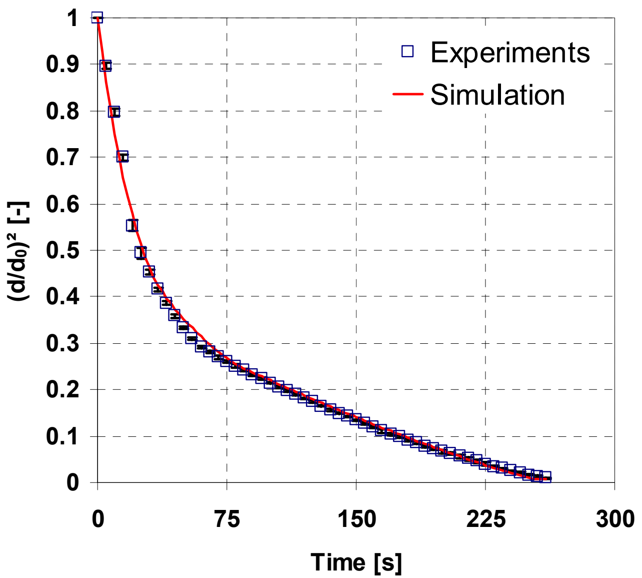


1.50 mm diameter droplets, containing 30% n-Heptane, 20% Methanol, 20% Ethanol, and 30% 1-Butanol; R.H. = 3%; T_d = 287.0K; T_s = 302.15K

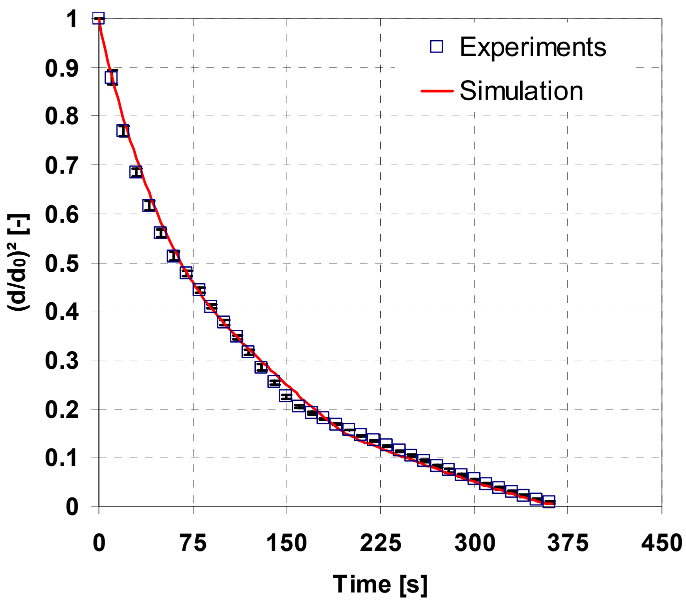


1.57 mm diameter droplets, containing 20% n-Heptane, 20% Methanol, 30% Ethanol, and 30% 1-Butanol; R.H. = 3%; T_d = 287.0K; T_s = 302.15K

Evaporation of five-component liquid droplets

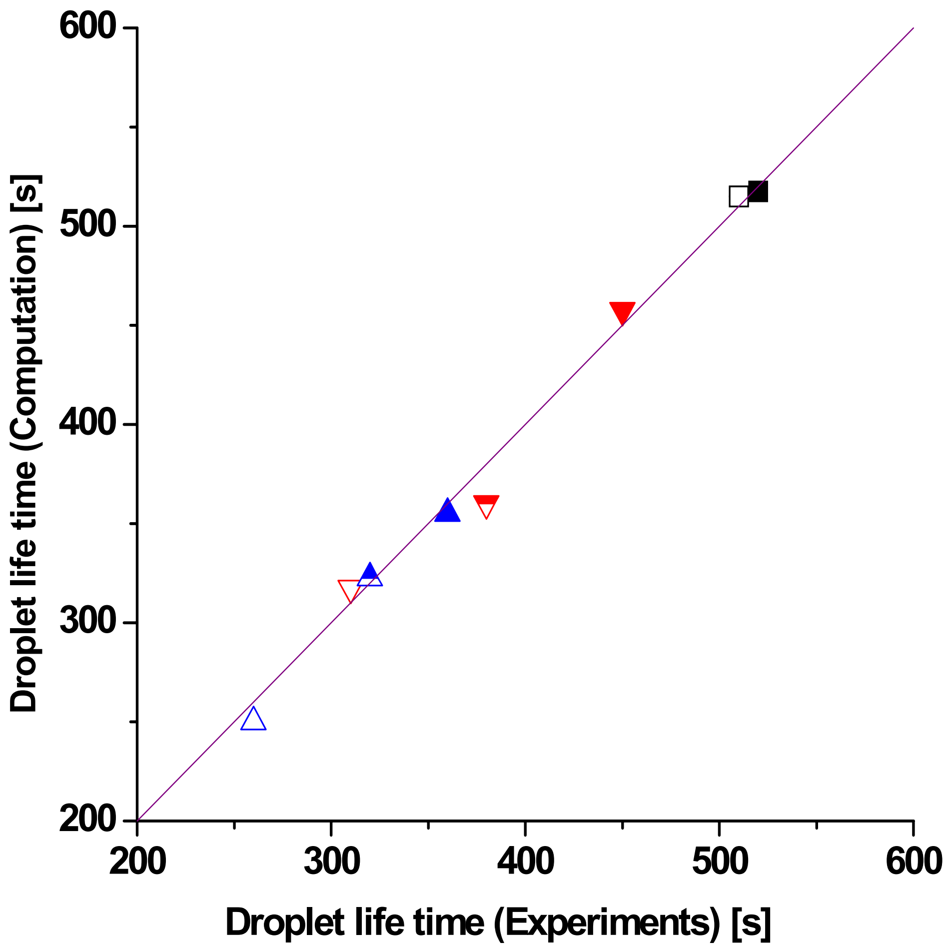


1.50 mm diameter droplets, containing 40% n-Heptane, 20% n-Decane, 20% Methanol, 10% Ethanol, and 10% 1-Butanol;
R.H. = 3%; T_d = 286.15K; T_s = 303.15K



1.70 mm diameter droplets, containing 15% n-Heptane, 15% n-Decane, 30% Methanol, 20% Ethanol, and 20% 1-Butanol;
R.H. = 2%; T_d = 286.15K; T_s = 303.15K

Comparison of lifetimes of droplets



Initial diameter of the droplets : ~ 1.65 mm
Initial droplet temperature : ~ 288.15 K
Air temperature : 301.15 K
Relative humidity : ~ 4%
Droplet containing initial volume fractions
- ■ 10% Methanol, 40% Ethanol and 50% 1-Butanol
- ⬒ 20% Methanol, 30% Ethanol and 50% 1-Butanol
- □ 30% Methanol, 20% Ethanol and 50% 1-Butanol

Initial diameter of the droplets : ~ 1.63 mm
Initial droplet temperature : ~ 280 K
Air temperature : 303.15 K
Relative humidity : ~ 5%
Droplet containing initial volume fractions
- ▼ 10% Methanol, 50% Ethanol and 40% n-Decane
- ▽ 20% Methanol, 50% Ethanol and 30% n-Decane
- ▽ 30% Methanol, 50% Ethanol and 20% n-Decane

Droplet containing initial volume fractions
Initial diameter of the droplets : ~ 1.62 mm
Initial droplet temperature : ~ 286.15 K
Air temperature : 302.3 K
Relative humidity : ~ 3%
Droplet containing initial volume fractions
- ▲ 30% Methanol, 20% Ethanol, 20% 1-Butanol 15% n-Heptane and 15% n-Decane
- ▲ 30% Methanol, 30% Ethanol, 10% 1-Butanol 20% n-Heptane and 10% n-Decane
- △ 20% Methanol, 10% Ethanol, 10% 1-Butanol 40% n-Heptane and 20% n-Decane

Conclusions

- Computational model for the simulation of the evaporation behaviour of multi-component liquid droplets was developed
- Verification experiments carried out with ultrasonically levitated single droplets of multi-component liquids
- Maximum deviation of 5% occurs in measured and computed lifetimes of the droplets of various multi-component mixtures
- The model predicts the evaporation rate of real fuels
- Helps in better understanding air-vapour mixture formation and, in the field of internal combustion engines,

  - Reduce fuel consumption
  - Leads to better use of fossil fuels
  - Reduces NO_X and CO_2 emissions
  - Leads to cleaner combustion