

Current research on droplet evaporation modelling at University of Bergamo

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Research lines

Modelling of droplet heating and evaporation

- ✓ variable properties : variable gas density
- ✓ Non-spherical drops : spheroids
- ✓ Multicomponent drops: Fick'law and Maxwell-Stefan

Mass transport in gases

Some definitions



$$\mathbf{N}^{(k)} = \frac{\mathbf{n}^{(k)}}{Mm^{(k)}}$$
$$\hat{\mathbf{j}}^{(k)} = \frac{\mathbf{j}^{(k)}}{Mm^{(k)}}$$

Molar fluxes

Mass transport in gases

Constitutive equations

The constitutive equations for the energy and mass fluxes can be obtained from non-equilibrium thermodynamics

$$\mathbf{q}^{h} = -\alpha_{00} \nabla \ln T - \sum_{n=1}^{N} \alpha_{0n} \frac{cRT}{\rho^{(n)}} \mathbf{d}^{(n)}$$
Dufour effect
$$\mathbf{q}_{jk} = \alpha_{kj}$$
Phenomenological coefficients
$$\mathbf{j}^{(p)} = -\alpha_{p0} \nabla \ln T - \rho^{(p)} \sum_{n=1}^{N} \alpha_{pn} \frac{cRT}{\rho^{(p)} \rho^{(n)}} \mathbf{d}^{(n)}$$
Soret effect
$$\mathbf{d}^{(p)} = \text{diffusional forces}$$

 $\widetilde{D}^{pn} = \alpha_{pn} \frac{cRT}{\rho^{(p)} \rho^{(n)}}$ Multicomponent Diffusion Coefficients $\alpha_{0p} = \alpha_{p0} = D_p^T$ generalised thermal Diffusion Coefficients

$$\mathbf{j}^{(p)} = -D_T^{(p)} \nabla \ln T - \boldsymbol{\rho}^{(p)} \sum_{n=0}^N \tilde{D}_{pn} \mathbf{d}^{(p)}$$

Mass transport in gases

Inversion of the previous equation set yields the Maxwell-Stefan equations (Soret effect will be neglected from now on)

$$\mathbf{d}^{(n)} = \sum_{\substack{k=1\\k\neq n}} C_{nk} \left(\frac{\mathbf{j}^{(k)}}{\rho^{(k)}} - \frac{\mathbf{j}^{(n)}}{\rho^{(n)}} \right) \qquad C_{pn} = \frac{y^{(p)} y^{(n)}}{D_{pn}} \qquad \text{Maxwell-Stefan}$$

Diffusion coefficients

The coefficients C_{pn} are related to the multicomponent diffusion coefficients by the relation [A1]:

$$\sum_{\substack{k=1\\k\neq j}}^{N} \sum_{\substack{n=1\\k\neq j}}^{N} \{ [\delta_{nk}(1-\delta_{ik}) - \delta_{ik}] \chi_j - \delta_{nj} \chi_k \} C_{in} \widetilde{D}^{kj} = \chi_i \chi_j$$

For low density gases D_{pn} are practically independent on composition and they can be obtained by measuring binary diffusion coefficients. <u>This is not true for high density gases and for liquid mixtures</u>.

[A1] C.F. Curtiss, R.B. Bird Multicomponent diffusion, Ind. Eng. Chem. Res , 1999, 38, 2515-2522.

$$\mathbf{d}^{(s)} = \begin{cases} \frac{y^{(s)}}{RT} \sum_{p=0}^{n} \left(\frac{\partial \mu^{m(s)}}{\partial y^{(p)}}\right)_{T,P,\chi_{q*s,p}} \nabla y_{p} + \frac{y^{(s)}}{RT} Mm^{(s)} \left(\frac{\tilde{\nu}^{m(s)}}{Mm^{(s)}} - \frac{1}{p}\right) \nabla P \\ p \neq s \\ -\frac{y^{(s)}Mm^{(s)}}{RT} \left(\mathbf{f}^{(s)} - \sum_{p=0}^{n} \chi^{(p)} \mathbf{f}^{(p)}\right) \end{cases}$$

For an ideal mixture of ideal gases, neglecting the pressure diffusion and the external forces diffusion the diffusional forces simplify to

$$\mathbf{d}^{(s)} = \nabla \mathbf{y}^{(s)}$$

In a fixed reference frame the mass fluxes are

 $\mathbf{n}^{(p)} = \mathbf{n}^T x^{(p)} + \mathbf{j}^{(p)}$ Mass form $\mathbf{N}^{(p)} = \mathbf{N}^T y^{(p)} + \mathbf{\hat{j}}^{(p)}$ Molar form

$$\nabla y^{(n)} = \sum_{\substack{k=1 \ k \neq n}} \frac{1}{cD_{nk}} \left(y^{(n)} \mathbf{N}^{(k)} - y^{(k)} \mathbf{N}^{(n)} \right)$$

Maxwell-Stefan equations

Mass transport in gases Binary mixtures

$$\nabla y^{(1)} = \frac{1}{cD_{12}} \left(y^{(1)} \mathsf{N}^{(2)} - y^{(2)} \mathsf{N}^{(1)} \right) \quad \text{inversion} \quad \mathsf{N}^{(1)} = \mathsf{N}^T y^{(1)} - cD_{12} \nabla y^{(1)} \\ \nabla y^{(2)} = \frac{1}{cD_{21}} \left(y^{(2)} \mathsf{N}^{(1)} - y^{(1)} \mathsf{N}^{(2)} \right) \quad \mathsf{N}^T = \mathsf{N}^{(1)} + \mathsf{N}^{(2)} \\ \mathsf{N}^T = \mathsf{N}^{(1)} + \mathsf{N}^{(2)} \quad \text{Fick's law}$$

$$\mathbf{n}^{(1)} = \chi^{(1)} [\mathbf{n}^{(1)} + \mathbf{n}^{(2)}] - \rho D_{12} \nabla \chi^{(1)}$$

$$\mathbf{n}^{(2)} = \chi^{(2)} [\mathbf{n}^{(1)} + \mathbf{n}^{(2)}] - \rho D_{12} \nabla \chi^{(2)}$$

Fick's law

Since D_{jk} are the same as in M-S equations, they can be measured in binary diffusion experiments.

Mass transport in gases Multicomponents mixtures

Multicomponents diffusion can be studied using an approximated form of the constitutive equation, derived by extrapolating Fick's law, which holds for low concentration of the diffusing species:

 $\mathbf{N}^{(s)} = \mathbf{N}^{(T)} \mathbf{y}^{(s)} - cD^{(s,m)} \nabla \mathbf{y}^{(s)} \qquad \text{Molar form}$ $\mathbf{n}^{(s)} = \mathbf{n}^{(T)} \mathbf{\chi}^{(s)} - \rho D^{(s,m)} \nabla \mathbf{\chi}^{(s)} \qquad \text{Mass form}$

for multicomponent mixtures the two forms are not equivalent

Simple analytical solutions of the above reported equations can be found imposing the constancy of the molar (c) or the mass (ρ) density respectively. These assumptions are not equivalent and then the two equations yield different solutions also for the case of binary mixtures

For binary mixture the solution of the molar form (with c=const) would yield exactly the same solution of the M-S system since for N=2 the two sets of equation are equivalent and the same assumption (c=const) is made.

Drop evaporation models

Single component spherical drop

Conservation equations $\nabla \mathbf{n}^{(s)} = \mathbf{0}$ $\mathbf{n}^{(s)} = \mathbf{n}^{(T)} \boldsymbol{\chi}^{(s)} - \rho D_{\nu} \nabla \boldsymbol{\chi}^{(s)}$ Constitutive equations $D_{v} = D_{v,g} = D_{g,v}$

In spherical symmetry the only non-nil component of the fluxes is the radial one. Integration of conservation equation yields:

Assuming a still drop surface and $\mathbf{n}^{(s)} = \frac{K^{(s)}}{4\pi r^2}$; no gas diffusion into the liquid, the gas flux is nil at drop surface and then it is nil everywhere:

$$\mathbf{n}^{(v)} = \frac{m_{ev}}{4\pi r^2};$$
$$\mathbf{n}^{(g)} = 0;$$



[A2] N.A. Fuchs, Vaporisation and droplet growth in gaseous media, Pergamon Press, London, 1959.

Droplet heating and evaporation with variable gas density





Variable gas density
Evaporation rate
$$G = \ln(\chi_g); \quad \tilde{U} = \frac{U4\pi R_0^2 \rho_{\infty}}{\dot{m}_{ev}}; \quad \tilde{\rho} = \frac{\rho}{\rho_{\infty}}$$
 $\tilde{U} = -\frac{\zeta^2}{\hat{m}_{ev}}G_{\zeta}$ $\tilde{\rho} = -\frac{\hat{m}_{ev}}{G_{\zeta}}$ $\tilde{\rho} = -\frac{\hat{m}_{ev}}{G_{\zeta}}$ The momentum equation yields $\tilde{\rho} = -\frac{\hat{m}_{ev}}{G_{\zeta}}$

$$\frac{\zeta^2 G_{\zeta}^2}{\left[\zeta^4 G_{\zeta}^2 - \Lambda(1 + \theta e^G) \widetilde{T}\right] \frac{\hat{m}_{ev}}{Sc}} \frac{d^2 \zeta^2 G_{\zeta}}{d\zeta^2} = -G_{\zeta\zeta} + G_{\zeta} \frac{\Lambda \left(G_{\zeta} \theta e^G \widetilde{T} + (1 + \theta e^G) \widetilde{T}_{\zeta}\right) + 2\zeta^3 G_{\zeta}^2}{\Lambda(1 + \theta e^G) \widetilde{T} - \zeta^4 G_{\zeta}^2}$$

 $\Lambda = \frac{RT_{\infty}R_0^2}{Mm_{\nu}D_{\nu}^2}$ $\theta = \frac{Mm_{\nu} - Mm_g}{Mm_g}$

In a large variety of conditions of practical interest the parameter Λ assumes quite large values; the asymptotic condition $\Lambda \rightarrow \infty$ yields the following simplified form of the equation

$$G_{\zeta\zeta} = G_{\zeta} \left[\frac{\theta e^G G_{\zeta}}{(1 + \theta e^G)} + \frac{\tilde{T}_{\zeta}}{\tilde{T}} \right]$$

[1] S. Tonini and G.E. Cossali, An analytical model of liquid drop evaporation in gaseous environment, International Journal of Thermal Sciences, 57, (2012), 45-53.

Variable gas density Evaporation rate

$$G(\zeta) = \ln\left(\frac{e^{AF(\zeta)+B}}{1-\theta e^{AF(\zeta)+B}}\right) \qquad \hat{P}_{\nu s} = \frac{P_{\nu s}Mm_{\nu}}{RT_{\infty}\rho_{\infty}} = \chi_{\nu s}\tilde{\rho}_{s}\tilde{T}_{s}.$$

Boundary conditions









Variable gas density Isothermal case (T_{drop}=T_{gas})



S-F model underestimate evaporation rate when M_{vap}/M_{gas} <1



Discrepancies increase with drop temperature and vapour molar weight



Variable gas density Extension to Re>0



The B.C. at free flow are moved to the film boundary

Thermal film thickness: $R_2 - R_0$ Diffusional film thickness: $R_3 - R_0$

The solution for the non-dimensional evaporation rate is now:

$$Y + (\tilde{T}_{s} - 1) \left(Y \frac{e^{-Y\zeta_{2}}}{(e^{-Y\zeta_{2}} - e^{-Y})} - \frac{e^{-Y\zeta_{3}} - e^{-Y}}{(e^{-\zeta_{2}Y} - e^{-Y})(1 - \zeta_{3})} \right) = \frac{\Gamma}{1 - \zeta_{3}} \ln(1 + B_{M}^{*})$$

$$\zeta_{2} = \frac{R_{0}}{R_{2}}$$

$$B_{M}^{*} = \frac{\hat{P}_{\nu s} - \chi_{\nu, \infty}}{\hat{P}_{\nu, cr} - \hat{P}_{\nu, s}}$$

$$\hat{P}_{\nu, cr} = 1 + \theta(1 - \chi_{\nu, \infty})$$

Variable gas density Extension to Re>0: thermal film thickness

The heat rate in non-dimensional form

$$\tilde{Q} = \frac{Q}{4\pi R_0 k T_\infty} = \left(\tilde{T}_s - 1\right) \frac{Y e^{-Y}}{e^{-Y\zeta_2} - e^{-Y}}$$

can be written by introducing the usual definition of Nusselt number

 $\tilde{Q} = \frac{Nu^*}{2} \left(\tilde{T}_s - 1 \right) \quad \text{then} \qquad \zeta_2 = 1 - \frac{1}{Y} \ln \left(1 + \frac{2Y}{Nu^*} \right)$ $Nu^* = \frac{2 + 0.6 \operatorname{Re}_f^{1/2} Pr_f^{1/3}}{1 + B_f} \qquad B_f = \frac{c_f (T_\infty - T_s)}{h_{LV}}$ Spalding number $Properties \qquad T_f = T_s + \alpha_f (T_\infty - T_s) \qquad \alpha_f = 1/2 \quad (\text{from [3]})$ $\chi_f = \chi_s + \alpha_f (\chi_\infty - \chi_s) \qquad \alpha_f = 1/3 \quad (\text{from [4]})$

[3] M. Renksizbulut and M.C. Yuen, 105 (1983) 384-388
[4] M.C. Yuen and L.W. Chen, Combust. Sci. Tech., 14 (1976), 147-154

Variable gas density Extension to Re>0: thermal film thickness

The diffusional film thickness is estimated from an analogy with the model of Abramzon and Sirignano, largely used to account for the convection effects on droplet evaporation without assuming explicit dependence of gas density on temperature and species concentrations

Abramzon-Sirignano model

$$Y^{A-S} = \frac{Sh^{A-S}}{2Le} \ln(1+B_M)$$
 $B_M = \frac{\chi_{\nu,s} - \chi_{\nu,\infty}}{1-\chi_{\nu,s}}; Sh^{A-S} = 2 + \frac{(Sh_0 - 2)}{F_M(B_M)}$
 $Sh_0 = 2 + 0.552 \operatorname{Re}_f^{1/2} Pr_f^{1/3}$ $F_M(B_M) = (1+B_M)^{0.7} \frac{\ln(1+B_M)}{B_M}$

For Re=0 $Y_{\text{Re}=0}^{A-S} = \frac{1}{Le} \ln(1+B_M) \qquad \qquad Y_{\text{Re}=0} + (\tilde{T}_s - 1) \left(\frac{Y_{\text{Re}=0}}{1 - e^{-Y_{\text{Re}=0}}} - 1\right) = \Gamma \ln(1+B_M^*)$ Abramzon-Sirignano $\Gamma = \frac{\hat{P}_{v,cr}}{Le}$

Variable gas density Extension to Re>0: thermal film thickness

RHS Abramzon-S	RHS This model			
$\frac{1}{Le}\ln(1+B_M)$	Re=0	$\Gamma \ln(1+B^*_M)$		
$\frac{Sh^{A-S}}{2Le}\ln(1+B_M)$	Re>0	$\frac{Sh^*}{2}\Gamma\ln(1+B_M^*)$		

This assumption yields

$$\zeta_3 = 1 - \frac{2}{Sh^*}$$
 $Sh^* = 2 + \frac{(Sh_0 - 2)}{F_M(B_M^*)}$

And the final relation for the non-dimensional evaporation rate is

$$Y + (\tilde{T}_s - 1) \frac{Nu^*}{2} \left[1 + \frac{2Y}{Nu^*} - \frac{Sh^*}{2Y} \left(e^{\frac{2Y}{Sh^*}} - 1 \right) \right] = \frac{Sh^*}{2} \Gamma \ln(1 + B_M^*)$$

Variable gas density Extension to Re>0: validation

Four experimental databases were selected among the ones available in the scientific literature: Ranz-Marshal, Downing, Eisenklam et al., Wong-Lin.

Many additional experimental data can be found in the open literature, but they were not included in this study since they do not report all the needed information about the operating conditions and experimental results requested to correctly reproduce the test cases.

Ranz-Marshal, Downing, Eisenklam et al., report data about steadystate (or quasi-steady state) evaporation experiments

Wong-Lin reports data about transient evaporation

Variable gas density

Extension to Re>0: validation (database [5])

The liquid temperature is either calculated through an energy balance or by imposing the values reported by [5] that are about 5K (water) to 10K (benzene) higher than the calculated ones

Quasi steady-state volumetric evaporation rate Liquid temperature: 278.6K - 301K (water) ; 270.9K- 276.7K (benzene).



Both models yield better results when the liquid temperature is calculated. The present model behaves slightly better for benzene.

[5] Ranz and Marshall, Chemical Engineering Progress, 48(4), (1952) 141-146.

Variable gas density

Extension to Re>0: validation (database [6])

Air/drop temperature difference for benzene drops as function of T_{gas}



Modelling of liquid temperature

variation was included in these

calculations, ITC and IMD were used

The model agrees well with the experimental measurements, particularly at higher air temperature conditions, where the non-uniformity of gas density is expected to play a major role



Time evolution of drop size for hexane drop evaporating in air at different T_{gas}

[6] Downing C.G., AIChE Journal, 12(4) (1966) 760-766.

Variable gas density Extension to Re>0: validation (database [7])

Drop diameter square over time for heptane drops. Gas temperature: 473K, 673K and 873K.



A-S model overpredict evaporation rates at higher temperatures. The air/drop temperature difference is equally predicted

[7] P. Eisenklam, S.A. Arunachalam and J.A Weston, 11th Symp. on Combustion, The Combustion Institute, Pittsburgh, P.A., (1967) 715-728.

Variable gas density Extension to Re>0: validation



The experimental data reported in [7] are not distinguished according to the air temperature (473K-873K)

The parameter Ψ was then calculated at each selected Reynolds number assuming the air temperature equal to 473K, 673K and 873K.

Then for both models, three sets of data predictions are plotted, the region comprised between the predictions at T_{gas} =473K and T_{gas} =873K should encompass the experimental data.

Variable gas density Extension to Re>0: validation (database [8])

Wong&Lin measured the temporal evolution of drop size and temperature for a decane drop evaporating in air at 1000K and with initial Reynolds number equal to 17.



The model predicts, with a satisfactory agreement, the drop size reduction and the temperature increase.

The effect of variable gas density taken into account by the model seems to play a dramatic role under high evaporating conditions.

[8] S.C. Wong and A.C. Lin, Journal of Fluid Mechanics, 237 (1992) 671-687

Droplet heating and evaporation with variable parameters

Next steps



Why non-spherical drops?

Drop-gas interaction activates many drop oscillation modes and actually no droplet in a gaseous stream can be steadily spherical, and the surface area increment is expected to increase the evaporation rates

Available studies are limited to numerical simulations. Mashayek [9] proposed a correlation for the instantaneous nondimensional evaporation rate of oscillating drop, derived from numerical simulations:

$$m_{ev} = \frac{m_{ev}}{4\pi R_0 \rho D_v} = \left[1 + G_n \mathcal{E}_n \left(1 + \cos\left(2\omega t\right)\right)\right] \ln\left(\frac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}}\right)$$

$$\epsilon_n = \sqrt{\frac{\beta - 1}{0.8}} \qquad \beta = \frac{A_{deformed}}{A_{sphere}} \qquad \frac{\beta}{1.196}$$

[9] F. Mashayek, Int. J. Heat Mass Transfer 44(8) (2001) 1527-1541

Non-spherical drops Why spheroids?

The oscillation modes of droplet in gaseous environment can be described (for small oscillation amplitude) by the generalised Lamb equation:

$$\omega_n^2 = \frac{n(n+1)(n-1)(n+2)}{(n+1)\rho_{inner} + n\rho_{outer}} \frac{\sigma}{R_0^3}$$

n=0: pure expansion (bubbles)n=1: translationn=2 oblate-prolate moden>2: more complex modes

For a liquid drop in a gas:
$$\omega_2 = \sqrt{\frac{8}{\rho_L} \frac{\sigma}{R_0^3}}$$

Non-linear theory yields more accurate (but more complex) results, among others the fact that the time spent in the oblate form is larger than that spent in a prolate form. Considering the effect of liquid viscosity, the higher modes are quickly damped and the mode n=2 is the only long lasting one.



Non-spherical drops spheroids

Oblate $a_1 > a_3$; $\varepsilon < 1$ Prolate $a_3 > a_1$; $\epsilon > 1$ $\frac{x^{2}}{a_{1}^{2}} + \frac{y^{2}}{a_{1}^{2}} + \frac{z^{2}}{a_{3}^{2}} = 1$ $\varepsilon = \frac{a_{3}}{a_{1}}$ 2a₁_ $2a_3$ Isovolume drop $R_0^3 = a_1^3 \varepsilon$ $\beta = \frac{A_{sd}}{A_{sphere}} = \frac{1}{2\varepsilon^{2/3}} \begin{cases} \varepsilon^2 \ln\left(\frac{1+\sqrt{1-\varepsilon^2}}{\varepsilon}\right) & -\frac{1}{2\varepsilon^2} \\ 1+\frac{\varepsilon^2 \operatorname{drc} \operatorname{tan}\left(\sqrt{\varepsilon^2-1}\right)}{\sqrt{1-\varepsilon^2}} & \operatorname{Oblate} \\ 1+\frac{\varepsilon^2 \operatorname{drc} \operatorname{tan}\left(\sqrt{\varepsilon^2-1}\right)}{1+\frac{\sqrt{1-\varepsilon^2-1}}{2\varepsilon^2}} & \operatorname{Prolate} \end{cases}$ Oblate Prolate

Non-spherical drops Spheroidal coordinates

Oblate $a_1 > a_3$; $\epsilon < 1$



 $x = a \cosh(\xi) \sin(\theta) \cos(\varphi)$ $y = a \cosh(\xi) \sin(\theta) \sin(\varphi)$ $z = a \sinh(\xi) \cos(\theta)$ Oblate spheroidal coordinates



Prolate $a_3 > a_1$; $\epsilon > 1$



 $x = a \sinh(\xi) \sin(\theta) \cos(\varphi)$ $y = a \sinh(\xi) \sin(\theta) \sin(\varphi)$ $z = a \cosh(\xi) \cos(\theta)$

Prolate spheroidal coordinates

Mathematical model

(α=g,v)

 $\nabla_{j} n_{j}^{(\alpha)} = 0$ Conservation equation $n_{j}^{(\alpha)} = \rho U_{j} \chi^{(\alpha)} - \rho D_{\nu} \nabla_{j} \chi^{(\alpha)}$ Constitutive equation

Constant gas density and diffusivity

Oblate and prolate cases can be treated in a unique manner:

$$\Phi_{\pm}(\xi) = \frac{e^{\xi} \pm s(\varepsilon)e^{-\xi}}{2} \qquad \qquad x = a \Phi_{-}(\xi)\sin(\theta)\cos(\varphi)$$
$$s(\varepsilon) = \begin{cases} -1 \text{ oblate} \\ +1 \text{ prolate} \end{cases} = sign(\varepsilon - 1) \qquad \qquad y = a \Phi_{-}(\xi)\sin(\theta)\sin(\varphi)$$
$$z = a \Phi_{+}(\xi)\cos(\theta)$$

in these coordinate systems the drop surface is defined by the simple equation $\xi = \xi_0$

The spheroidal drop has a volume corresponding to that of a sphere of radius R_0 ,

$$\xi_0 = \ln \sqrt{\frac{\epsilon^s + 1}{\epsilon^s - 1}}; \ a = R_0 \frac{|1 - \epsilon^2|^{1/2}}{\epsilon^{1/3}}$$

Non-spherical drops Mathematical model

Given the following B.C.
$$\xi = \xi_0$$
: $\chi^{(\alpha)}(\xi_0, \theta, \varphi) = \chi^{(\alpha)}_s$
 $\xi = \infty$: $\chi^{(\alpha)}(\infty, \theta, \varphi) = \chi^{(\alpha)}_\infty$

the only non-nil components of the flux vector is n_{ξ} (1-D solution exists)

Accounting for the proper scale factors, the conservation equations in normalised basis, after using the mass conservation equation $\nabla_j \rho U_j = 0$ becomes:

$$\rho U \frac{\partial \chi^{(\alpha)}}{\partial \xi} = \frac{D_{\nu}}{aS^2} \frac{\partial \rho \Phi_{-}(\xi) \frac{\partial \chi^{(\alpha)}}{\partial \xi}}{\partial \xi}$$
$$S^2(\xi, \theta) = \left[\Phi_{-}^2(\xi) + s(\varepsilon) \sin^2(\theta) \right]^{1/2} \Phi_{-}(\xi)$$
$$= \Phi_{-}(\xi) \left[\Phi_{-}^2(\xi) \cos^2(\theta) + \Phi_{+}^2(\xi) \sin^2(\theta) \right]^{1/2}$$

Mathematical model

$$\chi^{(\alpha)} = \begin{cases} K_0^{(\alpha)} e^{2K_2 \arctan(e^{\xi})} + \frac{K_1^{(\alpha)}}{K_2} & \text{oblate } (s = -1) \\ K_0^{(\alpha)} e^{K_2 \ln\left(\frac{e^{\xi}-1}{e^{\xi}+1}\right)} + \frac{K_1^{(\alpha)}}{K_2} & \text{prolate } (s = 1) \end{cases}$$

$$\alpha = v, g \quad \text{and applying the B.C.} \\ \chi_{v}(\xi) = 1 - (1 - \chi_{v,s}) \begin{cases} \left(\frac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}}\right)^{\frac{\arctan e^{\xi} - \arctan e^{\xi_{0}}}{\pi/2 - \arctan e^{\xi_{0}}} & \text{oblate (s=-1)} \\ \left(\frac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}}\right)^{1 - \frac{\ln(e^{\xi} + 1) - \ln(e^{\xi} - 1)}{\ln(e^{\xi_{0}} + 1) - \ln(e^{\xi_{0}} - 1)}} & \text{prolate (s=+1)} \end{cases}$$

And the evaporation rate can be evaluated as

$$\dot{m}_{ev} = \int_{A_{sphd}} \rho U dA = 2\pi a^2 C_0 \int_0^{\pi} \sin(\theta) d\theta = 4\pi a^2 \frac{\rho D_v}{a} K_2$$
$$= \frac{4\pi \rho D_v a}{\ln \left(-\frac{1 - \sqrt{s} e^{\xi_0}}{1 + \sqrt{s} e^{\xi_0}} \right)^{\sqrt{s}}} \ln \frac{1 - \chi_s^{(v)}}{1 - \chi_{\infty}^{(v)}}$$

Non-spherical drops Evaporation rate

The evaporation rate can be written as a "correction" of that found for a spherical drop

$$\widehat{m}_{ev} = \Gamma(\varepsilon) \ln \frac{1 - \chi_{\infty}^{(v)}}{1 - \chi_{s}^{(v)}} \quad \Gamma(\varepsilon) = \frac{\left|1 - \varepsilon^{2}\right|^{1/2}}{\varepsilon^{1/3}} \begin{cases} \frac{1}{\left(\pi - 2 \arctan\left(\sqrt{\frac{1 + \varepsilon}{1 - \varepsilon}}\right)\right)} & \text{oblate } (s = -1) \\ \frac{1}{\ln\left(\sqrt{\frac{s + 1}{s - 1}} + 1\right) - \ln\left(\sqrt{\frac{s + 1}{s - 1}} - 1\right)} & \text{prolate } (s = 1) \end{cases}$$

This can also be evaluated as a function of the spheroid area: $\beta = \frac{A_{sphd}}{A_{sph}} = \frac{A_{sphd}}{4\pi R_0^2}$



The prolate drop evaporates more rapidly than an oblate drop having the same volume and surface (not described by the model [9]).

$$Q = \frac{Q}{4\pi R_0 k_g T_{\infty}} = \Gamma(\varepsilon) \left(\tilde{T}_s - 1\right) \left(\frac{e^{-T}}{1 - e^{-Y}}\right) Y$$

is found for the
heat rate
$$Y = \frac{1}{Le} \ln \left(\frac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}}\right)$$

 $v \rightarrow$



Local flux

The vapour concentration gradients are related to the local surface curfature and so must be for the vapour flux.

[9] suggested a linear correlation with the local mean curvature.

From the solution $n_{\xi}^{(\nu)} = \frac{\varepsilon^{2/3}}{|1 - \varepsilon^2|S^2(\xi, \theta)|} \frac{m_{e\nu}}{4\pi R_0^2}$

And at drop surface:

 $n_{\xi,s}^{(\nu)} = \hat{n}_{\xi,s}^{(\nu)} \frac{m_{e\nu}}{4\pi R_0^2}$

0.08 χ^(v) 0.20







The curvature of a surface can be defined completely by evaluating the two principal curvatures: k_1 , k_2

Two independent curvature (mean and Gaussian curvatures) can be defined

$$k_m = k_1 + k_2$$
$$C_G = k_1 k_2$$

From a geometric view point they are quite different since C_G is an intrinsic property of the surface, and can be obtained from the surface metric only, while k_m depends on the 3-D space into which the surface is embedded.





Non-spherical drops Curvatures

Mahayek [11] proposed a correlation to express the local mass flux as a function of the surface curvature, based on the suggestion of Lian and Reitz [12] who studied the instability of evaporating liquid jets, postulating that the deformed surface may be locally considered as the surface of a spherical drop having the same mean curvature as that of the deformed surface, and that the local flux would be that of a spherical drop with that curvature radius.

From the present solution, the mass flux at drop surface is proportional to the fourth rooth of the nondimensional Gaussian curvature:





[11] F. Mashayek, Int. J. Heat Mass Transfer 44(8) (2001) 1517-1526.[12] Z.W. Lian, R.D. Reitz, Atomization Sprays 3 (3) (1993) 249-264.

Non-spherical drops Oscillating drops

The spheroid surface oscillates with

 $a_n(t) = a_n^0 e^{i\omega_n t}$

 $R(\theta) = R_0 \left(1 + \sum_{n=2} \frac{a_n(t)}{2n+1} P_n(\cos \theta) \right)$

$$\beta(t) = \frac{A_{spheroid}}{A_{sphere}} = 1 + \frac{2}{5} (a_2^0)^2 \sin^2(\omega_2 t) = 1 + \Delta\beta \sin^2(\omega_2 t)$$

Under the assumption of quasi-steady drop evaporation, the nondimensional instantaneous evaporation rate and heat rate depend on time by the relations:

$$\begin{split} \hat{m}_{ev} &= \Gamma(\beta(t)) \ln \left(\frac{1-\chi_{v,\infty}}{1-v_{v,\infty}}\right) = \Gamma(\beta(t)) \hat{m}_{ev}^{sphere} \\ \tilde{Q} &= \Gamma(\beta(t)) (\tilde{T}_s - 1) \left(\frac{e^{-\frac{\hat{m}_{ev}^{sphere}}{L_e}}}{1-e^{-\frac{\hat{m}_{ev}^{sphere}}{L_e}}}\right) \frac{\hat{m}_{ev}^{sphere}}{Le} \end{split}$$

Oscillating drops



Non-linear analysis shows that drops, which are released from an initially two lobed configuration, spend less time as a prolate form than as an oblate one. Here linear theory results are used.

> Mashayek [9] proposed a correlation for the instantaneous non-dimensional evaporation rate of oscillating drop.

$$\hat{m}_{ev}^{spheroid} = \left[1 + 0.6 \left(\frac{\beta - 1}{0.8}\right)^{1/2} \left(1 + \cos\left(2\omega t\right)\right)\right] \ln\left(\frac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}}\right)$$

It does not account for different behaviour from oblate to prolate

 $\Delta\beta$ = non-dimensional maximum excess area from the spherical state.

Quasi-steady state assumption

$$\tau_{oscill} \approx \sqrt{\frac{\rho_l R_0^3}{\sigma}}$$

The characteristic time scale of the oscillatory process (assuming n=2) can be defined as the inverse of the oscillation frequency:

quasi-steady-state assumption may be acceptable when: $t_{evap} \ll t_{oscill}$

Evaporation from a drop is an overlapping of mass and thermal diffusive (driven by the thermal α and mass diffusivity D_v coefficients respectively) and convective phenomena (Stefan flow, driven by a characteristic velocity U₀).

$$U_0 = \frac{\dot{m}_{e\nu}}{\beta 4\pi R_0^2 \rho} = \frac{\hat{m}_{e\nu}}{\beta} \frac{D_\nu}{R_0}$$

Characteristic timesMass transferHeat transferconvective $t_{conv} \approx \frac{R_0}{U}$ $t_{conv}^H \approx \frac{R_0}{U}$ diffusive $t_{diff} \approx \frac{R_0^2}{D_v}$ $t_{diff}^H \approx \frac{R_0^2}{\alpha} = \frac{t_{diff}}{L_e}$ convective-diffusive $t_{cd} \approx \frac{D_v}{U^2} = \frac{t_{conv}^2}{t_{diff}}$ $t_{cd}^H \approx \frac{\alpha}{U^2} = t_{cd}Le$

These characteristic times are not all independent

Quasi-steady state assumption



Since
$$\frac{\beta}{\hat{m}_{ev}} > 1$$
 for $\varepsilon \lesssim 42.7$
max[t_{cd}, t^{H}_{ev}] > max[t_{conv}, t^{H}_{conv}] > max[$t_{diff_{ev}}$

The evaporation characteristic time scale may be one of the three above mentioned characteristic times, but the condition t_{evap}<<t_{oscill} is certainly satisfied if: $\max[t_{cd}, t_{cd}^H] \ll t_{oscill}$

$$\frac{D_{\nu}^{2}(T_{film})\rho_{l}\ln^{4}(1-\chi_{\nu,s})}{2.074\sigma(T_{s})} = R_{lim} \gg R_{0}$$

$$\left(\frac{\beta}{\Gamma(\beta)}\right)^{2} \frac{R_{0}^{2}}{\left(\hat{m}_{ev}^{sphere}\right)^{2} D_{v}} \max[1, Le] = \max[t_{cd}, t_{cd}^{H}]$$

Quasi-steady state assumption

The temperature dependence of D_v and σ yield, for each value of R_{lim} , a relation between T_{gas} and T_{drop} that defines on a T_{gas} - T_{drop} plane a region where the condition t_{evap} < t_{oscil} holds

An inspection of the diagrams shows that the inequality (and then the quasi-steady assumption) may acceptably hold for small drops (few tenths of micron) in hot gaseous environment and for high volatility fluids.



Extend the results to a wider class of deformed drops

Find possible relation between local vapour flux and curvature Some results already obtained, a generalize theory for 1-D evaporation is available. Triaxial ellipsoid solved.

The 1-D evaporation approach support the conjecture that the proportionality of vapour flux and the fourth root of the nondimensional gaussian curvature may hold for a larger class of drop shapes.

$$n_{\xi,s}^{(\nu)} = \left(R_0^2 K_G\right)^{1/4} \frac{m_{e\nu}}{4\pi R_0^2}$$

Multicomponent drop evaporation

Multicomponent drop evaporation basic

A possible approach is through the approximation of single component: The vapour mixture is treated as a single component vapour and

 $\bar{D}^{(v,0)}$ is the diffusion coefficient of the mean vapour mixture in air, that can be calculated according to the Wilke and Lee formula

$$\begin{split} \bar{D}^{(\nu,0)} &= \frac{3.03 - \frac{0.98}{\sqrt{\bar{M}^{(\nu,0)}}} 10^{-2} T^{3/2}}{P \sqrt{\bar{M}^{(\nu,0)}} (\bar{\sigma}^{(\nu,0)})^2 \Omega_D} \\ \bar{M}^{(\nu,0)} &= \frac{n+1}{\sum_{j=0}^n \frac{1}{M_m^{(j)}}} \\ \bar{\sigma}^{(\nu,0)} &= \frac{\sum_{j=0}^n \sigma^{(j)}}{n+1} \end{split}$$

that takes into account the physical properties of each species.

The evaporation ratios for each species are calculated as:

The result is then again the usual formula: $\dot{m}_{ev}^{(T) \, [Model \, 1]} = 4\pi R_0 \rho_{ref} \bar{D}^{(v,0)} \ln \left(1 + B_M^{(m)}\right)$

$$\boldsymbol{\varepsilon}^{(k)} = \frac{m_{ev}^{(k)}}{m_{ev}^{(T)}} = \frac{\boldsymbol{\chi}_s^{(k)}}{\sum_{j=1}^N \boldsymbol{\chi}_s^{(j)}}$$

[13] S.S. Sazhin, et. al. International Journal of Heat and Mass Transfer 53 (2010) 4495-4505.

Multicomponent drop evaporation basic

A semi-empirical approach that account for different diffusivities of the species is reported in [14]

$$\dot{m}_{ev}^{(k) \ [Model \ 2]} = 4\pi R_V^{(k)} \rho_{ref} D^{(k,0)} \ln\left(1 + B_M^{(k)}\right)$$

$$R_V^{(k)} = R_0 \sqrt[3]{\varphi^{(k)}}$$

$$B_M^{(k)} = \frac{\chi_s^{(k)} - \chi_\infty^{(k)}}{1 - \chi_s^{(k)}}$$
Where $R_V^{(k)}$ is the function of the spectrum the liquid mixture diffusivity of pure

Where $R_V^{(k)}$ is the equivalent drop radius, function of the species volume fraction in the liquid mixture $\varphi^{(k)}$, $D^{(k,0)}$ is is the gas diffusivity of pure species k in air at reference condition.

[14] G. Brenn et al., International Journal of Heat and Mass Transfer 50 (2007) 5073--5086.

Multicomponent drop evaporation

Model equations

K=1,...,n stands for the n evaporating species, k=0 for the gas. D^(k,m) is the the mass diffusion coefficient for the species k in the gaseous mixture and it can be aproximated by Blanc's law [16] or Wilke's law [17].

$$D^{(k,m)} = \left(\sum_{j=0; \, j \neq k}^{n} \frac{\chi_{ref}^{(j)}}{D^{(k,j)}}\right)^{-1} \qquad D^{(k,m)} = \frac{1 - y_{ref}^{(k)}}{\sum_{j=0}^{n} \frac{y_{ref}^{(j)}}{D_{jk}}}$$

Blanc's law
Wilke's law

D^(k,m) depend on species concentrations and they are calculated at reference conditions

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[15] Zhang, L., Kong, S.-C., Fuel 95 (2012) 471-480
[16] M.A. Blanc, J. Phys. 7 (1908) 825.
[17] D.F. Fairbanks, C.R. Wilke, Ind. Eng. Chem. (1950) 471-475
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$$\chi_{ref}^{(j)} = \frac{2\chi_s^{(j)} + \chi_{\infty}^{(j)}}{3}$$

Multicomponent drop evaporation Solution



Multicomponent drop evaporation Extension to Re>0

Extension to Re>0 assumes that the evaporating drop is surrounded by different mass diffusional regions, which thickness depend on the physical properties of each species, based on the hypothesis that the interaction of the evaporating species is small (see also [18])

$$\begin{split} \dot{m}_{ev,c}^{(k)} &= \frac{Sh^{(k)}}{2} \dot{m}_{ev}^{(k)} \qquad \varepsilon_{c}^{(k)} &= \frac{Sh^{(k)}\varepsilon^{(k)}}{\sum_{j=1}^{n}Sh^{(j)}\varepsilon^{(j)}} \\ Sh^{(k)} &= 2 + \frac{Sh_{0}^{(k)} - 2}{F_{M}\left(B_{M}^{(m)}\right)} \qquad B_{M}^{(m)} &= \frac{\sum_{k=1}^{n}\chi_{s}^{(k)} - \sum_{k}^{n}\chi_{\infty}^{(k)}}{1 - \sum_{k=1}^{n}\chi_{s}^{(k)}} \\ Sh_{0}^{(k)} &= 2 + 0.552\sqrt{\operatorname{Re}}\sqrt[3]{Sc^{(k)}} \qquad B_{M}^{(m)} &= \frac{\left(1 + B_{M}^{(m)}\right)^{0.7}\log(1 + B_{M}^{(m)})}{B_{M}^{(m)}} \qquad \operatorname{Basically, an extension of Abramzon-Sirignano (1989) model to multicomponent} \\ Sc^{(k)} &= \frac{V}{D^{(k,m)}} \end{split}$$

[18] S. Tonini, G.E. Cossali, 2015, Int. J. Therm. Sci. 89 (2015) 245-253

$$\begin{split} \dot{m}_{ev}^{(T) \, [Model \, 1]} &= 4\pi R_0 \rho_{ref} \bar{D}^{(v,0)} \ln \left(1 + B_M^{(m)}\right) \qquad \bar{D}^{(v,0)} = \frac{3.03 - \frac{0.98}{\sqrt{M}^{(v,0)}} 10^{-2} T^{3/2}}{P \sqrt{M}^{(v,0)} (\bar{\sigma}^{(v,0)})^2 \Omega_D} \\ \dot{m}_{ev}^{(k) \, [Model \, 2]} &= 4\pi R_V^{(k)} \rho_{ref} \bar{D}^{(k,0)} \ln \left(1 + B_M^{(k)}\right) \\ R_V^{(k)} &= R_0 \sqrt[3]{\varphi^{(k)}} \qquad B_M^{(k)} = \frac{\chi_s^{(k)} - \chi_\infty^{(k)}}{1 - \chi_s^{(k)}} \\ \dot{m}_{ev}^{(T) \, [Model \, 3]} &= 4\pi R_0 \rho_{ref} \bar{D}^{(v,m)} \ln \left(1 + B_M^{(m)}\right) \qquad B_M^{(m)} = \frac{\sum_{k=1}^n \chi_s^{(k)} - \sum_k^n \chi_\infty^{(k)}}{1 - \sum_{k=1}^n \chi_s^{(k)}} \\ \bar{D}^{(v,m)} &= \frac{\sum_{k=1}^n \chi_{ref}^{(k)} D^{(k,m)}}{\sum_{k=1}^n \chi_{ref}^{(k)}} \end{split}$$



Alkanes							
n-octane	-	-	-	-	-	0.33	0.33
n-decane	-	-	-	-	-	0.33	-
n-dodecane	-	-	-	-	-	0.33	0.33
n-tetradecane	1.	0.8	0.6	0.4	0.	-	-
n-hexadecane	0.	0.2	0.4	0.6	1.	-	0.33

Experimental Database available for comparison [19]

$$\delta m_{ev}^{[j]} = \frac{\dot{m}_{ev}^{[Model \, j]}}{\dot{m}_{ev}^{[Model \, 0]}}$$

Model 1 and 3 are in good agreement (model 3 is almost coincident) with the detailed multidiffusion model

Model 2, noticeably underestimates the evaporation rate for all the multicomponent drop test cases.

[19] J. Wilms, Evaporation of Multicomponent Droplets, PhD Thesis, Universität Stuttgart, 2005.



Model 1 and model 3 yields results quite close to that of the multidiffusion model for all the temperature ranges. Model 2 underestimates.



The effect of vapour composition at free stream conditions ($\chi_{oo}^{(k)}$) is tested for two drop compositions. The drop and gas temperatures are equal to 300 K and 500 K, respectively, and Re=0. The vapour mass fraction at free stream conditions of the first species in the drop composition has been varied from 0 up to the corresponding value at drop surface.

The simpler models (1 and 3) deviate at larger values of $\chi_{oo}^{(k)}$ for alkanes. This suggests that the detailed model should be preferred in case of fuel spray simulations, where the presence of vaporised fuel in the gas phase is higher, due to the evaporation of different liquid drops.



Multicomponent drop evaporation

Maxwell-Stefan equations

$$\begin{aligned} \nabla y^{(n)} &= \sum_{\substack{k=1 \ k \neq n}} \frac{1}{cD_{nk}} \left(y^{(n)} \mathbf{N}^{(k)} - y^{(k)} \mathbf{N}^{(n)} \right) \\ \text{Radial symmetry: } \zeta &= \mathbf{R}_0 / \mathbf{r} \qquad \hat{N}_{ev}^{(k)} = \frac{N_{ev}^{(k)}}{4\pi R_0 cD_{ref}} \qquad \varphi^{pk} = \frac{D_{ref}}{D_{pk}} \qquad \mathbf{v}^{(k)} = \frac{N_{ev}^{(k)}}{\sum_{p=1}^n N_{ev}^{(p)}} \\ \frac{dy^{(p)}}{d\zeta} &= -\hat{N}_{ev}^{(T)} \sum_{k=0}^n \varphi^{pk} (y^{(p)} \mathbf{v}^{(k)} - y^{(k)} \mathbf{v}^{(p)}) \qquad \sum_{k=0}^n y^{(k)} = 1 \\ \text{n independent equations} \end{aligned}$$

$$\begin{aligned} \frac{d}{d\zeta} \Psi &= \mathcal{A} \Psi + \mathbf{B} \\ \frac{d}{d\zeta} \Psi &= \mathcal{A} \Psi + \mathbf{B} \end{aligned} \qquad \mathcal{A} = \hat{N}_{ev}^{(T)} \begin{bmatrix} -\sum_{k=1}^{n} \varphi^{1k} v^{(k)} & v^{(1)}(\varphi^{12} - \varphi^{10}) & \dots & v^{(1)}(\varphi^{1n} - \varphi^{10}) \\ v^{(2)}(\varphi^{21} - \varphi^{20}) & -\sum_{k=1}^{n} \varphi^{2k} v^{(k)} & \dots & v^{(2)}(\varphi^{2n} - \varphi^{20}) \\ \dots & \dots & \dots & \dots \\ v^{(n)}(\varphi^{n1} - \varphi^{n0}) & v^{(n)}(\varphi^{n2} - \varphi^{n0}) & \dots & -\sum_{k=1}^{n} \varphi^{nk} v^{(k)} \end{bmatrix} \\ \Psi &= \begin{bmatrix} y^{(1)} & \dots & y^{(n)} \end{bmatrix}^{T} \\ \mathbf{B} &= \hat{N}_{ev}^{(T)} \begin{bmatrix} v^{(1)} \varphi^{10}, v^{(2)} \varphi^{20}, \dots, v^{(n)} \varphi^{n0} \end{bmatrix}^{T} \end{aligned}$$

Multicomponent drop evaporation Solution

A simple solution can be found assuming a constant value of the molar density c.

$$\boldsymbol{\Psi} = \boldsymbol{e}^{\mathcal{A}\boldsymbol{\zeta}} \cdot \boldsymbol{\mathsf{C}}_0 - \mathcal{A}^{-1}\boldsymbol{\mathsf{B}}$$

the vector \mathbf{C}_0 has to be determined from the B.C.:

$$\begin{split} \boldsymbol{\Psi}(1) &= \left[y_s^{(1)}, \dots, y_s^{(n)} \right] = \boldsymbol{\Psi}_s \\ \boldsymbol{\Psi}(0) &= \left[y_{\infty}^{(1)}, \dots, y_{\infty}^{(n)} \right] = \boldsymbol{\Psi}_{\infty} \end{split}$$

$$e^{\mathcal{A}}(\mathcal{A}\Psi_{\infty} + \mathbf{B}) - (\mathcal{A}\Psi_{s} + \mathbf{B}) = 0 \qquad \text{N+1}$$

$$\sum_{k} v^{(k)} = 1$$

N+1 algebraic equations for the n+1 unknown $\begin{pmatrix} v^{(k)}, \hat{N}_{ev}^{(T)} \end{pmatrix}$

[20] S. Tonini, G.E. Cossali, 2015, submitted to Int. J. Heat and Mass Transf.

Multicomponent drop evaporation

Fick's law based models



$$\varepsilon^{(k)} = \frac{Mm^{(k)}v^{(k)}}{\sum_{p=1}^{n}Mm^{(p)}v^{(p)}}; \quad m_{ev}^{(T)} = N_{ev}^{(T)}\sum_{p=1}^{n}Mm^{(p)}v^{(p)}$$

The two solutions are different also for single component drops, but in such case the solution of the molar form would yield exactly the same solution of the M-S model since in that case the two sets of equations are equivalent and the same assumption (c=const.) is made.

Multicomponent drop evaporation

Comparison

4x10⁴

Isothermal (T_{drop}=T_{gas})





50% ethanol / 50% acetone

S-M F^{molar}

Both the Fick's models underpredict the evaporation rate and the differences increase with the temperature.

Evaporation rate fractions predicted by the Fick's models, for the selected range of temperatures, differs from the S-M model predictions by 4% to 8%.

Same behaviour for other mixtures.

But for some combinations the difference may be larger

Total evaporation rate differs considerably for certain species combinations, mass fractions and temperature

The effect of non-isothermal drop evaporation is taken into account only through the values of the reference temperature at which molar and mass densities and diffusion coefficients are calculated

Multicomponent drop evaporation

Future developments

