Multicomponent-Liquid-Fuel Vaporization with Complex Configuration

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Major Goals: for multicomponent-liquid-fuel vaporization in a general geometrical situation, predict vaporization rate, interface scalars and scalar gas-phase profiles for any value of the Lewis number, with transient heat and mass diffusion in the liquid interiors.

Background

- Define mass-flux potential
- Transform the gas field equation to Laplace's equation assuming only Stefan convection
- Method of images to solve gas field with interaction droplets
- Reduce scalar properties to function of mass-flux potential only

Correlations and approach to solve the gas phase

Continuity: $\quad \nabla \cdot (\rho \vec{V}) = 0 \xrightarrow{\;\;\rho \vec{V} = \nabla \phi\;\;} \nabla^2 \phi = 0$

$\phi_S = 0$, ϕ_∞ determined by vaporization rates.

Species: $\quad \nabla \cdot (\rho \vec{V} Y_n - \rho D_n \nabla Y_n) = 0$

Energy: $\quad \nabla \cdot (\rho \vec{V} h_\varepsilon - \lambda \nabla T) = 0$

$$Le_{\varepsilon,n} = \frac{\overline{\lambda / c_{p,\varepsilon}}}{\overline{\rho D_n}}, \quad B_{M,n} = \frac{Y_{n,S}}{\varepsilon_n - Y_{n,S}}, \quad B_{H,\varepsilon} = \frac{h_{\varepsilon,\infty} - h_{\varepsilon,S}}{L_{eff}}$$

$$\Phi = \phi / \phi_\infty = \phi \Big/ \overline{\rho D_n} \ln[1 + B_{M,n}]$$

and satisfy: $\quad \nabla^2 \Phi = 0 ; \quad \Phi_{S=0} ; \quad \Phi_\infty = 1$

Correlations and approach to solve the gas phase (cont.)

Reduce scalar properties to function of mass flux potential only:

$$\frac{Y_n - \varepsilon_n}{Y_{n,S} - \varepsilon_n} = [1 + B_{M,n}]^{\overline{\rho D_n} \int_0^\Phi d\Phi' /(\rho D_n)}$$

$$\frac{h_\varepsilon - h_{\varepsilon,S} + L_{eff}}{L_{eff}} = [1 + B_{M,n}]^{\overline{\rho D_n} \int_0^\Phi d\Phi' /(\lambda/c_{p,\varepsilon})}$$

Determine $Y_{n,s}$,

$$Y_{n,s} = W_n X_{n,lS} \sum_{k=1}^{N} (Y_{k,S}/W_k) \, e^{L_n/RT_{b,n}} e^{-L_n/RT_s} \quad (n-1,...,N-2)$$

Determine ε_n and L_{eff},

$$[1 + B_{M,n}]^{1/Le_{\varepsilon,n}} = 1 + B_{H,\varepsilon} \quad (n = 1,...N-2)$$

Governing equations for liquid phase

$$\frac{\partial Y_{l,n}}{\partial t} = \frac{D_{l,n}}{R^2}\frac{\partial^2 Y_{l,n}}{\partial \varsigma^2} + [\frac{2D_{l,n}}{R^2 \varsigma} + \varsigma\, \dot{R}]\frac{\partial Y_{l,n}}{\partial \varsigma}$$

$$\frac{\partial T_l}{\partial t} = \frac{\alpha_l}{R^2}\frac{\partial^2 T_l}{\partial \varsigma^2} + [\frac{2\alpha_l}{R^2 \varsigma} + \varsigma\, \dot{R}]\frac{\partial T_l}{\partial \varsigma}$$

$$ICs:\ Y_{l,n}(\varsigma, t=0) = Y_{l,n0};\ T_l(\varsigma, t=0) = T_{l0}$$

$$BCs:\ \varepsilon_n = Y_{l,n}(\varsigma=1,t) + \frac{D_{l,n}}{R\dot{R}}\frac{\partial Y_{l,n}}{\partial \varsigma}(\varsigma=1,t)$$

$$\lambda_l \frac{\partial T_l}{\partial \varsigma}(\varsigma=1,t) = -\rho_l R\dot{R}\,[\frac{\sum_{k=1}^{N-2}\varepsilon_k(h_{k,\infty}-h_{k,S})}{(1+B_{M,n})^{1/Le_{\varepsilon,n}}-1} - \sum_{k=1}^{N-2}\varepsilon_k L_k]$$

Points of numerical calculation

- Eight droplets in a cubic array, with initial distance between droplets 10 times of initial droplet radius, and the ambient pressure 1 atm;

- The droplet is composed of three species: heptane, octane and decane ;

- Variable gas-phase properties ;

- The gas-phase mass diffusivities are binary mass diffusivities in nitrogen and vary in space and time;

- The liquid-phase diffusivity of a species is determined by weighting its binary mass diffusivities in other two species based on mass fraction, the binary mass diffusivities are given by semi-empirical equations.

Surface temperature and species mass fraction at the liquid surface

$T_\infty = 2000K$; $[Y_{l,0,1}, Y_{l,0,2}, Y_{l,0,3}] = [1/3, 1/3, 1/3]$. Surface temperature increases with time. Surface mass fraction of volatile components decreases while mass fraction of non-volatile components increases.
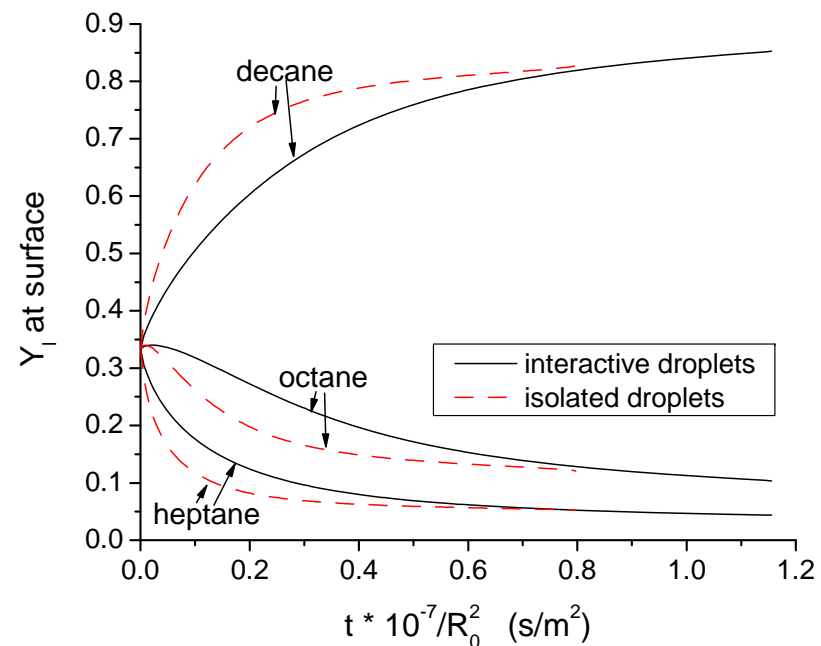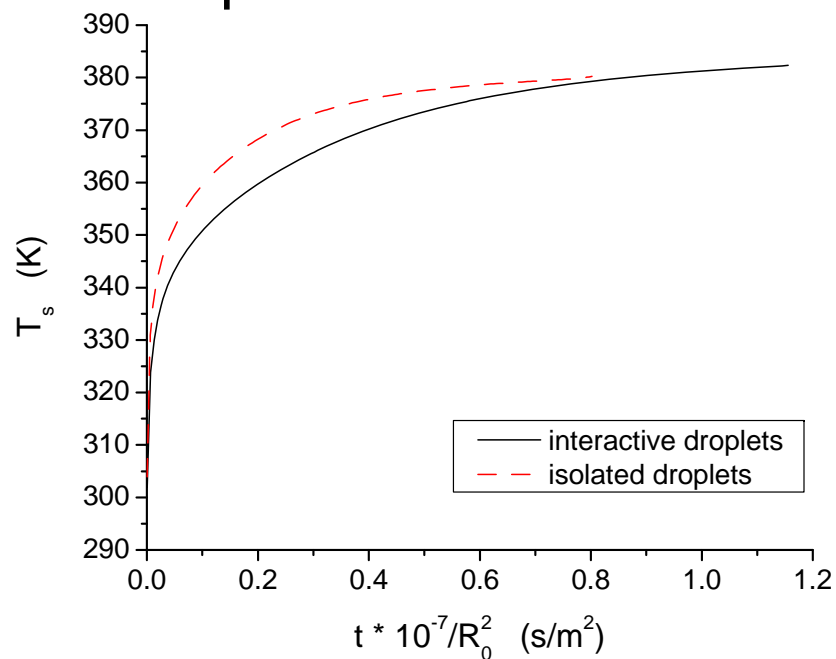
Actual boiling point

$1/T_{bi} - 1/T_{bi,pure} = R.\ln(X_{i,ls})/L_i$. Actual boiling point of volatile components increases while actual boiling point of non-volatile components decreases. The temperature at any location in the droplet will not exceed any component's actual boiling point at that location at any time.
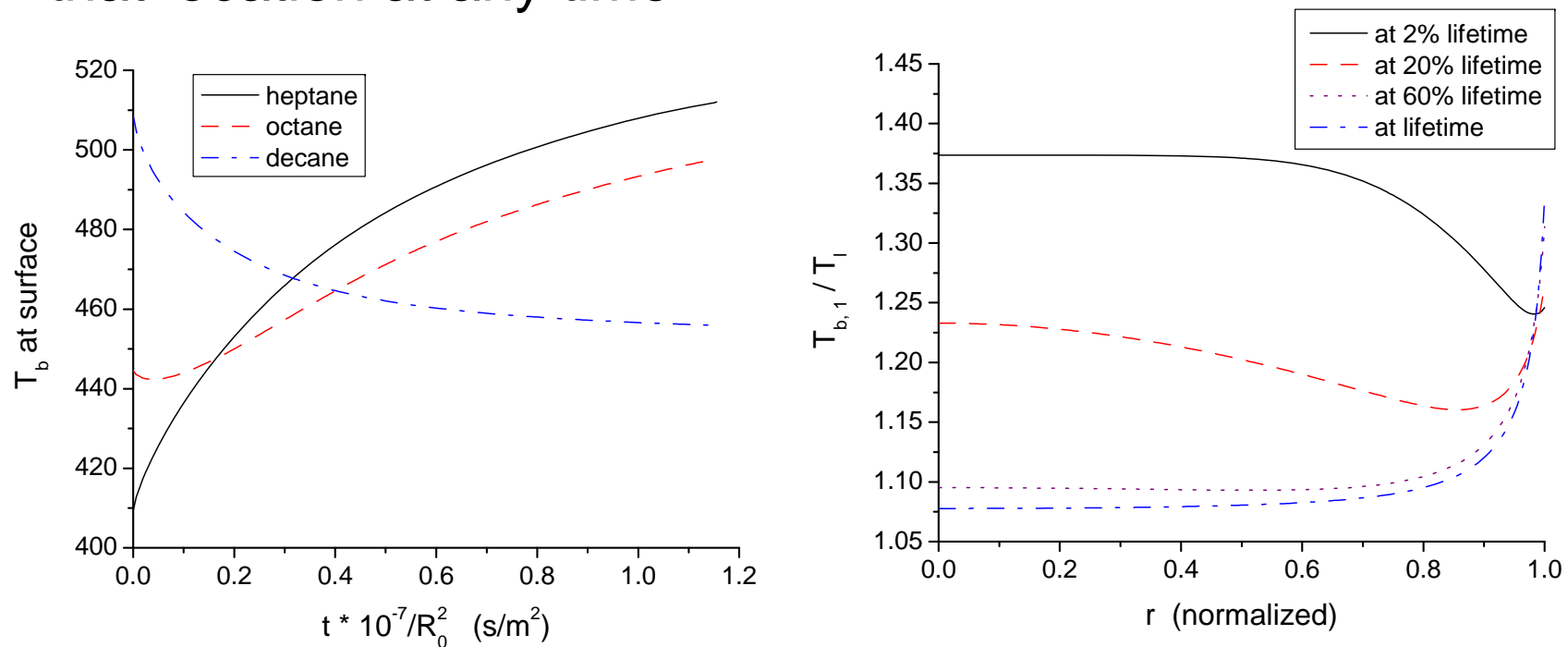
The shape of radius squared curves

The rate of decrease of radius squared normally become larger with time. But when the ambient temperature is very low, $B_{M,n}$ may decrease with time due to a strong distillation effect, and the $(R/R_0)^2 \sim t$ curve may consequently become concave.
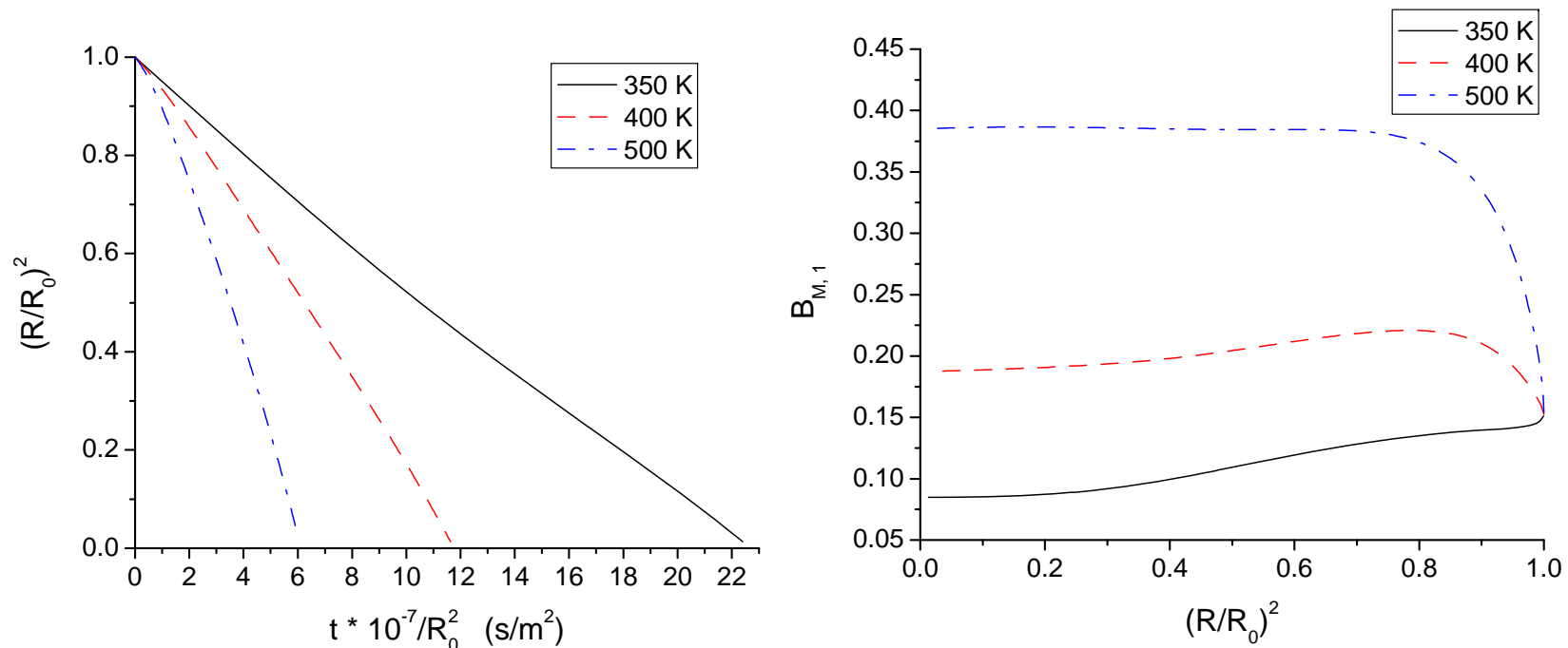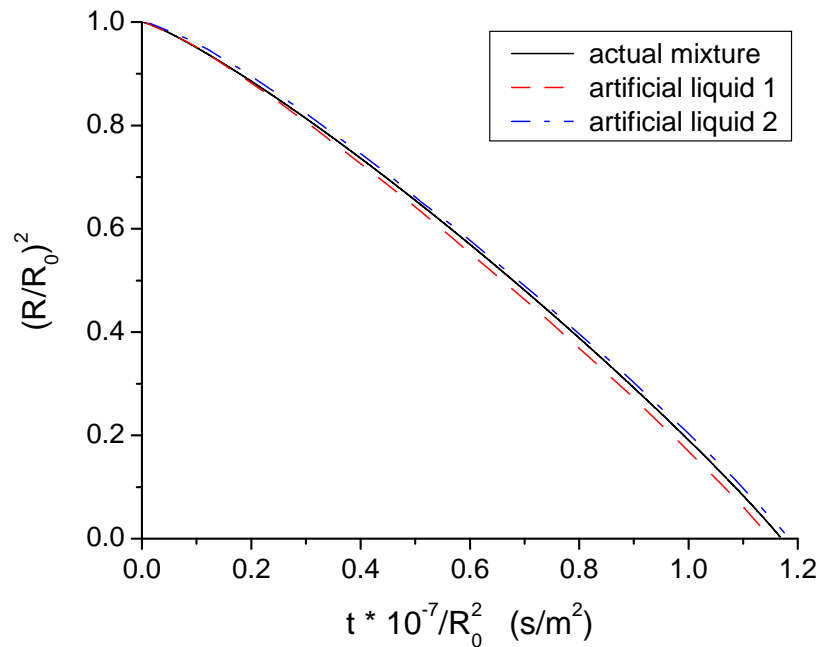
Comparisons of different cases

Higher ambient temperature always leads to faster vaporization rate. The mixture with greater fractions of the more volatile components has slightly faster radius squared rate of change.
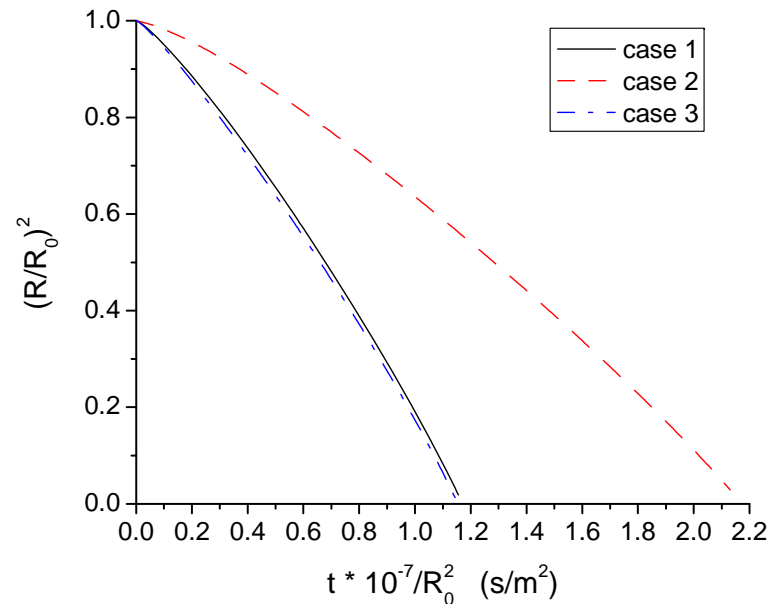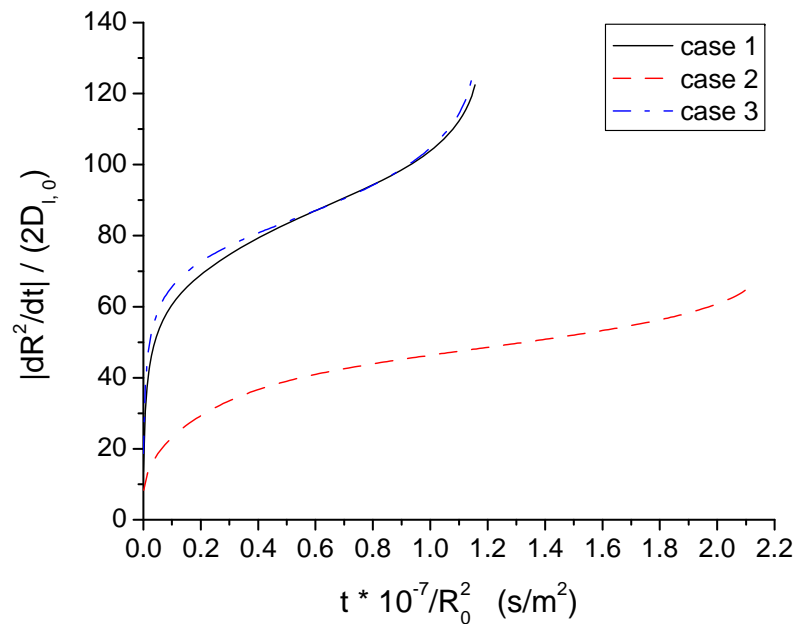
case 1: 2000K, 1/3,1/3,1/3; case 2: 1000K, 1/3,1/3,1/3; case 3: 2000K, 2/3,1/6,1/6.

Artificial liquid

An artificial single-component liquid is created to serve as a surrogate for the multicomponent. An average of the component properties is considered. The mass fractions of the more volatile components become smaller than their initial value in the process of the vaporization of the mixture, so less weighting should be put on the more volatile components in order to have a radius squared rate of change closer to the value for the actual mixture.

actual mixture: 2000K, 1/3,1/3,1/3; artificial liquid 1: 1/3,1/3,1/3; artificial liquid 2: 1/6,1/6,2/3.
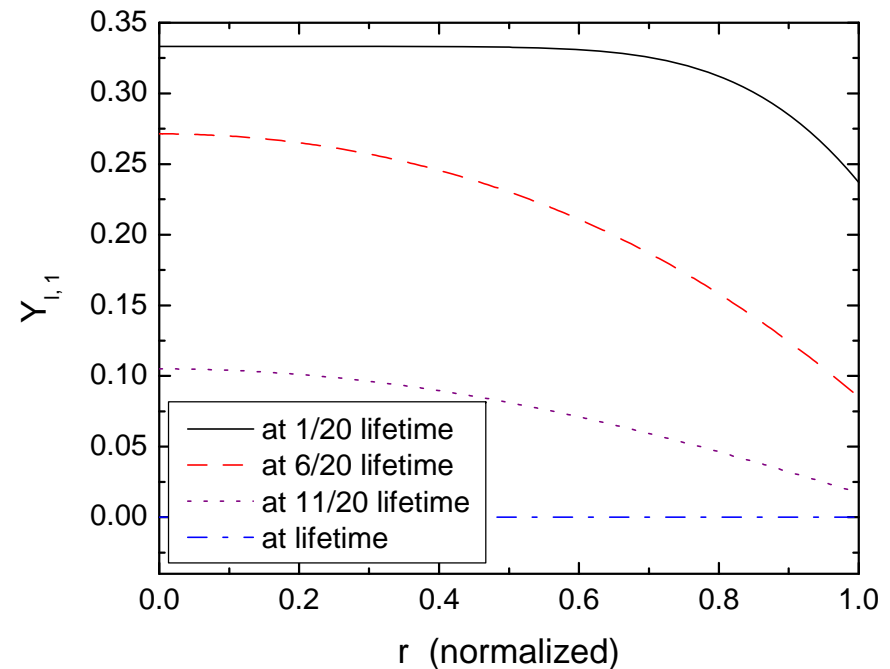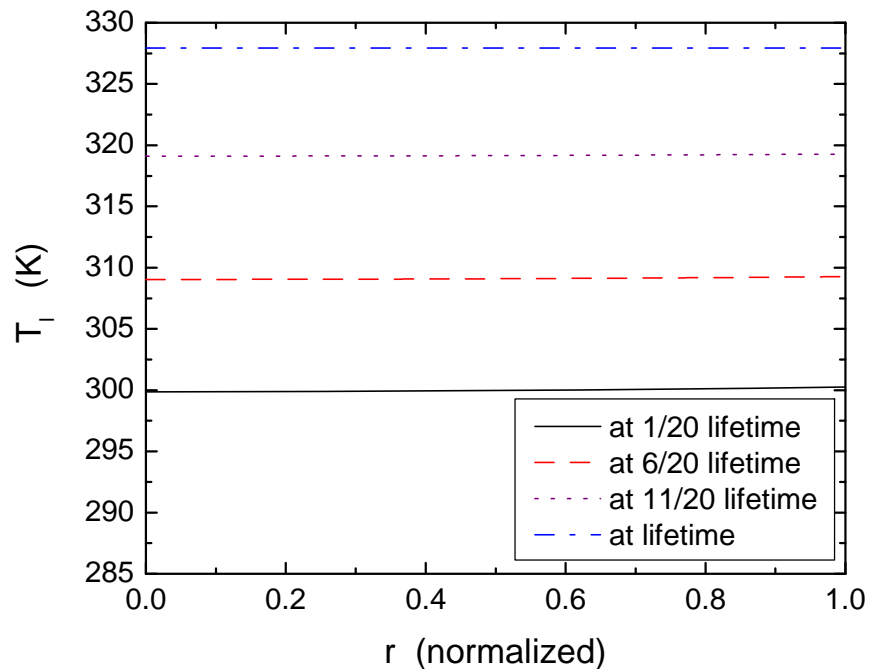
Profiles in the liquid phase ($T_\infty = 2000K$)

The profiles of temperature and composition inside the droplets change with time while the changes of surface temperature and surface composition become slower with time. As heat conduction in the liquid phase is much faster than mass diffusion, the temperature becomes nearly uniform and constant after some time while the profiles of species mass fraction still varies.
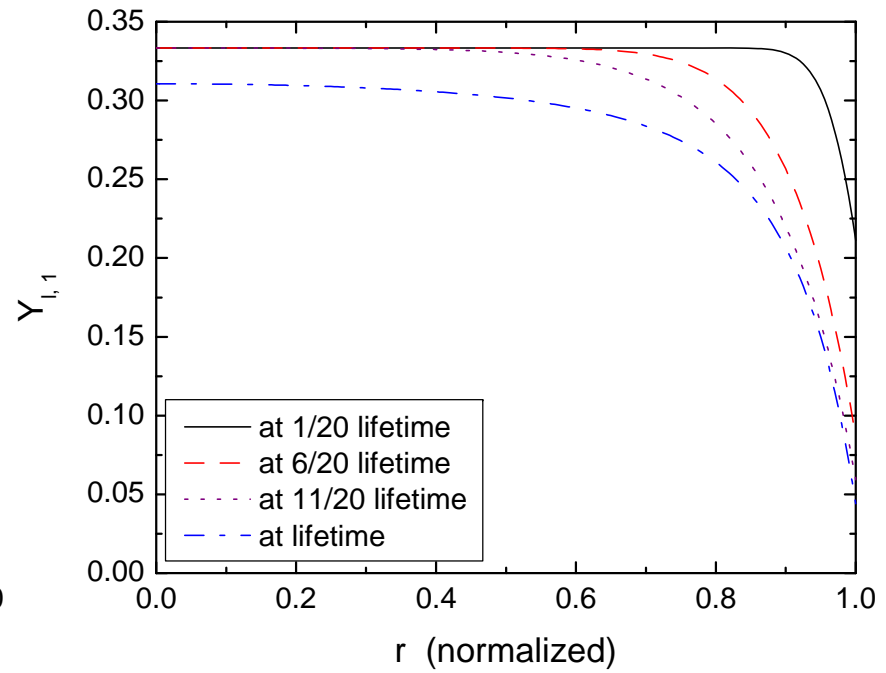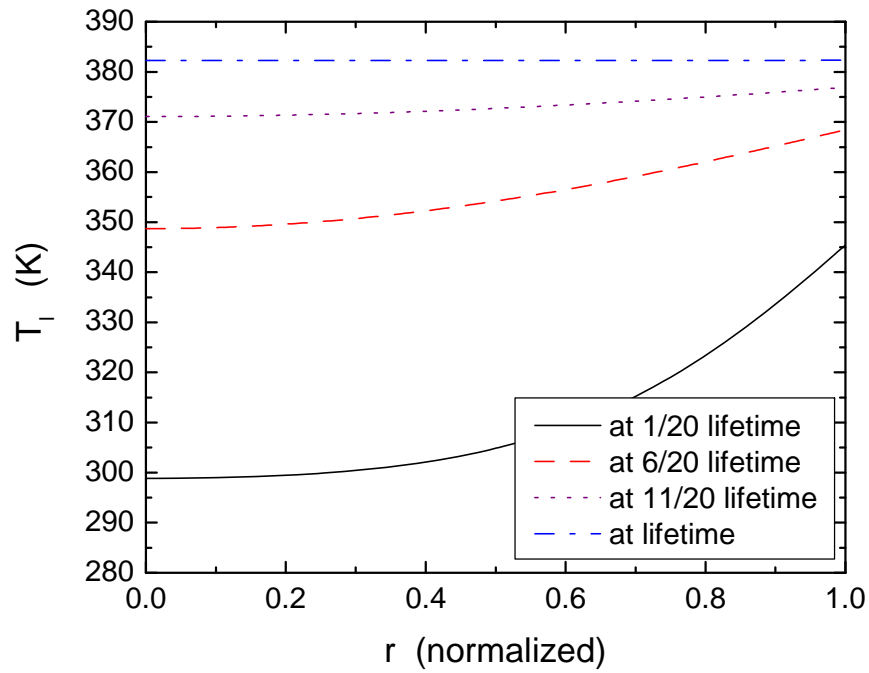
Profiles in the liquid phase ($T_\infty = 350K$)

Lower ambient temperature always leads to more uniform profiles because it results in longer lifetime and allows more time for heat and species diffusion in the droplets. In the case of 350K ambient temperature, the temperature profiles are nearly uniform all the time but the mass fraction profiles are not, so the slow vaporization limit is not strictly satisfied for multicomponent case even at low ambient temperature 350K.

Profiles in the liquid phase ($T_\infty = 3000K$)

In the case of 3000K ambient temperature, the temperature and mass fraction profiles become steeper but still don't produce a sufficiently thin diffusion layer to satisfy strictly the fast vaporization limiting conditions.
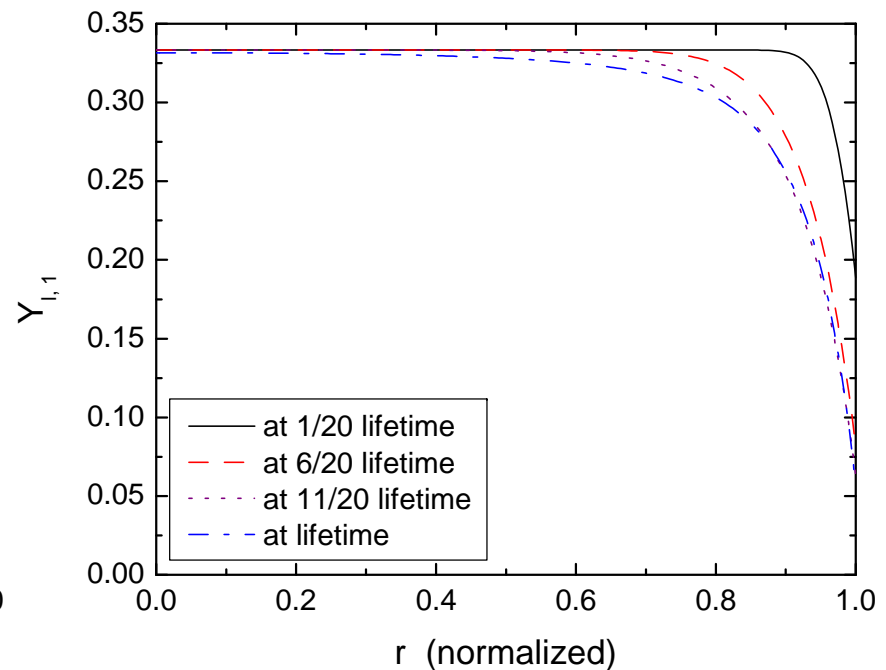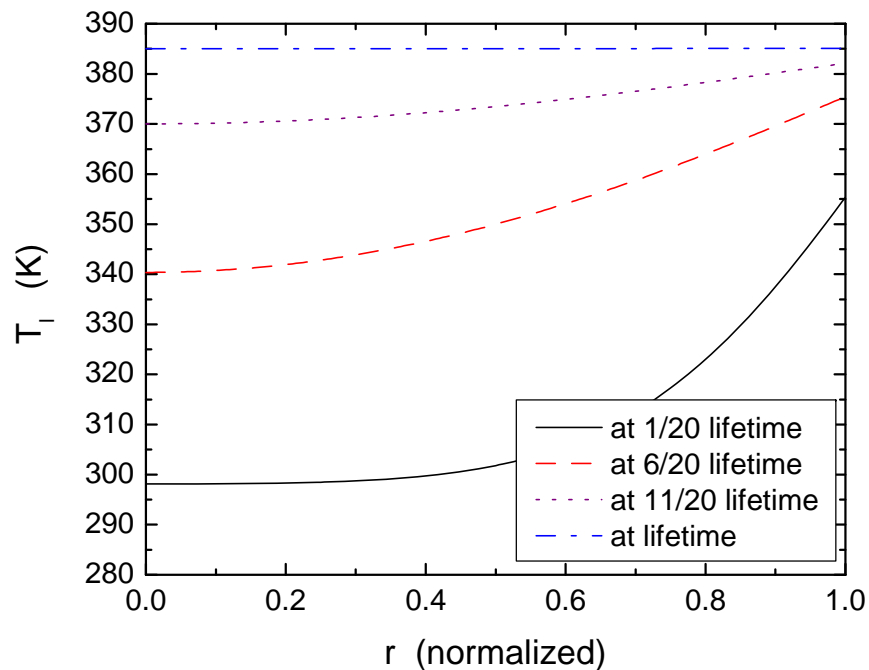
Major conclusions

- The revised definition of the Lewis number and the new heat transfer number $B_{H,\varepsilon}$ are shown to be very useful in the analysis and calculation.
- Liquid temperatures may exceed the pure-form boiling point but are always lower than the actual boiling point in a liquid blend, thus no gasification inside the liquid occurs.
- At low ambient temperature the rate of decrease of radius squared may decreases with time due to a strong distillation effect.
- The slow vaporization limit model predicts the transient behavior well only for single-component case at low ambient temperature (350K).
- The fast vaporization limit model doesn't predict the transient behavior well even at the ambient temperature of 3000K.

Future work

- Extend the calculation to involve forced convection in the gas phase
- Consider internal circulation in the liquid phase

Thank you!