

Theoretical Developments in Group Combustion of Droplets and Sprays

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Collaborations: Guang Wu, current student; Randall Imaoka, former student, US Navy; Forman A. Williams on 4-step reaction.

- Early Studies: 1971-81, quasi-steady gas, Stefan convection; 1978-1993, transients, convection, internal circulation**
- Recent extensions of group combustion / array theory to transient liquid phase, larger arrays, non-unitary Lewis number, variable properties, and multicomponent fuel.**
- Convective burning of periodic arrays in two directions, periodic arrays in one direction, and finite arrays.**

Early Pioneering Studies: Quasi-steady Behavior, Stefan Convection

Spalding (1951) and Godsave (1953)— spherically symmetric single droplet burning.

Chiu and co-workers (1971-83)— classified group combustion, identified similarity parameter.

Labowsky & Rosner (1978) identified a group combustion similarity parameter whose square is equivalent to the Chiu number.

Labowsky (1978) introduced mass-flux potential governed by Laplace's equation for vaporizing droplet array. Modifications in droplet Nusselt and Sherwood numbers are implicit. Scalars become "one-dimensional" functions of potential only.

Twardus and Brzustowski (1977), Umemura et al. (1981a,b) considered two burning droplets with implicitly modified Nusselt and Sherwood numbers

Early Pioneering Studies: Transient Liquid Heating

Law and Sirignano (1977) – considered liquid-phase heat conduction.

Early Pioneering Studies: Convection, Internal Circulation, Transient Liquid Heating

Prakash and Sirignano (1978, 1980) considered convective heating and vaporization of single droplet with internal circulation and transient liquid heat transport.

Lara-Urbaneja and Sirignano (1981) extended convective analysis to multicomponent fuel.

Raju and Sirignano (1990) and Chiang and Sirignano (1993a,b) extended convective studies to two and three tandem droplets.

Major Assumptions, non-convective case

- **Stefan convection only**
- **Fourier heat conduction**
- **Fickian mass diffusion, multicomponent flow**
- **Unitary Lewis number**
- **One-step oxidation kinetics**
- **Single-component fuel**
- **Low Mach number : negligible kinetic energy;
pressure gradients affect momentum balance but
not energy balance**
- **Negligible radiation**
- **Phase-equilibrium law gives $Y_{Fs} (T_s)$**
- **No oxygen at liquid surface (diffusion flame)**

Basic Gas-Phase Equations

Species conservation

$$L(Y_i) \equiv \rho \frac{\partial Y_i}{\partial t} + \rho \mathbf{u} \cdot \nabla Y_i - \nabla \cdot (\rho D \nabla Y_i) = \rho \dot{w}_i ; i = F, O, P$$

Energy

$$L(h) \equiv \rho \frac{\partial h}{\partial t} + \rho \mathbf{u} \cdot \nabla h - \nabla \cdot (\rho D \nabla h) = -\rho \dot{w}_F Q + \frac{\partial p}{\partial t}$$

Sensible enthalpy definition

$$h = \sum_i Y_i \int_{T_{ref}}^T c_{pi}(T') dT' = \sum_i Y_i h_i = \int_{T_{ref}}^T c_p(T') dT'$$

$$c_p \nabla T = \nabla h - \sum_i h_i \nabla Y_i$$

Plus continuity and momentum equations

Problem Formulation

A transfer number and an effective latent heat of vaporization can be defined.

$$B = \frac{h_{\infty} - h_s + \nu Q Y_{O\infty}}{L_{eff}} = \frac{\nu Y_{O\infty} + Y_{FS}}{1 - Y_{FS}}$$

$$L_{eff} = L + \frac{\dot{q}_l}{\left| \rho \vec{V} \right|_s}$$

Coupling functions

$$\alpha_1 = h + \nu Q Y_o$$

$$\alpha_2 = Y_F - \nu Y_o$$

Super-Scalar Formulation

Consider $L_{eff} / (1 - Y_{Fs}(T_s))$ to be uniform over gas-liquid interfaces. Then, a super scalar S can be constructed which is uniform over the gas (but possibly time-varying).

$$S = \alpha_1 + \frac{L_{eff}}{1 - Y_{Fs}} \alpha_2 = h + v \left(Q - \frac{L_{eff}}{1 - Y_{Fs}} \right) Y_O + \frac{L_{eff}}{1 - Y_{Fs}} Y_F$$

$$S = S_\infty(t) = h_\infty + v \left(Q - \frac{L_{eff}}{1 - Y_{Fs}} \right) Y_{O_\infty} + \frac{L_{eff} Y_{F_\infty}}{1 - Y_{Fs}} = h_f$$

The limiting diffusion flame enthalpy and temperature can readily be determined and is independent of the particular geometrical configuration.

Mass, energy, and species conservation equations

Create the mass-flux potential

$$\nabla \cdot (\rho \vec{V}) = 0 \quad ; \quad \rho \vec{V} = \overline{\rho D} \ln(1 + B) \nabla \Phi \quad ; \quad \nabla^2 \Phi = 0$$

$$\nabla \cdot (\rho \vec{V} \alpha_i - \rho D \nabla \alpha_i) = 0$$

A solution can be found where $\nabla \Phi$ is aligned with the velocity; i.e., diffusion is directed along a streamline created by Stefan convection. Solutions have the form

$$\alpha_i = a_i + b_i (1 + B)^\Phi$$

$p = \rho R T = p_\infty$ A uniform pressure assumption can replace the momentum equation

Comments

- **S-Z variables are conserved gas-phase scalars, neither created or destroyed by chemical reaction since no source term appears.**
- **S-Z variables are not passive scalars; they can affect the velocity field. Also they can be affected by the velocity field.**
- **The scalar variables are functions of the mass-flux potential Φ without implicit dependence on position or time, universally valid for any configuration.**
- **The normalized Φ satisfies Laplace's equation without dependence on scalar constraints.**
- **The potential value at the thin flame and the flame temperature are independent of configuration.**
- **Variable properties have important consequences.**
- **Burning rate and vaporization rate do depend on configuration.**

Problem Formulation

Enthalpies, composition, flame locations, and $\overline{\rho D}$ can be obtained for a fixed liquid-surface temperature

$$\overline{\rho D} = \overline{\lambda / c_p} = \left(\int_0^1 \frac{d\Phi}{\lambda / c_p} \right)^{-1}$$

$$(1+B) \overline{\rho D} \int_0^{\Phi} \frac{d\Phi'}{\lambda / c_p} = 1 + \frac{h - h_s + \nu Q Y_O}{L_{eff}} = 1 + \frac{Y_F - Y_{FS} - \nu Y_O}{Y_{FS} - 1}$$

$$\overline{\rho D} \int_0^{\Phi_F} \frac{d\Phi'}{\lambda / c_p} = \frac{-\ln(1 - Y_{FS})}{\ln(1 + B)}$$

Unsteady combustion with liquid heating

The diffusion equation in the liquid

$$\frac{\partial T}{\partial t} = \frac{\alpha_l}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right)$$

is normalized by

$$\hat{t} = \frac{t}{t_{iso}} \qquad \hat{r} = \frac{r}{a} \qquad \hat{a} = \frac{a}{a_0}$$

Liquid-phase temperatures are now governed by

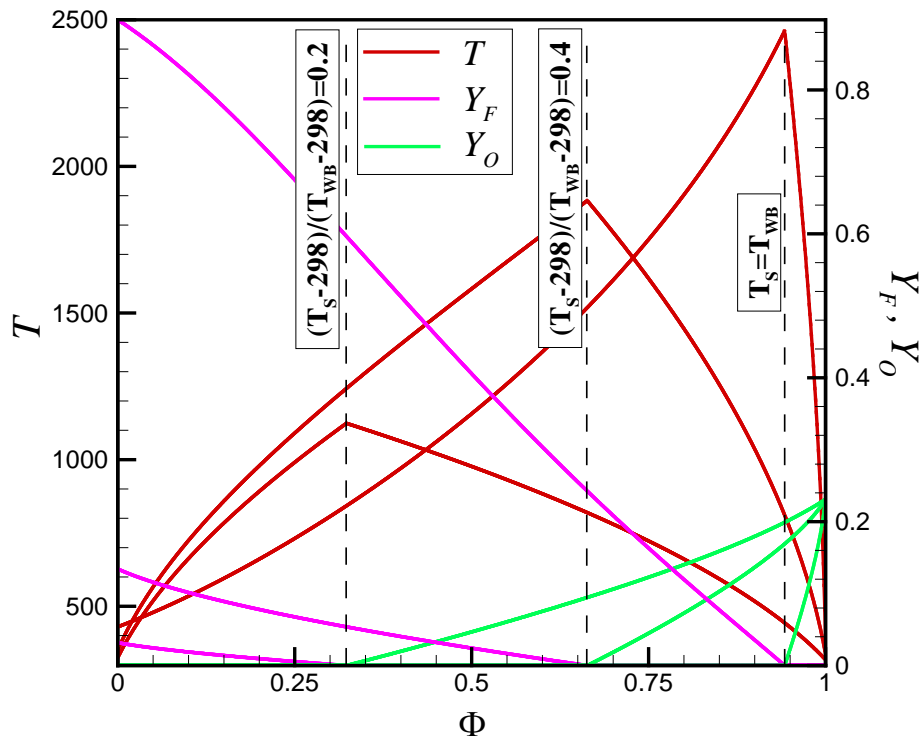
$$\frac{\partial T}{\partial \hat{t}} = \frac{\alpha_l t_{iso}}{(a_0 \hat{a})^2} \frac{\partial^2 T}{\partial \hat{r}^2} + \left(\frac{2\alpha_l t_{iso}}{(a_0 \hat{a})^2 \hat{r}} + \frac{\hat{r}}{2\hat{a}^2} \frac{d\hat{a}^2}{d\hat{t}} \right) \frac{\partial T}{\partial \hat{r}}$$

Droplet radii are obtained by solving

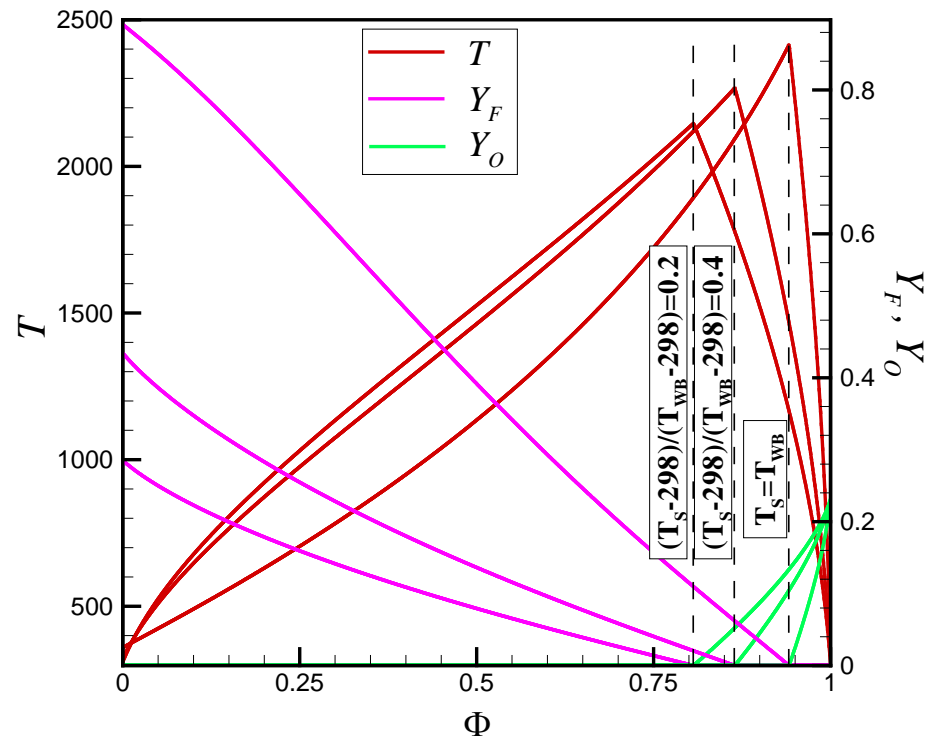
$$\frac{d\hat{a}^2}{d\hat{t}} = - \frac{\ln(1+B)}{\ln(1+B_{WB})} \eta_A$$

Mixture temperature, fuel and oxidizer mass fractions for decane and heptane

$$T_\infty = 298K, Y_{O_\infty} = 0.231$$



Decane; $T_{WB} = 429.73K$



Heptane; $T_{WB} = 359.36K$

Factors Affecting Flame Position

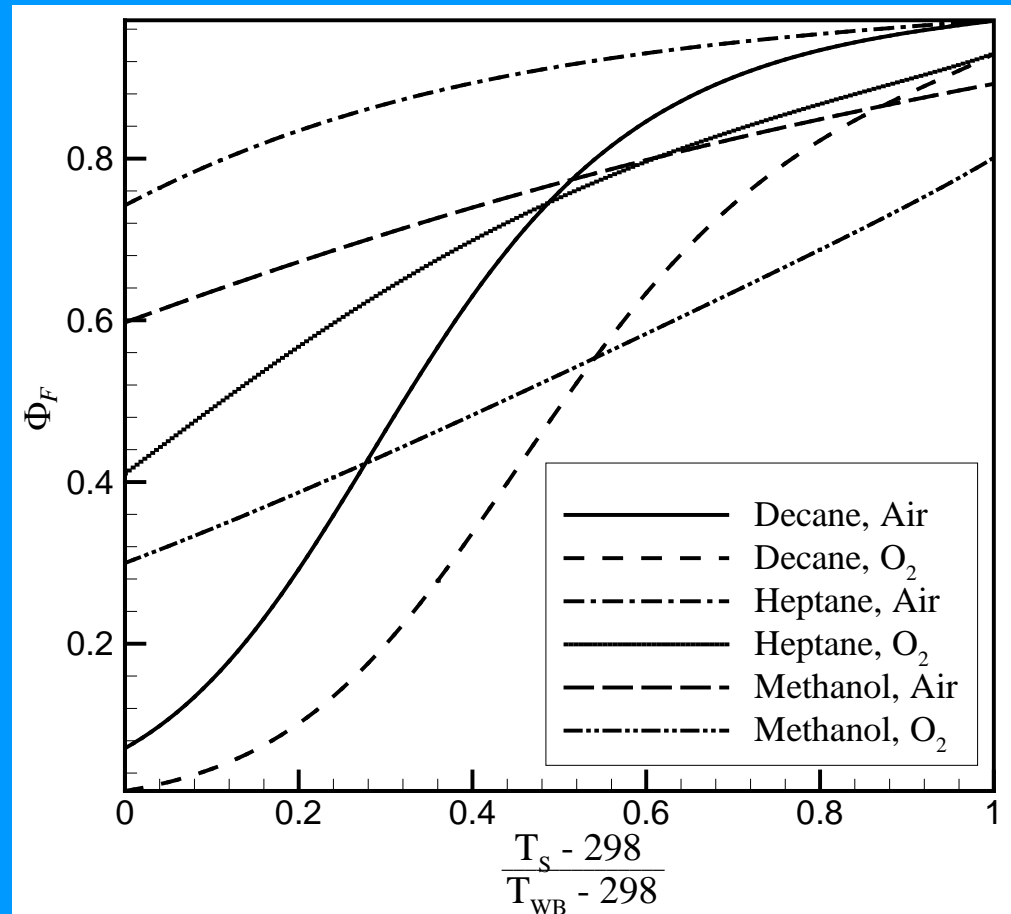
- Droplet temperatures
- Ambient oxidizer mass fraction
- Type of fuel
- Ambient pressure
- Ambient temperature

Flames become approximately spherical at large distances from the droplet array

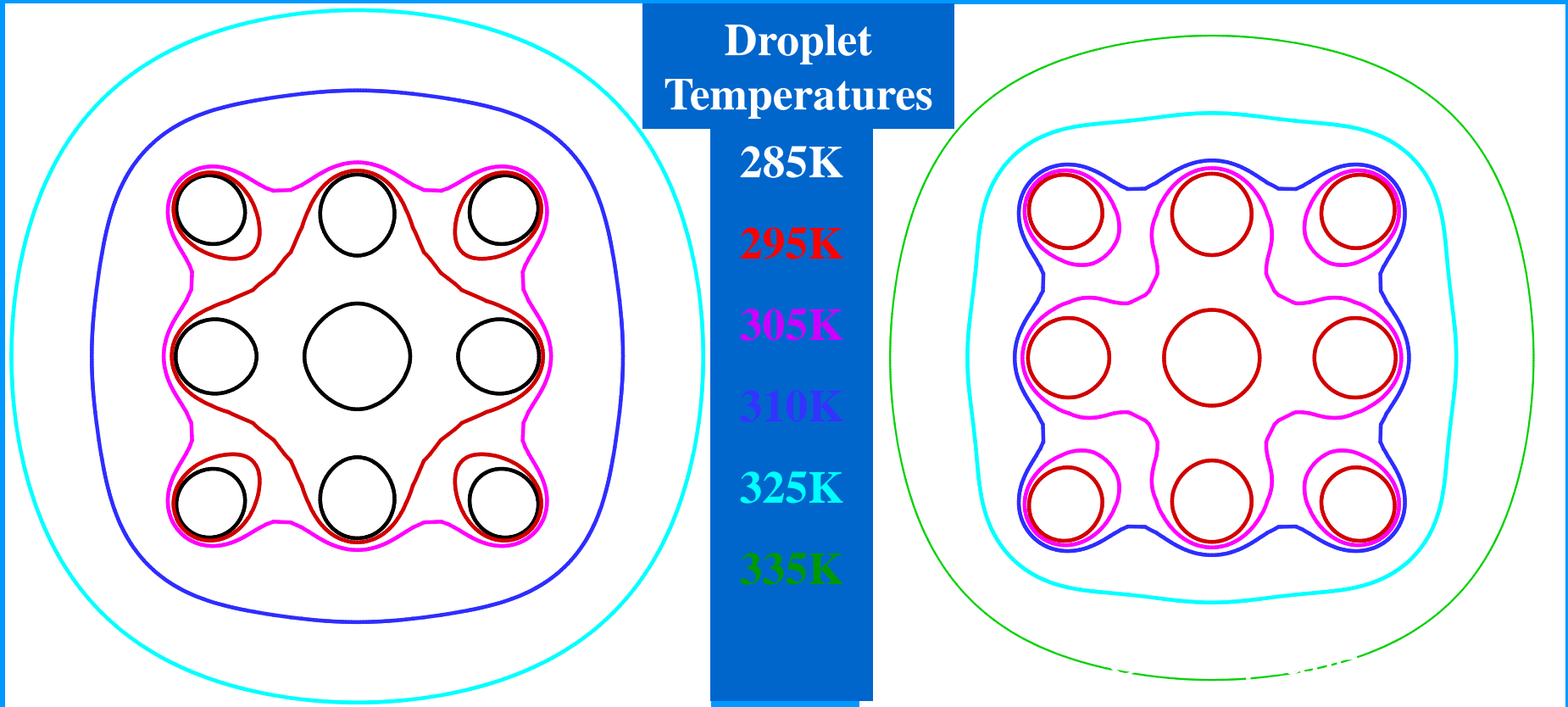
$$\Phi^*(r) = 1 - \frac{aN\eta_A}{r}$$

Droplets at wet-bulb temperatures had a spherical flame for all droplet arrays studied

Flame locations in air and oxygen vs. droplet surface temperature



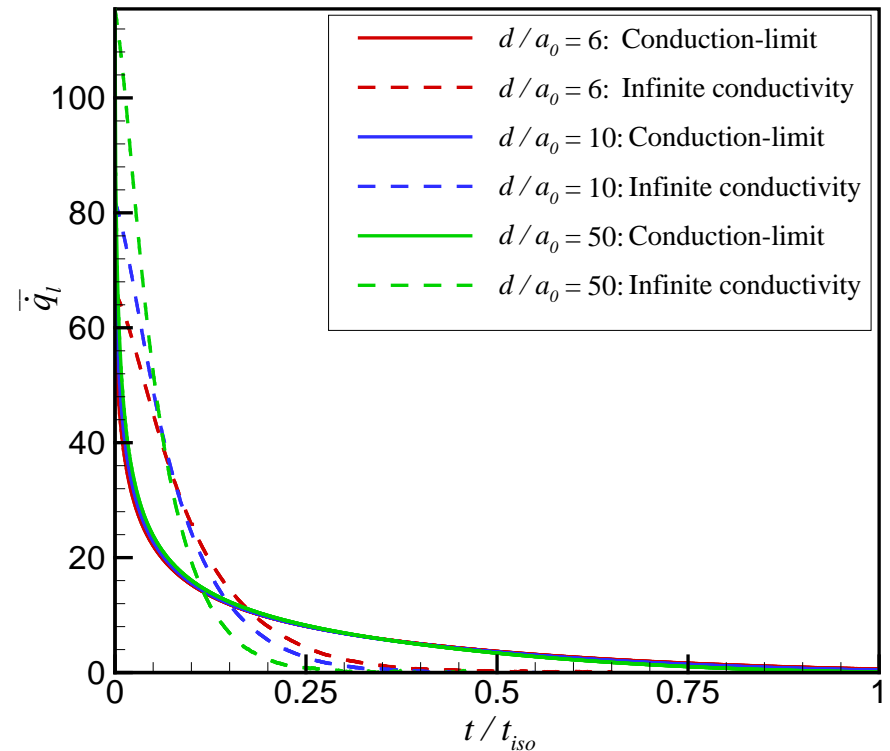
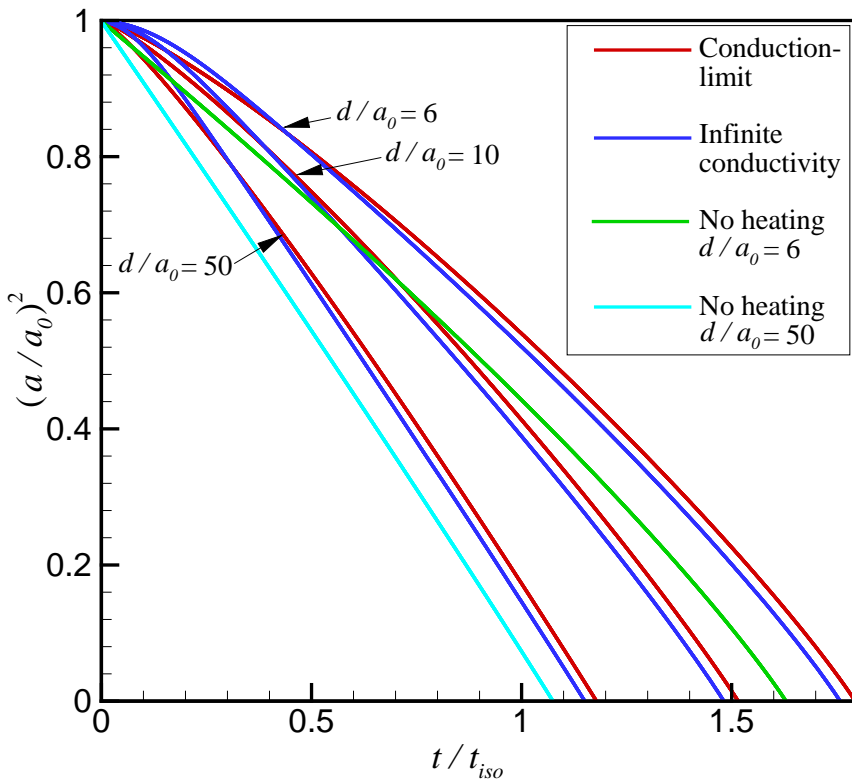
Flame locations in the central and outer planes of a 27-drop cubic array with $d/a = 5$ for decane/air at various droplet temperatures ($T_{wet-bulb} = 430.8 K$)



- 285K: 27 individual-droplet flames
- 295K: 7 droplets burn as a group plus 20 individual-droplet flames
- 305K: 19 droplets burn as a group plus 8 individual-droplet flames
- 310K: 27 droplets burn as a group

Square of normalized radius and heat flux (kW/m²) vs. time for cubic arrays of 8 heptane drops with different initial spacing

$$T_{\infty} = 298K; Y_{O\infty} = 0.231$$



The gas-phase for any geometry is governed by

$$\nabla^2 \Phi = 0$$

with b. c.'s $\Phi = 0$ **on the liquid surfaces**

$\Phi = 1$ **far from the droplets**

$\Phi(x, y, z, t)$ does not depend on properties, scalar solutions, or boundary values.

Normalized droplet and array vaporization rates are

$$\eta_j = \frac{\dot{m}_j}{\dot{m}_{iso}} = \frac{1}{4\pi a_j} \iint \nabla \Phi \cdot d\vec{A}_j$$

$$\eta_A = \frac{\sum_{j=1}^N \dot{m}_j}{N\dot{m}_{iso}} = \frac{1}{4\pi a_j N} \sum_{j=1}^N \iint \nabla \Phi \cdot d\vec{A}_j = \frac{1}{N} \sum_{j=1}^N \eta_j$$

Vaporization Rates

The similarity parameter ξ can be expressed in terms of the liquid / array volume ratio V_l / V_A and N . For uniform spacing, $\xi = (d/a)N^{-0.72}$

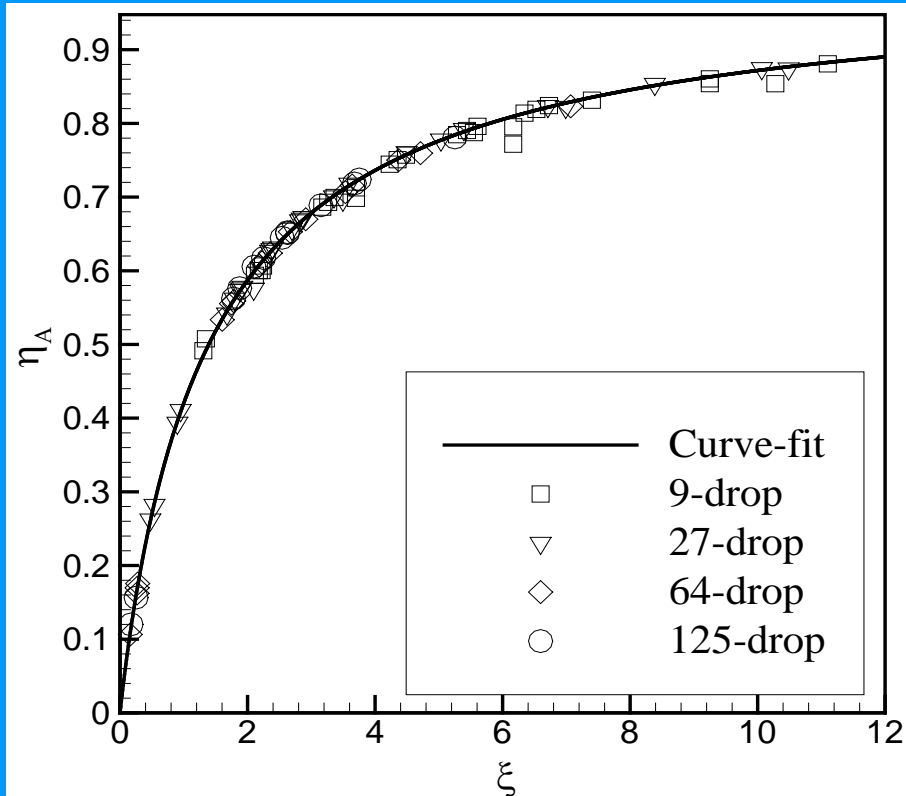
$$\xi = \frac{\left(\frac{4\pi V_A}{3V_l} \right)^{1/3}}{N^{0.72}}$$

For uniform spacing, the similarity parameter is almost identical to the reciprocal of the Chiu number: $1/G = \text{constant } (d/a)N^{-2/3}$.

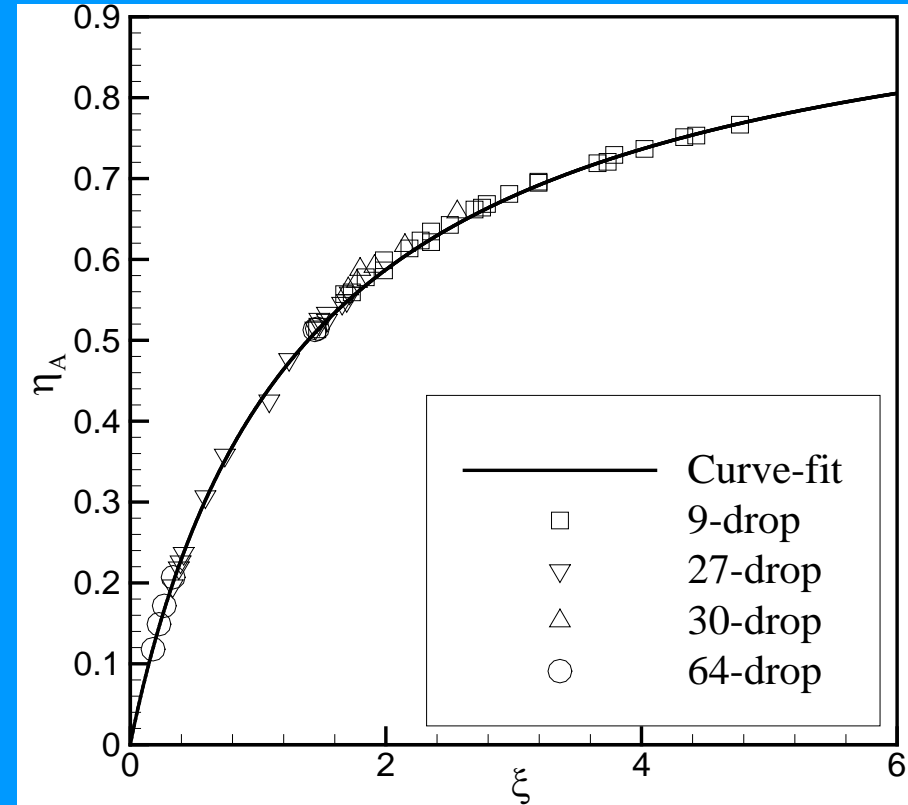
Vaporization rate can be obtained from the correlation for η_A .

$$\frac{\dot{m}_A}{\rho D \ln(1+B)V_A^{1/3}} = (4\pi N)^{2/3} \left(\frac{3V_l}{V_A} \right)^{1/3} \left\{ 1 - \frac{1}{1 + 0.7257\xi^{0.9717}} \right\}$$

η_A vs. ξ for arrays with variable radii



η_A vs. ξ for arrays with non-uniform spacing



Up to 1000 droplets with uniform radii and spacing have been shown to fit on this correlation curve. That is, an octant with three symmetry planes and up to 125 droplets was considered.

Findings

- **The scalar variables are a function of the mass-flux potential Φ without explicit dependence on position or time, universally valid for any configuration.**
- **The normalized Φ satisfies Laplace's equation without dependence on scalar constraints.**
- **Peripheral droplets can vaporize substantially faster than inner droplets.**
- **Arrays of different size and spacing can be characterized by a similarity parameter.**
- **An optimal number of droplets exists and depends only on the fuel / array volume ratio.**
- **Droplet lifetimes are increased due to interactions and / or due to transient droplet heating.**

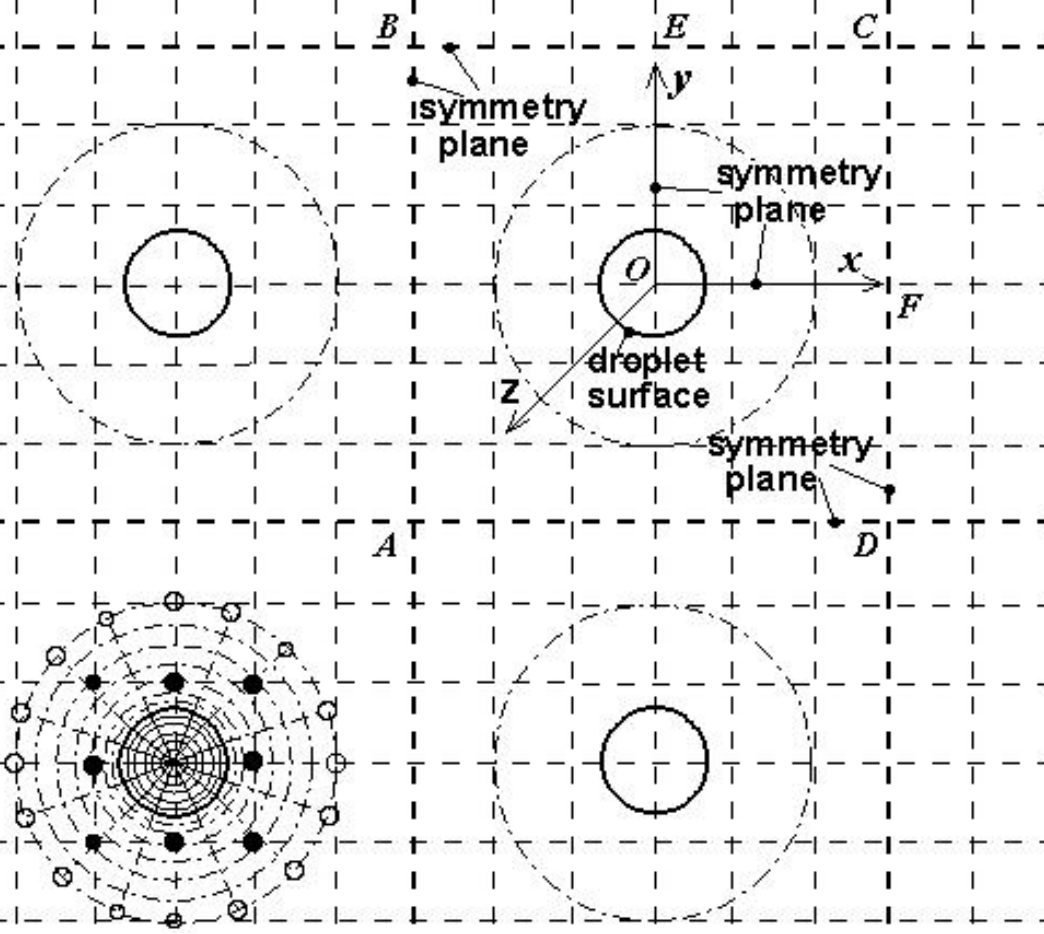
Findings and Extensions

- Different modes of combustion exist depending on fuel, droplet temperatures, and ambience.
- Combustion modes can change during the array lifetime due to decreasing droplet size and / or droplet heating.
- Individual droplet burning was not observed for droplets at wet-bulb temperatures.
- A spherically symmetric solution exists for large distances from the droplet array.
- The analysis has been extended to the general case of non-unitary Lewis number.
- An extension to arrays of vaporizing multicomponent droplets has been made.

Convective Burning of Fuel-Droplet Arrays

- Accurate numerical studies on the burning of fuel droplets should consider droplet interactions, size regression, droplet deceleration, internal circulation inside the droplet, variable properties, transient droplet heating, and the effect of surface tension.
- Numerical studies have been made on the burning of an isolated convective droplet previously, with considerations of all the above effects except for droplet interactions: Wu and Sirignano, *Combustion and Flame* 157, pp. 970-981, 2010.
- This study investigates numerically the transient convective burning of interactive fuel droplets in a model 3-D array, i.e., an infinite periodic array, with considerations of all the above effects. The transient flame shape, temperature, velocity, and burning rates will be studied as a function of initial spacing amongst droplets, initial Reynolds number, initial Damkohler number, and initial droplet radius.

Single layer array and grid



- Spherical mesh inside and around each droplet, and Cartesian mesh for the rest, with interpolations at the interfaces;
- The spherical mesh is updated as the droplet surface regresses;
- Free stream flow is normal to this plane.

Model and Numerical Scheme

- A global single-step chemical reaction mechanism models oxidation kinetics. Later, a four-step mechanism is examined.
- The initial octane droplet radius is 25 microns, the ambient air temperature and pressure are 1500 K and 20 atm.
- Navier-Stokes, energy and species equations with BCs and ICs are solved in multicomponent gas phase and matched with liquid-phase solutions for Navier-stokes and energy equations.
- Used Semi-Implicit Method for Pressure linked Equations (SIMPLE), staggered mesh, forward time scheme, boundary conditions with 2nd order precision, and ADI to sweep in all the three directions for each time step.
- Stream velocity and mesh in r direction are updated over time to consider the droplet deceleration and surface regression.

Initial parameters

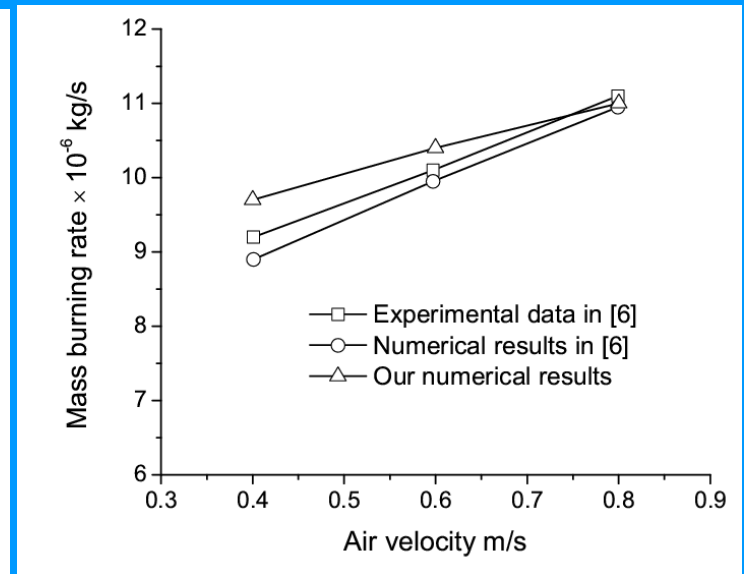
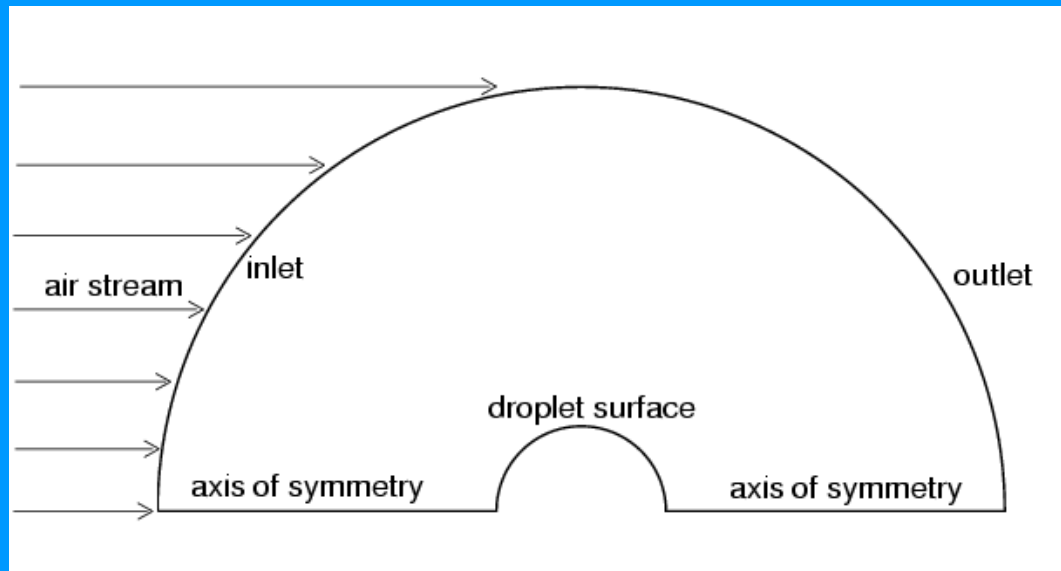
- initial droplet radius R_0 or diameter d_0
- initial relative stream velocity $U'_{\infty,0}$
- initial droplet spacing sp_0

- initial Reynolds number $Re_0 = \frac{\rho_{\infty} U'_{\infty,0} d_0}{\mu_{\infty}}$
- initial Damkohler number $Da_0 = \frac{d_0 / U'_{\infty,0}}{\rho_{\infty} Y_F^o / (\omega^o M_F)}$

where Y_F^o and ω^o are the reference mass fraction for the fuel vapor and reference reaction rate.

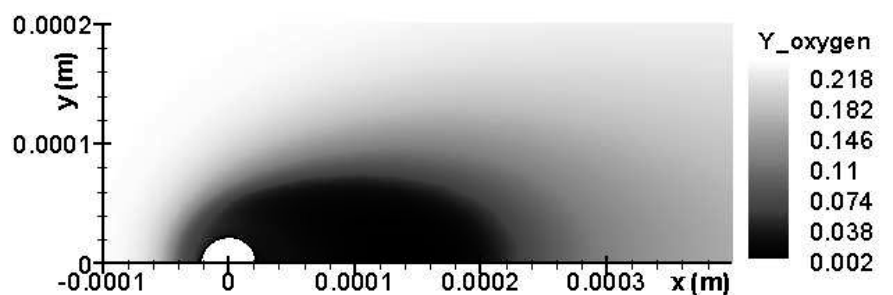
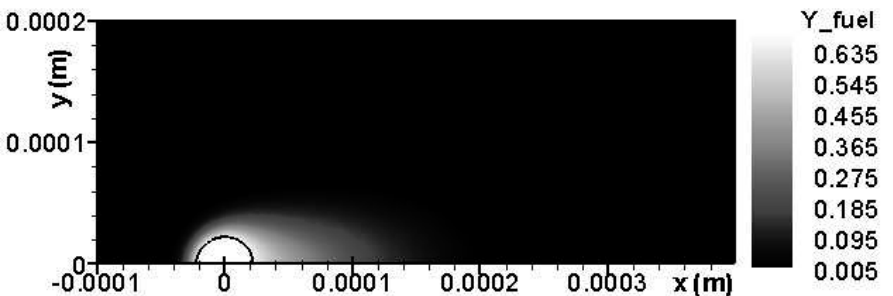
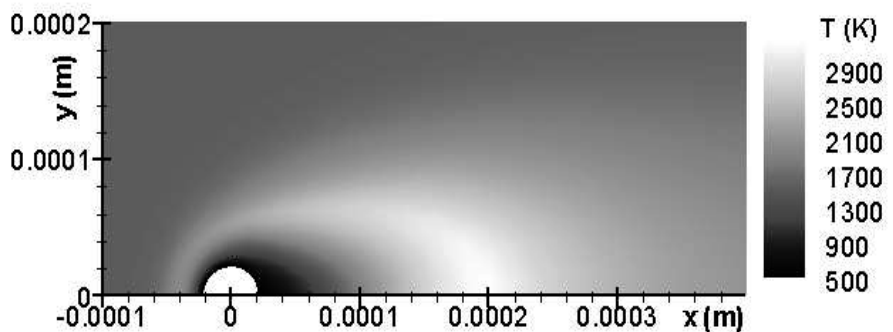
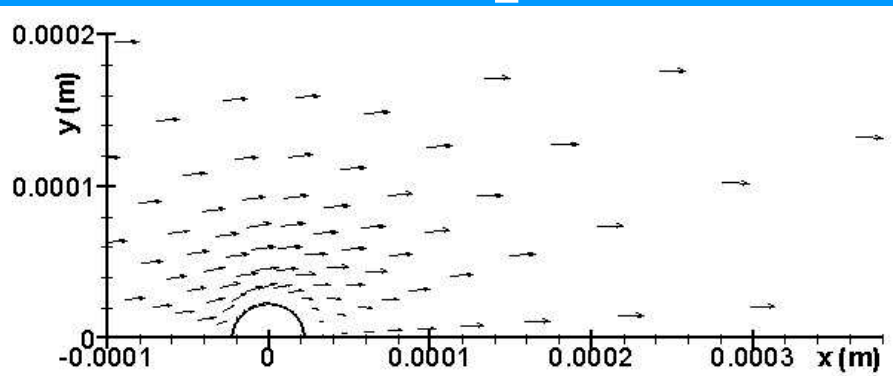
Benchmarking of Code

A single isolated droplet was analyzed first using an axisymmetric code with a spherical mesh. The hybrid spherical / Cartesian 3D mesh was checked against these results.



Computational results compared favorably with steady-state, porous-plug experiments [Raghavan, Babu, Sundararajan, and Natarajan, IJHMT 48 (2005) 5354–70]. Agreement on bifurcation in steady-state at certain velocities to wake flames. Also, our transient results do predict transition in time from wake flame to envelope flame as droplet decelerates and residence time increases.

Envelope Flame



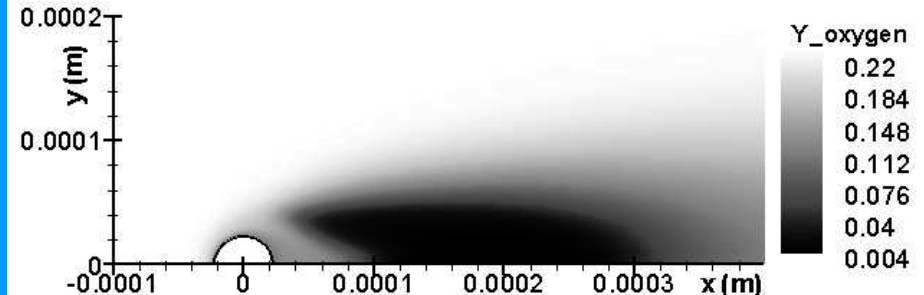
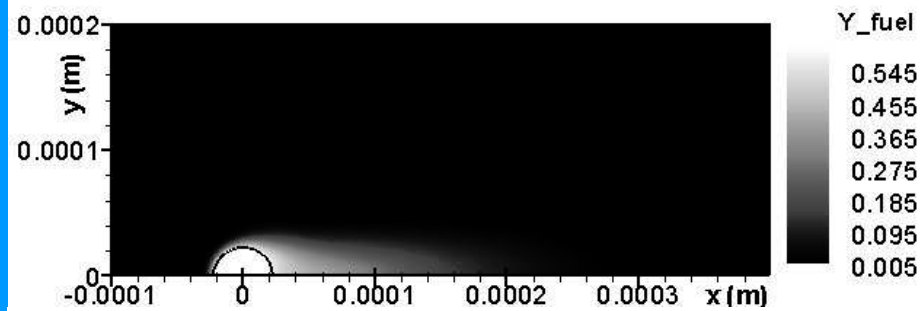
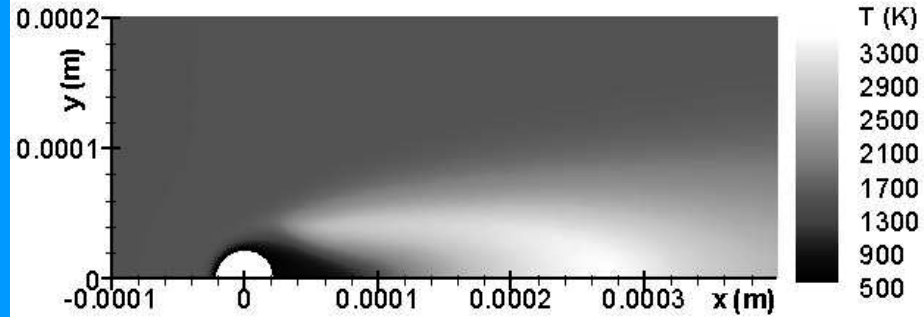
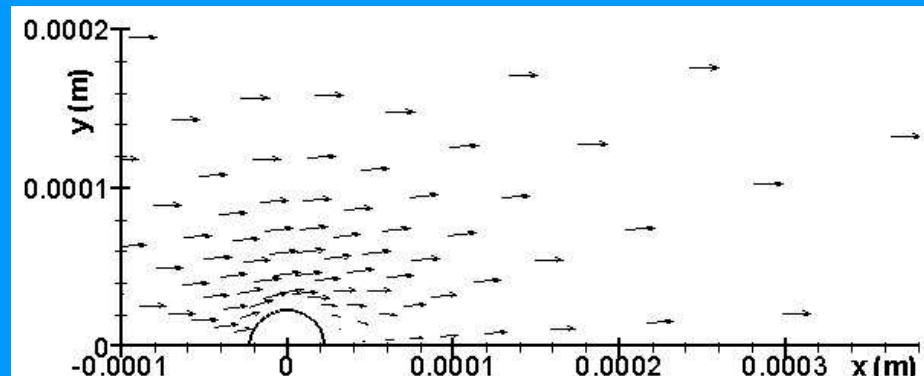
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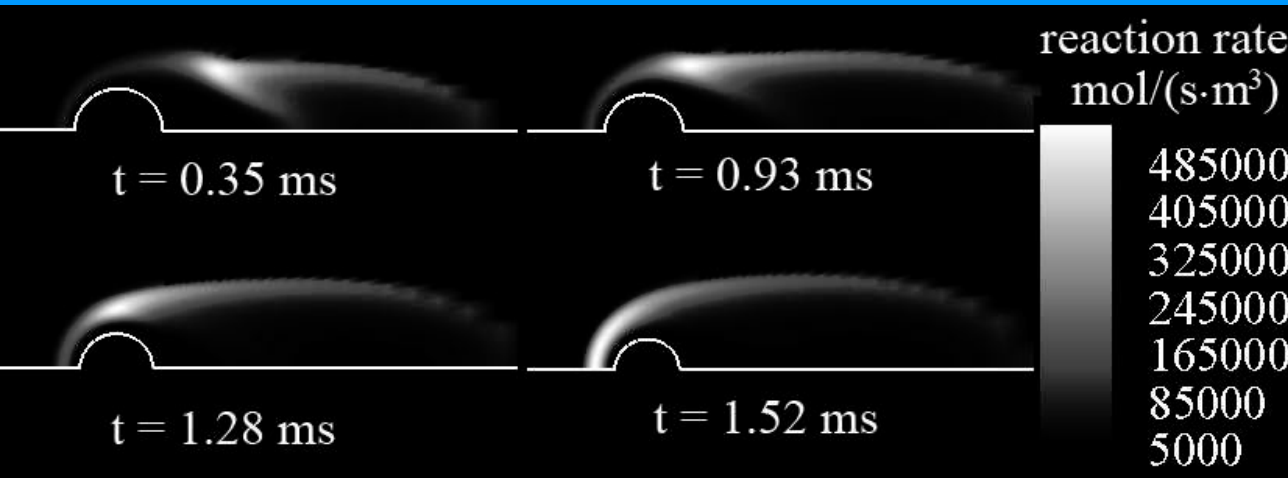
Y_F

Y_O

Wake Flame

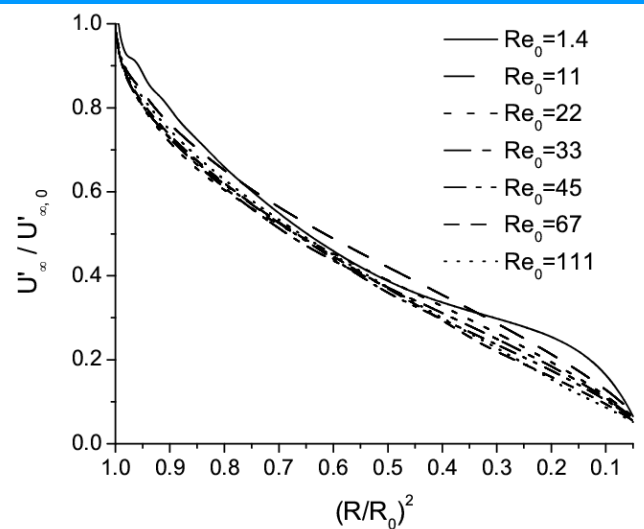
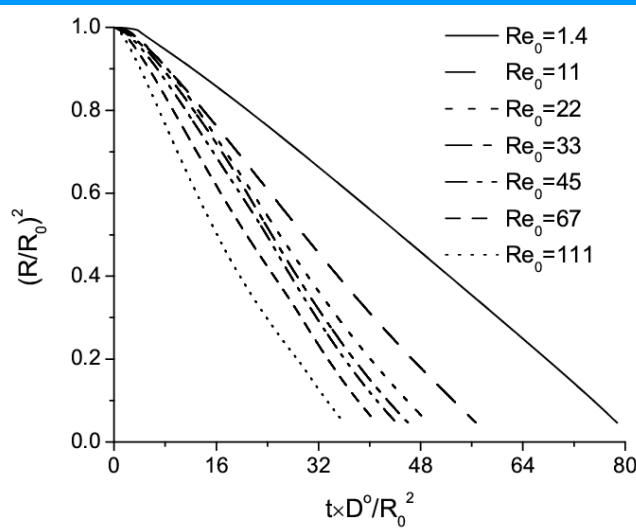


For lower initial Reynolds number (Re) and/ or higher initial Damkohler number (Da), flame is initially an envelope flame and remains so for lifetime.



For higher initial Reynolds number and /or lower initial Damkohler number, flame is initially a wake flame but transitions later to an envelope flame as droplet slows.

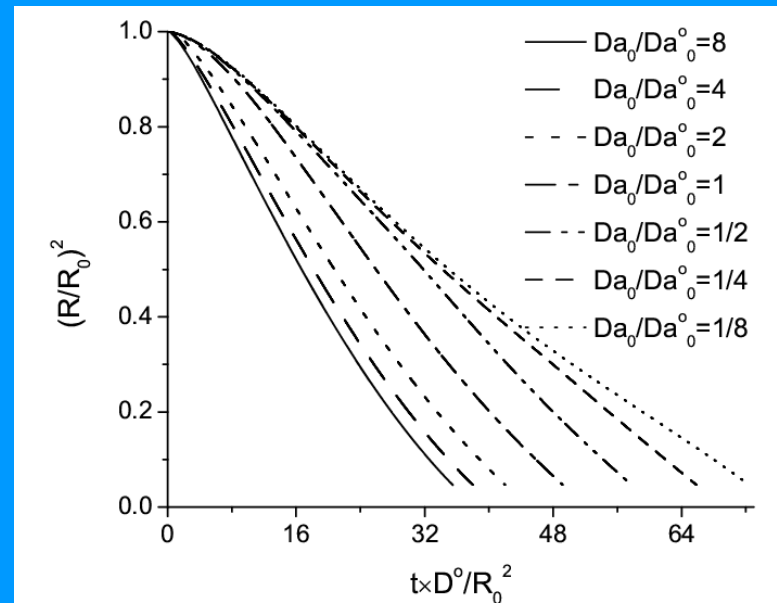
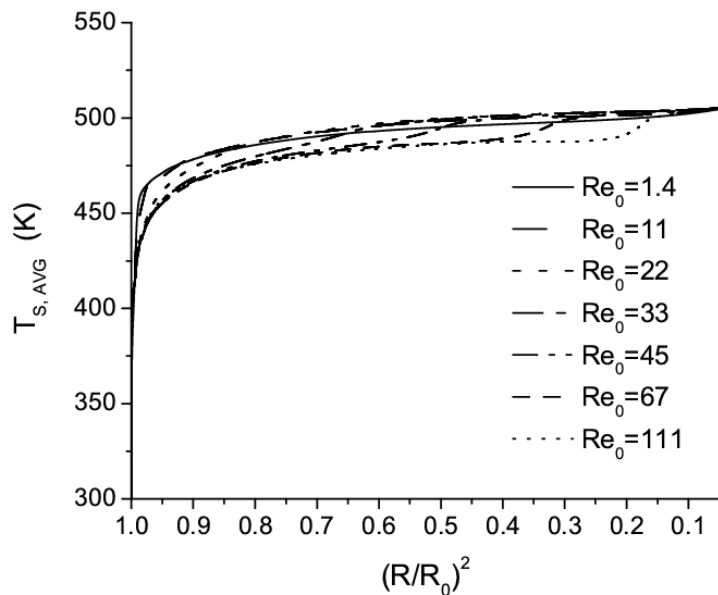
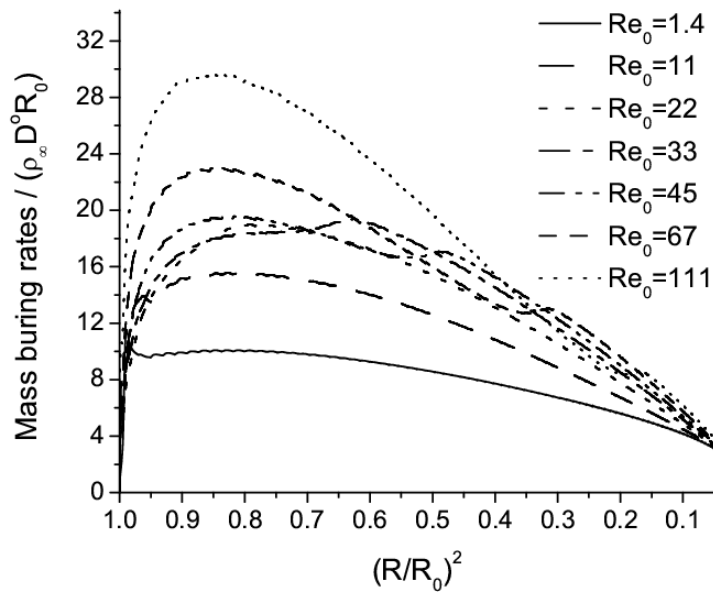
Both droplet size and relative velocity decrease with time. The deviation from classical R^2 law increases as Re becomes larger.



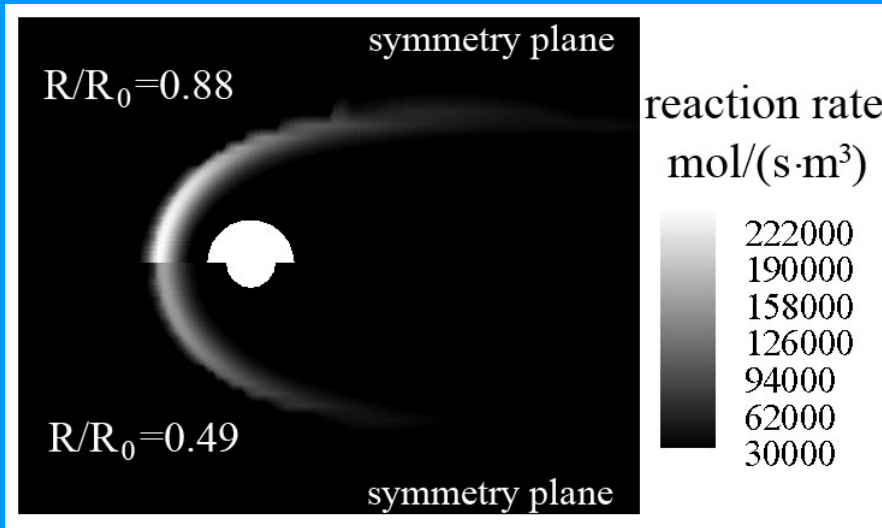
Droplet velocity decrease has a greater effect on residence time increase than droplet size decrease has on residence time decrease. So, residence time increases with time, allowing transition to envelope flame.

All of these qualitative features found in the single-droplet results persist for the transient vaporization and burning of arrays.

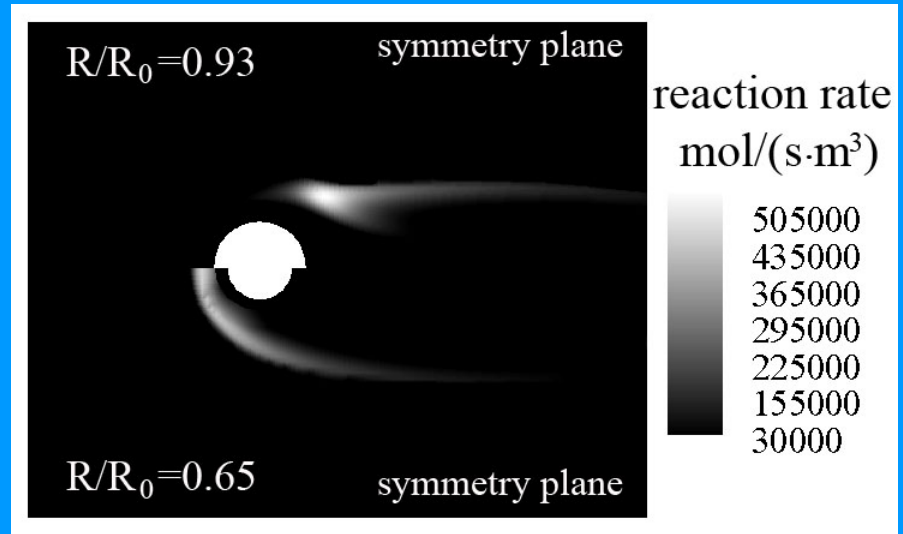
Burning rate increases with initial Re. For higher Re cases, transition to envelope flame occurs, causing a sudden increase in burning rate and liquid surface temperature.
Vaporization rate increases with Da; so, the flame is not thin and not completely diffusion-controlled.



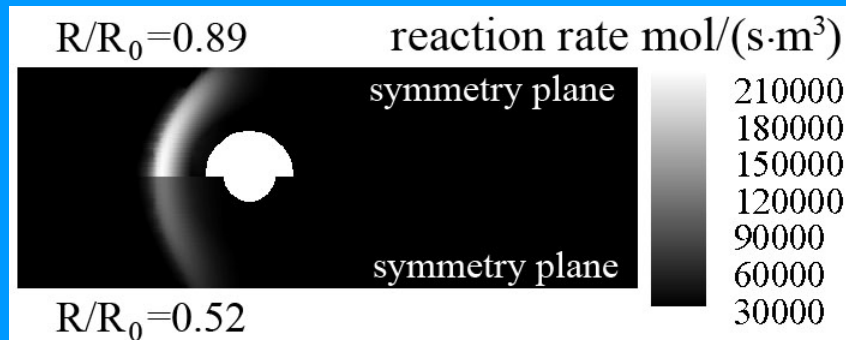
Flame shapes for different sp_0 Or Re_0



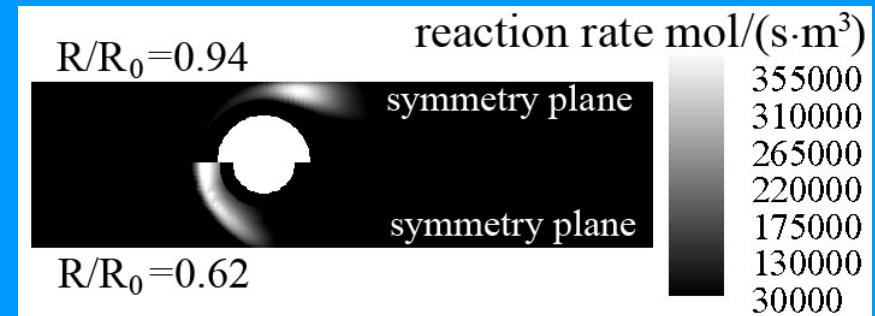
$Re_0 = 9 (Da_0 = 1.5), sp_0 = 5.9d_0$



$Re_0 = 45 (Da_0 = 0.3), sp_0 = 5.9d_0$



$Re_0 = 9 (Da_0 = 1.5), sp_0 = 2.4d_0$



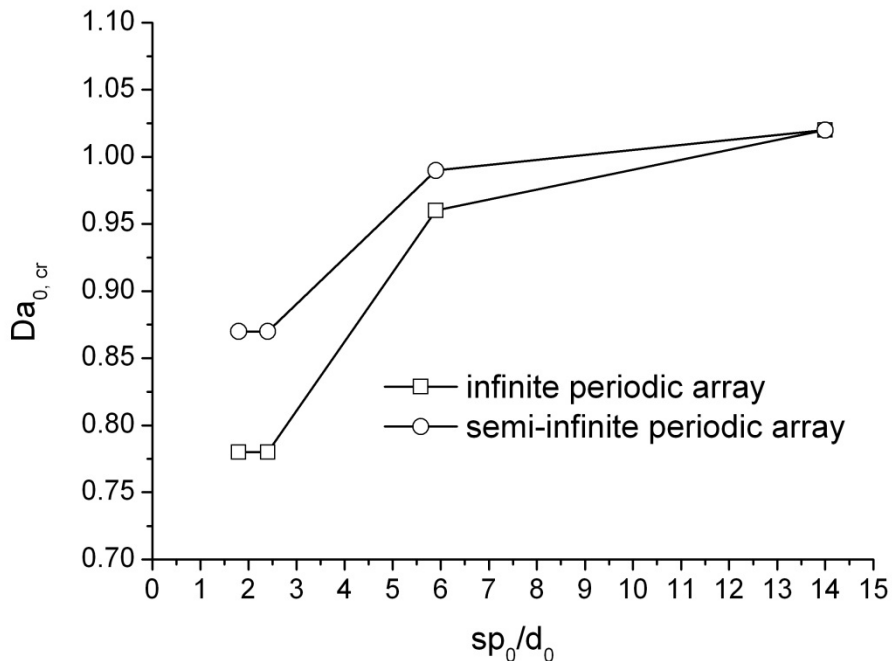
$Re_0 = 45 (Da_0 = 0.3), sp_0 = 1.8d_0$

- An initial envelope flame remains an envelope flame; an initial wake flame develops from a wake flame to an envelope flame.
- The flame remains with the initial individual or group character. The standoff distance does not change significantly during the lifetime.

Critical initial Damkohler number above which an initial envelope flame occurs

Residence time increases with Da .
greater Da and residence time.

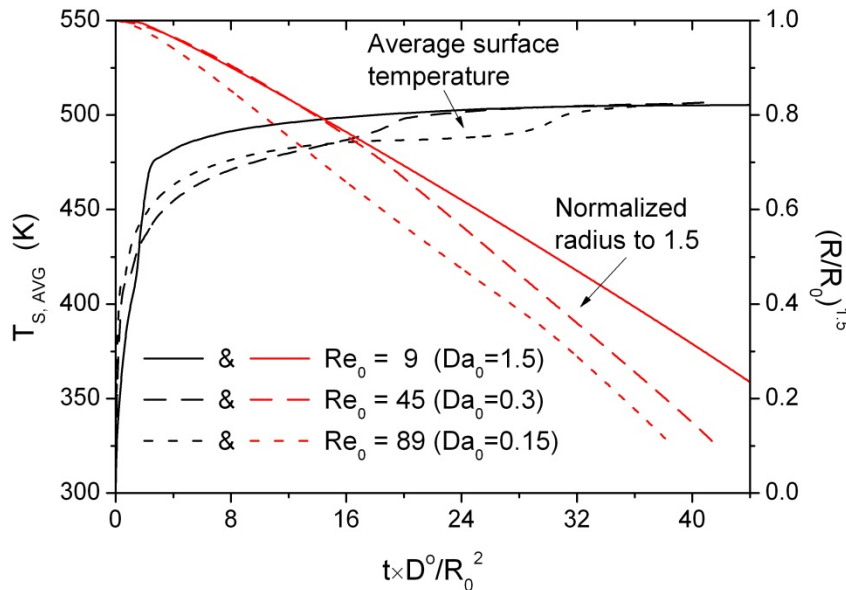
Envelope flame requires



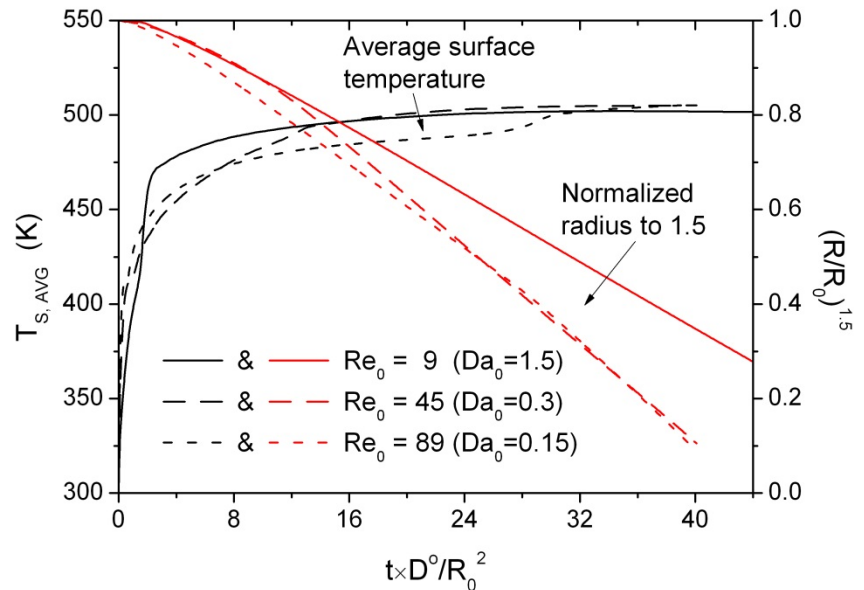
These results apply for any initial Reynolds number value.

- The critical initial Damkohler number decreases with decreasing initial droplet spacing at intermediate spacing, but has no substantial change when the initial droplet spacing becomes too small.
- The critical initial Damkohler number for a semi-infinite periodic array (with one line of droplets) is greater than that for an infinite periodic array because the overall droplet spacing is effectively greater for a semi-infinite periodic array.

Temporal behavior for different initial Reynolds number



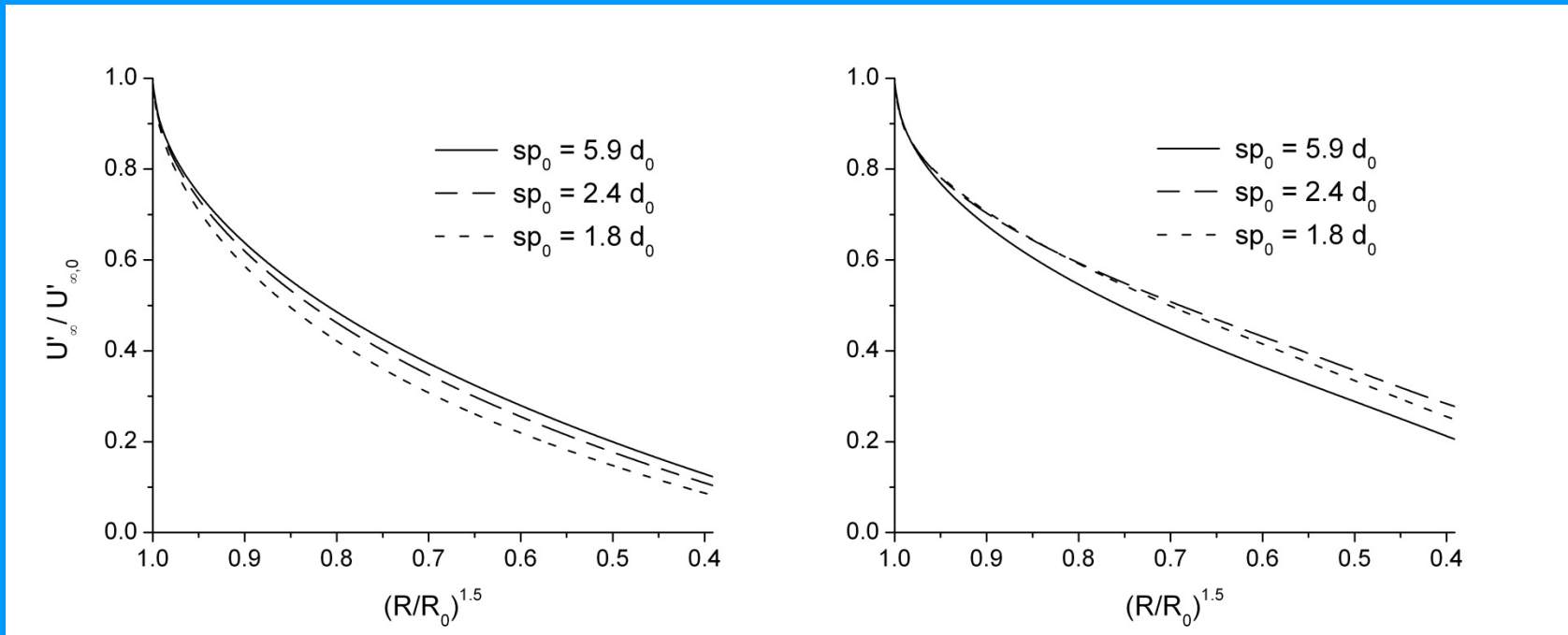
$$sp_0 = 5.9d_0$$



$$sp_0 = 2.4d_0$$

- The instant of wake-to-envelope transition is postponed as initial Reynolds number increases and initial Damkohler number decreases.
- Smaller initial Reynolds number may yield greater burning rate (for some period during the lifetime) because of an earlier wake-to-envelope transition.
- Asymptotically, $R^{1.5}$ is linear in time.

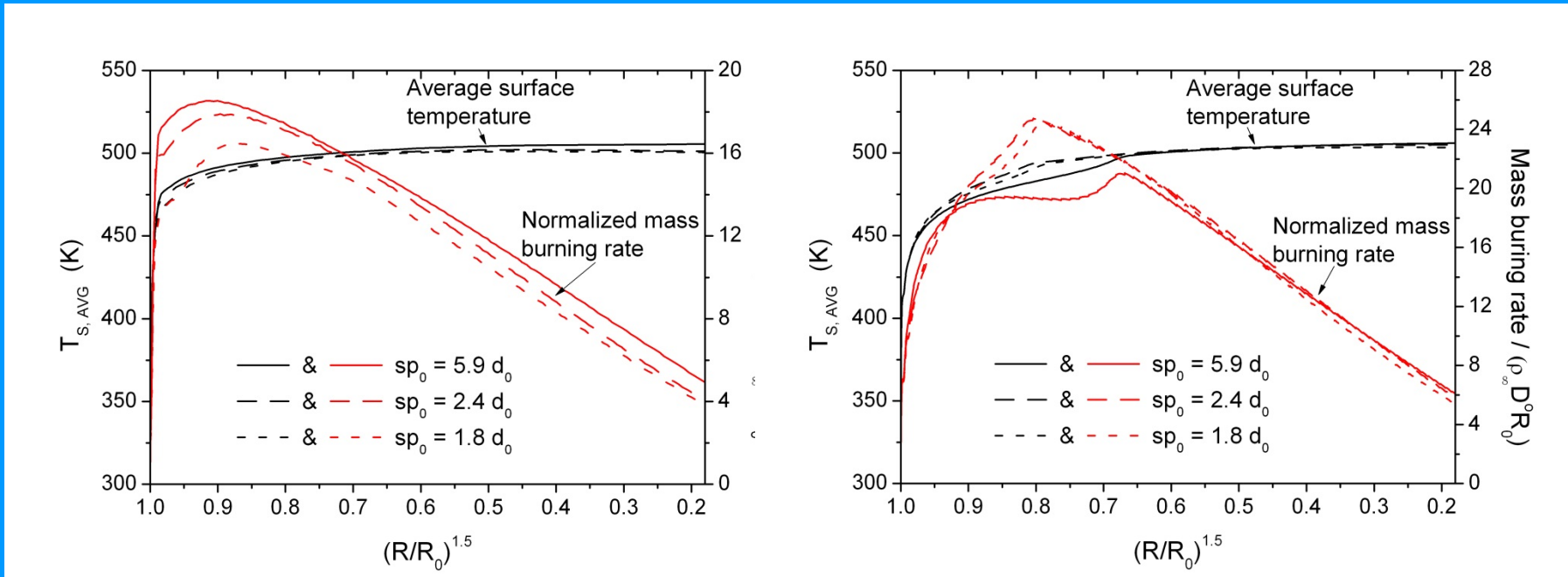
Temporal behavior for different initial droplet spacing (1)



$Re_0 = 89$ without chemical reaction $Re_0 = 89$ with chemical reaction

- The drag and the rate of decrease of the relative stream velocity is affected by the gas velocity between the adjacent droplets.
- Without chemical reaction, the gas velocity between the adjacent droplets and the drag increase as the initial droplet spacing decreases.
- With reaction, the gas velocity between the adjacent droplets is also modified by the flame, and decreases first and then increases as the initial droplet spacing decreases. These qualitative results apply for other initial Re values.

Temporal behavior for different initial droplet spacing (2)



$$Re_0 = 9 \quad (Da_0 = 1.5)$$

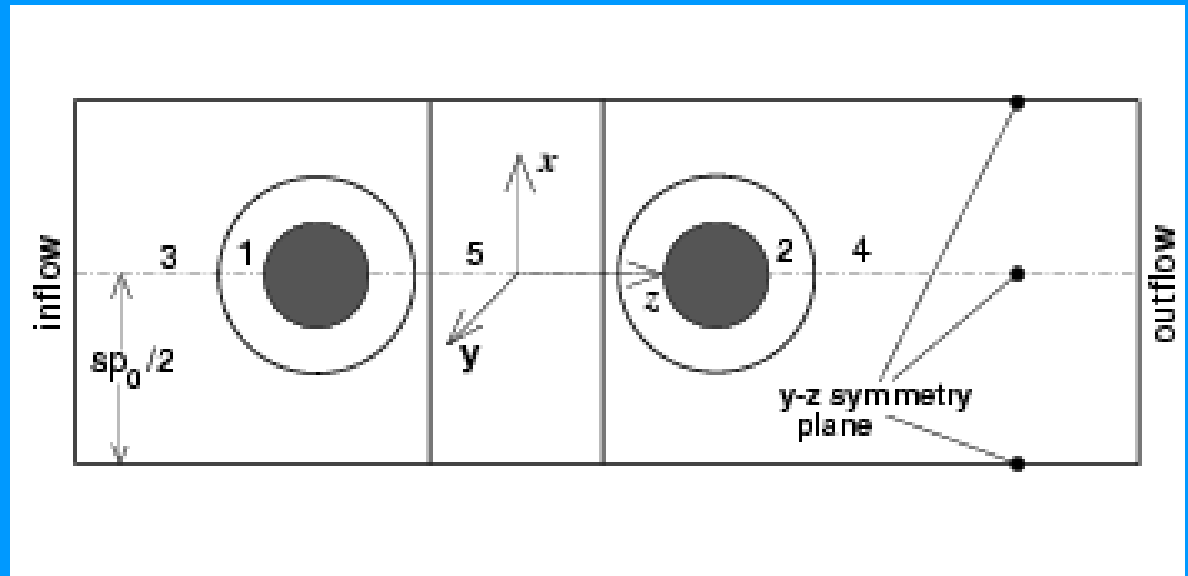
$$Re_0 = 45 \quad (Da_0 = 0.3)$$

- The instant of wake-to-envelope transition advances first and then is delayed as the initial droplet spacing decreases, because of the gas velocity behavior between the adjacent droplets.
- The burning rate is influenced by the interactions amongst droplets and the instant of wake-to-envelope transition.

Periodic Arrays with Two Layers

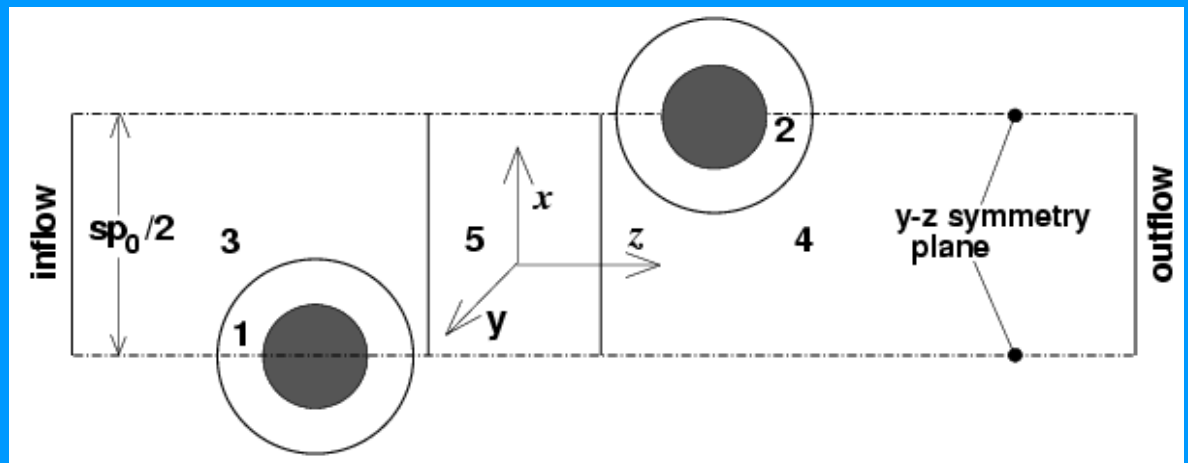
Droplets in Tandem

The second layer of periodic array has a droplet immediately aft of front droplet.

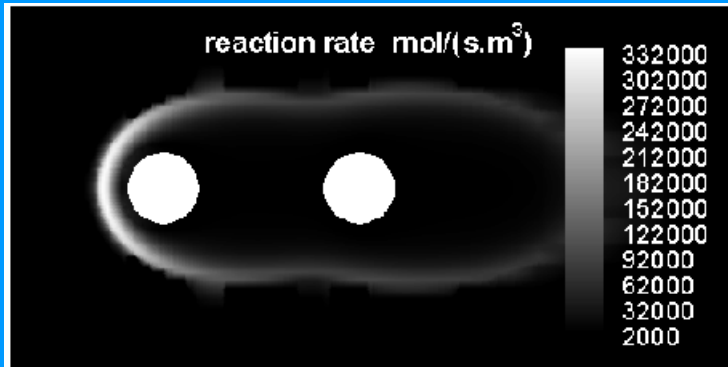


Staggered Droplets

The second layer of periodic array has a droplet offset in both transverse directions from front droplet.

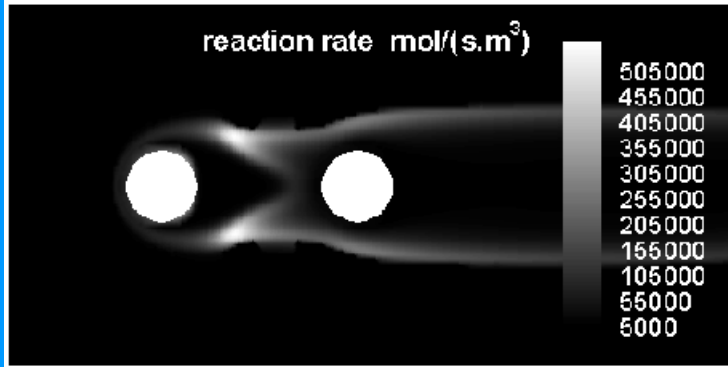


Flame Structure for Periodic Array with Tandem Droplets



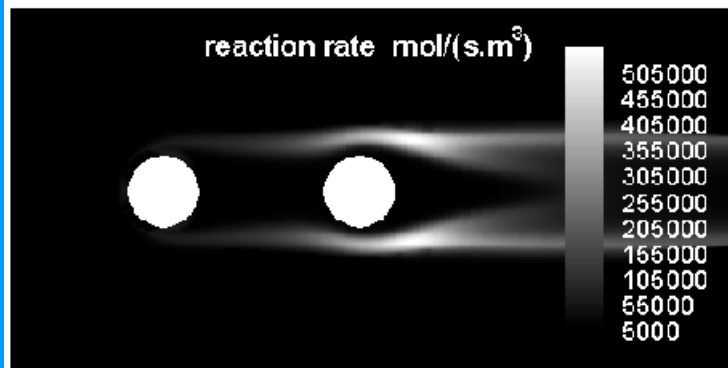
$s/R_0 = 5.6$

$Re_0 = 11$



$s/R_0 = 5.6$

$Re_0 = 45$



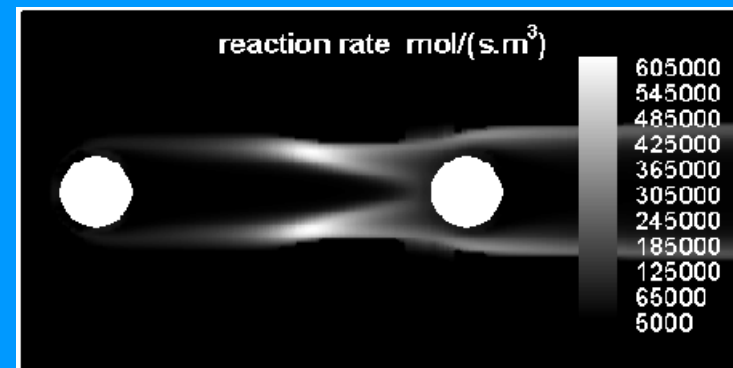
$s/R_0 = 5.6$

$Re_0 = 110$

Transverse spacing of
5.9 d_0 for all cases.

*Residence time affects
flame structure
through velocity, drop
size, and spacing*

$s/R_0 = 10.6, Re_0 = 110$



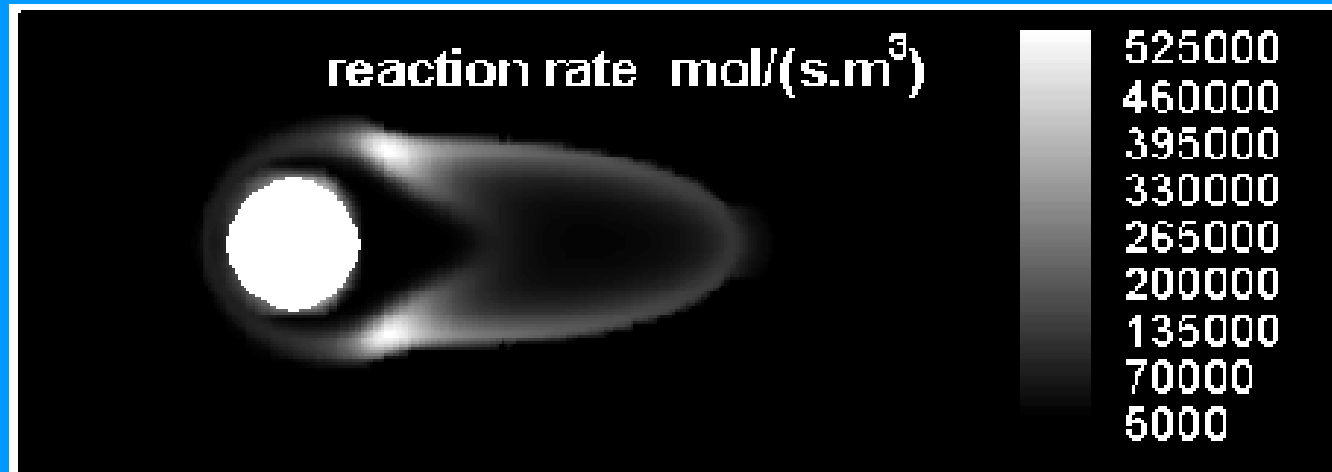
Flame Structure for Periodic Array with Two Staggered Layers

Transverse Spacing = $3.8 d_0$

$s/R_0 = 5.6$

$Re_0 = 45$

Front Droplet



Aft Droplets



Concluding remarks (1)

- In the transient process for a droplet array, an initial envelope flame remains an envelope flame, and an initial wake flame has a tendency to develop from a wake flame to an envelope flame. Similarly to isolated droplets, the flame standoff distance does not vary significantly during the lifetime.
- Generally, if a flame is initially a separated, individual flame for each droplet (or a group flame for many droplets), it remains a separated flame (or group flame) for a long time.
- For an initial wake flame, the wake-to-envelope transition time advances as the initial droplet spacing (intermediate) is decreased, but then delays as the initial droplet spacing is further reduced.
- The critical initial Damkohler number for the determination of an initial envelope or wake flame does not vary with initial Reynolds number and decreases with decreasing initial droplet spacing for intermediate spacing values, but has no substantial change when the initial droplet spacing becomes too small.

Concluding remarks (2)

- **Burning rate is influenced by the Reynolds number, wake-to-envelope transition time, and interaction amongst droplets. Smaller initial droplet spacing or initial Reynolds number may yield greater burning rate (for some period during the lifetime) because of an earlier wake-to-envelope transition.**
- **Lower ambient temperature yields smaller initial Damkohler number and slower droplet heating, and thereby a later wake-to-envelope transition and smaller mass burning rate.**
- **At lower ambient pressure, the average surface temperature is much smaller due to a lower boiling point, and the wake-to-envelope transition also occurs later due to a smaller initial Damkohler number which favors a wake flame.**
- **Downstream droplets downstream decelerate more slowly than the front droplets due to reduced drag and are more likely to hold envelope flames.**

Thank you for your attention.