Transient convective burning of a periodic fuel-droplet array

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Abstract

The transient convective burning of fuel-droplets interacting within 3-D infinite periodic arrays in a hot gas stream is numerically studied for the first time, with considerations of droplet regression, deceleration due to the drag of the droplets, internal liquid motion, variable properties, non-uniform liquid temperature, surface tension, and n-octane one-step oxidation kinetics. Depending upon the initial conditions and other constraints, a flame is established early as either a wake flame or an envelope flame. 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. The flame shows no strong tendency to modify significantly the standoff distance during the lifetime of the droplet. For an initial wake flame, the moment of wake-to-envelope transition is advanced as the initial droplet spacing (intermediate) is decreased, but tends to be postponed as the initial droplet spacing is further reduced. The burning rate at smaller initial droplet spacing or smaller initial Reynolds number might be greater for some period during the lifetime because of an earlier wake-to-envelope transition which elevates the average surface temperature. Lower ambient temperature yields a later wake-to-envelope transition time and smaller mass burning rate. At the lower ambient pressure with the same initial relative stream velocity, the average surface temperature is reduced, the wake-to-envelope transition is later, and the mass burning rate is smaller. Validation of our analysis is made by comparing with the results of an isolated droplet Wu and Sirignano [11].

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1. Introduction

A spray environment is characterized by droplet interactions as well as gas stream convection. Multi-droplets break the axi-symmetry assumption, and the gas-stream convection requires flow-field solutions with internal circulation and relative motion amongst droplets. So, an accurate simulation requires the numerical solution of the 3-dimensional Navier–Stokes, energy and species equations, combined with appropriate boundary conditions. For an accurate 3-D transient calculation, the computational cost may reach the available limit.

There are several relevant studies on convective vaporization of droplets. Asano et al. [1] investigated the interactions on drag coefficients and mass transfer coefficients of two adjacent spheres analytically by assuming steady flow and constant properties. They proposed correlations to account for the interactions for different geometric parameters. Patnaik [2] studied numerically...
the interaction between two vaporizing droplets moving in tandem, by solving the two droplets separately and neglecting the effects of the change of spacing between droplets. Raju and Sirignano [3] examined the same problem by using the implicit finite-difference method together with a grid-generation scheme to solve the transport equations for the whole domain. They [2,3] assumed constant thermo-physical properties expect for the density. Chiang et al. [4] found for a single vaporizing droplet that the drag coefficient can be overestimated by at least 20% with constant physical properties; so thermal dependence of physical properties must be considered for high-temperature calculation. The vaporizing droplets moving in tandem with variable properties were numerically investigated by Chiang and Sirignano [5,6].

Other relevant studies exist for isolated burning fuel droplets in convective flows. Aouina and Maas [7] numerically simulated the heating, vaporization, and ignition of a cold droplet injected in a hot gas flow. The time and position of ignition and the 2-D gas-phase contours up to and during the time of ignition were investigated. Dwyer et al. [8,9] studied the influence of surface tension on the burning of a convective methanol droplet, and concluded that the surface tension forces caused by surface mass-fraction gradients of water were important. Raghavan et al. [10] made experimental and numerical investigations of convective droplet burning. The stream velocity and droplet radius were kept constant and the interior of the droplet was not modeled. Wu and Sirignano [11] extended their work with considerations of transient heating of the droplet, droplet regression, deceleration due to the drag of the droplet, internal circulation inside the droplet, and the effect of surface tension. They found that the flame had always the tendency of wake-to-envelope transition for the decelerating relative stream velocity.

Kim et al. [12] studied three-dimensional flow over two spheres (solid or liquid) placed side by side without vaporization. They found that the drag of the droplets does not change much for different intermediate droplet spacing, but is increased significantly as the droplets get close. Some important work has been done on burning convective droplet arrays. Stapf et al. [13] numerically studied the combustion of 10 moving droplets in a disc-shaped configuration with an overset gridding scheme. The chemistry was treated with global and detailed reaction kinetics in a two-stage model. Their following paper [14] made a more detailed study on unsteady vaporization and ignition of an array of six droplets arranged with centers in a plane. The relative positions of the droplets were assumed unchanged. The array geometry had a strong influence on the flow field and the physical–chemical processes. Neither paper considered internal circulation, treating the liquid phase as one dimensional. A more complete review of droplet vaporization and burning is given by Sirignano [15].

The task of this study is to numerically simulate convecting, burning and interactive droplets in 3-D periodic arrays, by solving the Navier–Stokes, energy and species equations. Droplet regression, deceleration of the stream flow due to the drag of the droplets, internal circulation, variable properties, non-uniform surface temperature, and surface tension are considered. The transient flame shape, surface temperature, relative stream velocity, and burning rate are studied for different initial relative stream velocity, initial droplet spacing, and ambient temperature and pressure. Particularly, the flame transition (from a wake flame to an envelope flame) time and its influence on the burning rate are determined.

2. Problem formulation

The single-component n-octane droplets form a periodic array in a hot gas stream. The array is infinite in both cross-flow directions but has only one droplet layer in the flow direction. Figure 1 indicates a large number of droplets with the same initial size, uniform distribution in the x–y plane, and perpendicular flow direction to this plane (in the z direction). As the 3-dimensional flows are periodic along the two directions in the plane, only one droplet (with the domain of ABCD in Fig. 1) is considered in the calculation using four symmetry planes. In fact, the actual domain for the calculation can be further reduced into OECF with only a quarter of the droplet due to symmetries.

The free-stream air flow has velocity $U_\infty$, pressure $p_\infty$, and temperature $T_\infty$. The initial droplet
temperature $T_{s,0}$ is uniform and low compared to the boiling point. The droplets are first heated and vaporized, and then ignited and burned. Internal circulation is caused by the shear stress at the gas-side droplet surface and the non-uniform distribution of surface tension around the droplet surface. Although the droplets have a time-varying velocity $U_d$, we consider that they are not moving by instantaneously having an inertial frame of reference moving at the droplet velocity [4–6]. The relative velocity becomes: $U''_{\text{rel}} = U_{\infty} - U_d$. This is justified because all the droplets are identical and the relative motion amongst the droplets is zero for this array. As the droplets are slowed by the drag and vaporization occurs, the relative velocity and droplet radius are updated continuously.

The following assumptions are made: (1) the Mach number is much less than unity and the dissipation terms are neglected; (2) the natural convection and other gravity effects are negligible (with Grashof number and the ratio of the gravitational force and the drag force below 0.01 in this study); (3) the droplets remain spherical; (4) the gas mixture is an ideal gas; (5) the liquid-phase properties variation is neglected; and (6) the radiation is neglected. These assumptions can be justified by the quantitative results for constraints that are of practical relevance.

The variables have been non-dimensionalized and are listed as follows: radial position $r = \frac{\rho}{\rho_0}$, time $\tilde{t} = \frac{U_{\infty,0}}{d_0}$, velocity vector or components $\tilde{u} = \frac{u}{U_{\infty,0}}$, pressure $\tilde{p} = \frac{p}{p_\infty U_{\infty,0}}$, density $\tilde{\rho} = \frac{\rho}{\rho_{\infty}}$, enthalpy $\tilde{h} = \frac{h}{c_p(T_{\infty,0} - T_{\text{ad}})}$, temperature $\tilde{T} = \frac{T - T_{\text{ad}}}{T_{s,0} - T_{\text{ad}}}$, molecular weight $\tilde{M} = \frac{M}{M_p}$, specific heat $\tilde{c}_p = \frac{c_p}{c_{p,\infty}}$, dynamic viscosity $\tilde{\mu} = \frac{\mu}{\mu_{\infty}}$, thermal conductivity $\tilde{\lambda} = \frac{\lambda}{\lambda_{\infty}}$, thermal diffusivity $\tilde{\alpha} = \frac{\alpha}{\alpha_{\infty}}$, mass diffusivity $\tilde{D}_\text{m} = \frac{D_m}{D_{m,\infty}}$, shear stress tensor $\tilde{\tau} = \frac{\tau}{\mu_{\infty} U_{\infty,0}}$, reaction rate $\tilde{\omega} = \frac{\omega}{\dot{\rho}_{\text{in}}}$, surface tension $\tilde{\sigma} = \frac{\sigma}{\sigma_0}$, where $d_0$ and $U_{\infty,0}$ denote the initial droplet diameter and the initial relative stream velocity. The superscript ‘O’ denotes the reference value, and the subscripts ‘F’, ‘I’, ‘\infty’ and ‘O’ denote the fuel vapor, the ith species, the ambient value and the initial value, respectively. There are certain dimensionless numbers generated: initial Reynolds number $Re_0 = \frac{\rho U_{\infty,0} d_0}{\mu_{\infty}}$, Prandtl number $Pr_{\infty} = \frac{c_p}{\alpha_{\infty}}$, Schmidt number $Sc_{\infty,0} = \frac{\alpha_{\infty}}{D_{m,\infty}}$, Spalding transfer number $Bo = \frac{\rho c_p(T_{\infty,0} - T_{\text{ad}})}{\lambda}$, initial Weber number $We_0 = \frac{\rho U_{\infty,0}^2 d_0}{\sigma_0}$, and initial Damkohler number $Da_0 = \frac{d_0 / U_{\infty,0}}{Y_p / (\omega v_{DF})}$ (where $Y_p$ is the reference mass fraction for the fuel vapor).

The governing equations for both gas and liquid phases are

$$\frac{\partial \rho_0 \tilde{u}}{\partial \tilde{t}} + \nabla \cdot (\rho_0 \tilde{u} \tilde{u}) = \nabla \cdot (F_\rho) + S_\rho,$$

with $\Phi = 1$ for the continuity equation, $\tilde{u}$ for the momentum equation, $h$ for the energy equation, and $Y_i$ for the gas-phase species equation. For the continuity equation, $F_1 = S_1 = 0$. For the momentum equation, $F_2 = \frac{1}{Re \tilde{\sigma}}$ and $S_2 = -\nabla \tilde{p}$, in which $\tilde{\sigma}$ is the shear stress tensor in the form for the Newtonian compressible fluid. For the energy equation, $F_3 = \frac{\rho \tilde{c}_p}{Re\tilde{c}_p} \nabla h$, $S_3 = \nabla \cdot (\tilde{\rho} \tilde{D}_\text{m} \nabla Y_i) / (Re_0 Sc_{\infty,0}) - \nabla \cdot (\tilde{p} \tilde{c}_p \Sigma_i \tilde{D}_\text{m} \nabla Y_i) / (Re_0 Pr_{\infty}) + \frac{\tilde{q}_{\text{in}} \tilde{D}_\text{m}}{Re_0 \tilde{c}_p} (T - T_{\text{ad}})$ for the gas phase, and 0 for the liquid phase. $q$ is the heat of combustion. The reaction rate is given by $\tilde{\omega} = \tilde{a} \tilde{c}_p \tilde{F}^{[\text{Fuel}]^{b}}$, with $A = 4.6 \times 10^{11}$, $E_a = 1.255 \times 10^{5}$, $a = 0.25$, $b = 1.5$ for n-octane, from Westbrook and Dryer [16]. The reference value of the reaction rate $\tilde{\omega}^0$ is calculated based on $T_{\infty,\rho_{\text{in}}}, Y_{i,\rho_{\text{in}}}$, and the stoichiometric mass fraction for the fuel vapor $Y_p^0$. The values of $\tilde{\omega}^0$ and the initial Damkohler number $Da_0$ will be very sensitive to the choice of the reference temperature, and $T_{\infty,\rho_{\text{in}}}$ is a good choice for high ambient temperature where autoignition becomes possible. The temperature is obtained from the enthalpy. For the gas-phase species equation, $F_{Y_i} = \frac{\rho_{\text{in}}}{Re_0 Sc_{\infty,0}} \nabla Y_i$, and $S_{Y_i} = \tilde{\omega} \tilde{M} Y_i Y_p^0 Da_0$, in which $\tilde{M}$ and $s_i$ are the normalized molecular weight, and stoichiometric number for the ith species which represents moles of this species produced (+) or consumed (−) for each mole of fuel consumed.

The gas-phase continuity, momentum, energy and species equations and liquid-phase continuity, momentum and energy equations are coupled and solved simultaneously. There are totally $N = 5$ species including the fuel vapor, oxygen, water vapor, carbon dioxide, and nitrogen considered in the calculation. The species equations are applied to the first four species, while the concentration of nitrogen is obtained from the relation that the mass fraction for all the species sums to unity. The computational domain for the gas phase in Fig. 1 will be divided into $N_d$ ($N_d$ is the number of droplets and is 1 in this paper due to symmetry planes for the periodic array configurations) spherical domains, with one of these domains around each droplet, and one cartesian domain for the rest. For the liquid phase, each droplet has one separate spherical domain. The detailed form of the momentum equation in spherical coordinates and cartesian coordinates is provided in [17].

The droplet surface regresses during vaporization, and the droplet radius is a function of time $\tilde{R}(\tilde{t})$. Therefore, the liquid-phase domain shrinks while the gas-phase domain expands. To consider this, the radial position $\tilde{r}$ for the liquid phase is normalized by $\tilde{R}(\tilde{t})$: $\tilde{x} = \tilde{r} / \tilde{R}(\tilde{t})$, and the governing
equations for the liquid phase are modified accordingly: substitute \( \tilde{r} \) for \( R(\tilde{t}) \cdot \xi \), and replace \( \frac{\partial \Phi}{\partial \tilde{r}} = (\tilde{\Phi}) \) represents \( \tilde{p}, \tilde{u}_x, \tilde{u}_y, \tilde{u}_z, \) or \( \tilde{h} \) term with \( \frac{\partial \tilde{\Phi}}{\partial \tilde{r}} + \frac{\xi}{R(\tilde{t})} \frac{\partial \Phi}{\partial \tilde{t}} \). However, the radial position \( \tilde{r} \) for the gas-phase spherical domains is not normalized by \( R(\tilde{t}) \) in contrast with the liquid phase and thus mesh adjustment is required for the gas phase. Details regarding the mesh adjustment are provided in Wu and Sirignano [11].

The outer boundaries of the cartesian domain are the inflow and outflow boundaries of the gas stream, and the symmetry planes, with the boundary conditions \( \tilde{u}_x = \tilde{u}_y = 0, \quad \tilde{u}_z = \tilde{U} \tilde{u}_x, \tilde{T} = 1, \quad Y_i = 0.233 \) for \( O_2 \) and 0 for others at the inflow boundary, \( \partial(\tilde{u}_x, \tilde{u}_y, \tilde{u}_z, \tilde{Y}_i) / \partial \tilde{x} = 0 \) at the outflow boundary, \( \tilde{u}_x = 0, \partial(\tilde{u}_y, \tilde{u}_z, \tilde{Y}_i) / \partial \tilde{y} = 0 \) at the symmetry planes in the \( x \) direction, and \( \tilde{u}_y = 0, \partial(\tilde{u}_x, \tilde{u}_z, \tilde{Y}_i) / \partial \tilde{z} = 0 \) at the symmetry planes in the \( y \) direction. Matching conditions at the droplet surface are the same as the isolated droplet calculation [11], except the conditions for \( \tilde{u}_y \) which are similarly derived from continuity of tangential velocity and shear stress in \( \phi \) direction. Boundary conditions at the ends of \( \theta \) and \( \phi \) directions for the spherical domains can be derived based on continuity and the features of the flow, with \( \partial(\tilde{u}_x, \tilde{u}_y, \tilde{u}_z, \tilde{Y}_i) / \partial \tilde{\phi} = 0 \) at \( \theta = 0 \) and \( \pi \), and \( \tilde{u}_\phi = 0, \partial(\tilde{u}_x, \tilde{u}_y, \tilde{Y}_i) / \partial \tilde{\theta} = 0 \) at \( \phi = 0 \) and \( \pi / 2 \). Boundary conditions at the interfaces of gas-phase spherical domains and the cartesian domain are given by the continuity of the calculated quantities and their first derivatives: \( \{ \tilde{u}, \tilde{h}, \tilde{Y}_i \} _A \{ \tilde{u}, \tilde{h}, \tilde{Y}_i \} _B \) with “A” denoting gas-phase spherical domains and “B” denoting the cartesian domain.

The droplets are slowed by the drag \( C_D \) in the transient process, including pressure drag, friction drag and thrust drag. The instantaneous velocity of any of the droplets is thus determined by

\[
\frac{d\tilde{r}}{dt} = -\frac{8 \pi \tilde{r} \tilde{U}^2 \tilde{C}_D}{3}.
\]

3. Solution procedure

The thermodynamic and transport properties for the gas mixture are calculated by polynomials and semi-empirical equations [18–20]. The data [16] is used for the calculation of chemical reaction rates. The momentum equations, energy equation and species equations (gas phase only) are solved in order for each domain. Then, the temperature distributions are obtained by solving the differential form of \( \tilde{h} = h(T, \tilde{Y}_i) \). The droplet radius and relative velocity between the droplets and the free stream are updated instantaneously after each time step.

The gridding scheme for the 3-dimensional multi-droplet calculation is demonstrated in the left lower quarter of Fig. 1. Spherical grids are used for the spherical domains and cartesian grids are used for the cartesian domain. The sections represented by the solid lines are the spherical domains for the liquid phase. The sections represented by the dash-dot lines are the spherical domains for the gas phase. Their inner boundaries are the surface of the droplets, and their outer boundaries are the spheres with larger diameter and the same center as the droplets, as represented by the hollow circles in Fig. 1. The section represented by the dash lines is the cartesian domain for the gas phase. Its inner boundaries are the surfaces composed of the nodes inside and close to the outer boundary of the gas-phase spherical domains, as represented by the solid circles in Fig. 1. Its outer boundary is the free stream. Overlapping areas exist between the outer boundaries of the gas-phase spherical domains and the inner boundary of the cartesian domain. Interpolations are needed to get the boundary conditions at the interface of the two types of domains in the gas phase.

The Semi-Implicit Method for PressureLinked Equations (SIMPLE) is used to solve the coupled Navier-Stokes, energy and species equations for both gas and liquid phases. Staggered grids are used with four different control volumes for the three components of velocity and pressure correction (temperature, mass fraction or scalar properties) respectively. Forward time and central difference scheme are applied. For the iterations at each time step, the Alternating Direction Implicit (ADI) method is used to sweep in all the three directions. The grid and time-step independence have been tested, with the following selection for the size of mesh and time step giving a good balance between solution accuracy and computational economy. For the spherical domains, the mesh size is \( \Delta \theta = \pi / 40 \) in the \( \theta \) direction and \( \Delta \phi = \pi / 40 \) in the \( \phi \) direction for both liquid and gas phase; the mesh size in the \( r \) direction is \( \Delta r = 0.02R \) for the liquid phase and \( \Delta r = 0.01R \) for the gas phase. As the droplet surface regresses, the new cells added to the gas-phase spherical domain always have a mesh size of \( \Delta r = 0.01R \). For the cartesian domain, the mesh is uniform with \( \Delta x \) (or \( \Delta y, \Delta z \) = 0.1R) within a cube with side length of 4R and the center located at the droplet center, but diverges with a factor of 1.2 with distance away from this cube. The cartesian domain has a length of 32R in the \( z \) direction (the flow direction). The domain sizes in the \( x \) and \( y \) directions are determined by the droplet spacing in the two directions. The time step size is fixed and it takes about 10^5 time steps for 99% of the droplet volume to be vaporized. Each calculation requires about 60 h of time on the Pentium based computers. The errors due to the mesh-update scheme in the gas phase are found to be small, and have negligible influence on the stability of the calculations.
In order to validate the 3-D hybrid gridding scheme and the codes, we calculated the transient burning of an isolated droplet with the 3-D hybrid grid and two other simplified schemes: 2-D spherical grid [11] and 3-D spherical grid, which are only applicable for an isolated droplet. The ambient pressure, ambient temperature, and initial droplet radius are 20 atm, 1500 K, and 25 \( \mu m \). The transient average temperature around the droplet surface and the instantaneous radius squared of the droplet are compared for the three grids, at two different initial Reynolds numbers: \( Re_0 = 45 \) (\( Da_0 = 0.3 \)) and \( Re_0 = 89 \) (\( Da_0 = 0.15 \)), respectively. The results for the 2-D spherical grid and the 3-D spherical grid agree very well for both of the two initial Reynolds numbers. So, Fig. 2 only includes the comparisons of the results for the 3-D spherical grid and the 3-D hybrid grid, showing that the transient behaviors for the two grids are very close, at both \( Re_0 = 45 \) and \( Re_0 = 89 \).

4. Results and discussion

The initial relative stream velocity \( U'_{\infty,0} \) and the initial spacing amongst droplets \( sp_0 \) are varied to study the effects of forced convection and droplet interaction, at the ambient temperature \( T_\infty = 1500 \) K, ambient pressure \( p_\infty = 20 \) atm, and initial droplet radius \( R_0 = 25 \) \( \mu m \). The change in the initial relative stream velocity changes the initial Reynolds number \( Re_0 \) and Damkohler number \( Da_0 \). The ambient temperature and pressure are varied for other cases to study the influence of the ambient conditions.

Fig. 3a–d show the contours of the chemical reaction rate at two instants during the lifetime, for four cases with different initial relative stream velocity or initial droplet spacing. The initial flame shape is either an envelope flame or a wake flame, and either a connected flame, also known as a group flame, or a separated flame, as determined by the initial relative stream velocity and the initial droplet spacing. In the transient process, 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. This can be explained from the increasing surface temperature, decreasing Reynolds number (due to the decrease of both droplet radius and relative stream velocity), and increasing Damkohler number (due to the faster decrease of relative stream velocity than the droplet radius) over time, all of

![Fig. 2. Comparisons for the 3-D spherical grid and the 3-D hybrid grid, at two different initial Reynolds numbers for an isolated burning fuel droplet.](image)

![Fig. 3. The contours of the chemical reaction rate at two instants during the lifetime, for four cases: (a) \( Re_0 = 9 \) (\( Da_0 = 1.5 \)) and \( sp_0 = 5.9 \) \( d_0 \), with the initial flame shape envelope and separated; (b) \( Re_0 = 45 \) (\( Da_0 = 0.3 \)) and \( sp_0 = 5.9 \) \( d_0 \), with the initial flame shape wake and separated; (c) \( Re_0 = 9 \) (\( Da_0 = 1.5 \)) and \( sp_0 = 2.4 \) \( d_0 \), with the initial flame shape envelope and connected; (d) \( Re_0 = 45 \) (\( Da_0 = 0.3 \)) and \( sp_0 = 1.8 \) \( d_0 \), with the initial flame shape wake and connected.](image)
which favor an envelope flame. The flame shows no strong tendency to modify significantly the standoff distance during the lifetime of the droplet; i.e., an initially separated flame remains a separated flame and an initially connected flame remains a connected flame, if the initial flame is not too close to the critical state from a separated flame to a connected flame. This can be explained from the general balance of the regression of the droplet surface over time which tends to shrink the flame, and the decreasing Reynolds number and increasing surface temperature over time which tend to increase the flame stand-off. Both the decrease of the Reynolds number and the increase of the surface temperature allow the fuel vapor to diffuse and advect farther from the droplet surface and thus increase the flame stand-off.

The comparisons of the instantaneous average surface temperature and normalized radius to three halves power for different initial Reynolds number at the same initial droplet spacing \((2.4 d_0)\) are shown in Fig. 4. The flame is initially an envelope flame for \(Re_0 = 9\) \((Da_0 = 1.5)\), and a wake flame for \(Re_0 = 45\) \((Da_0 = 0.3)\) and \(Re_0 = 89\) \((Da_0 = 0.15)\), which transitions into an envelope flame later during the lifetime as indicated by the sharp increase of the average surface temperature. For the situation without liquid heating, chemical reaction and decrease of the relative stream velocity, the curve of the instantaneous radius to three halves power is found to be almost linear during the lifetime. Otherwise with those considerations, the curve is obviously convex during the period of fast initial liquid heating, but generally linear afterward due to the balance of the slower liquid heating (which makes the curve tend to be convex) and the decreasing Reynolds number (which makes the curve tend to be concave), with a modest jump of the slope during the wake-to-envelope transition (which elevates the liquid surface temperature and thus elevates the vaporization rate) for an initial wake flame. The decreasing \((R/R_0)^{1.5}\) is therefore used as the normalized time scale in the following plots for convenience. As greater initial Reynolds number (and smaller initial Damkohler number) postpones the wake-to-envelope transition which elevates the vaporization rate for an initial wake flame, the burning rate for the greater initial Reynolds number may be smaller for some period during the lifetime (e.g., the cases of \(Re_0 = 45\) \((Da_0 = 0.3)\) and \(Re_0 = 89\) \((Da_0 = 0.15)\) in Fig. 4).

The instantaneous relative stream velocity with different initial droplet spacing at the initial Reynolds number \(Re_0 = 89\) \((Da_0 = 0.15)\) is compared in Fig. 5. The comparisons are also made for the special situation without chemical reaction, to understand the influence of the initial droplet spacing on the relative stream velocity. Without chemical reaction, the rate of decrease of the relative stream velocity over time increases with decreasing spacing, with the increase greater from 2.4 \(d_0\) to 1.8 \(d_0\) than from 5.9 \(d_0\) to 2.4 \(d_0\). This occurs because gas velocity between the adjacent droplets and the droplet drag increase slowly with the decreasing initial droplet spacing when the initial droplet spacing is intermediate, but rise increasingly fast with the decreasing initial droplet spacing when the initial droplet spacing is close to the thickness of the velocity boundary layer (named “velocity-increase effect” of the flow between the adjacent droplets). With chemical reaction, the gas velocity between the adjacent droplets and the drag of the droplets are also modified by the presence of the flame, i.e., with a tendency to decrease with the decreasing initial droplet spacing. This occurs because smaller droplet spacing results in a cooler, denser region between the adjacent droplets due to the presence of the fuel vapor and thus smaller reaction rate in the region between the adjacent droplets. (This behavior is named the “velocity-decrease effect” of the flow between the adjacent droplets.) Therefore, the rate of decrease of the relative stream velocity for the situation with the chemical reaction is influenced by two opposing factors.

![Fig. 4. Comparisons for different initial Reynolds number, at \(sp_0 = 2.4 d_0\).](image)

![Fig. 5. Comparisons of the instantaneous relative stream velocity for different initial droplet spacing \(sp_0\) (at \(Re_0 = 89\), under the situations with and without chemical reaction.](image)
shown in Fig. 5, as the initial droplet spacing is decreased from $5.9 \, d_0$ to $2.4 \, d_0$, the “velocity-increase effect” of the flow between the adjacent droplets is less than the “velocity-decrease effect” and the rate of decrease of the relative stream velocity decreases; however, as the initial droplet spacing is further reduced to $1.8 \, d_0$, the “velocity-increase effect” of the flow between the adjacent droplets becomes more important because of smaller initial droplet spacing, and the rate of decrease of the relative stream velocity starts to increase.

The instantaneous average surface temperature and normalized mass burning rate at different initial droplet spacing are compared in Fig. 6a and b, for $Re_0 = 9$ and 45, respectively. For $Re_0 = 9$ ($Da_0 = 1.5$) with an envelope flame during the lifetime, the increase of the surface temperature is faster at the greater initial droplet spacing due to a higher flame temperature resulting from less interaction amongst droplets and greater chemical reaction rate. For $Re_0 = 45$ ($Da_0 = 0.3$) with an initial wake flame, the wake-to-envelope transition during the lifetime is indicated by the sharp increase of the average surface temperature and the mass burning rate in Fig. 6b. As discussed previously, the flow between the adjacent droplets is slowed as the initial droplet spacing is decreased from $5.9 \, d_0$ to $2.4 \, d_0$, but increased as the initial droplet spacing is decreased from $2.4 \, d_0$ to $1.8 \, d_0$. This can also explain that the instant of wake-to-envelope transition is advanced as the initial droplet spacing is decreased from $5.9 \, d_0$ to $2.4 \, d_0$, but tends to be postponed as the initial droplet spacing is decreased from $2.4 \, d_0$ to $1.8 \, d_0$. The initial droplet spacing affects the mass burning rate by the influence on the interaction of fuel vapor amongst droplets and the time of wake-to-envelope transition for an initial wake flame. At $Re_0 = 9$ with an envelope flame all the time, the mass burning rate is greater for greater initial droplet spacing because of smaller interaction of fuel vapor amongst droplets. At $Re_0 = 45$ for which the wake-to-envelope transition occurs early, the differences of the mass burning rate are primarily due to the differences in the wake-to-envelope transition times for different initial droplet spacing, and the case of $sp_0 = 2.4d_0$ with the earliest transition has the greatest overall burning rate.

The ambient temperature or pressure is changed for some cases to study the influence of the ambient conditions. The instantaneous average surface temperature and normalized mass burning rate are compared for different ambient temperature ($T_\infty = 1500$ and $1200$ K) but the same ambient pressure ($p_\infty = 20$ atm), at $Re_0 = 45$ and 89, and $sp_0 = 2.4d_0$. As the ambient temperature is decreased from 1500 to 1200 K, the initial relative stream velocity decreases (for the same initial Reynolds number) and the initial residence time increases; however, the initial Damkohler number decreases (from 0.3 to 0.04 for $Re_0 = 45$ and from 0.15 to 0.02 for $Re_0 = 89$) because of greater increase of the reference chemical reaction time than the initial residence time. Therefore, the cases with the lower ambient temperature have later wake-to-envelope transition and smaller mass burning rate, due to the smaller initial Damkohler number which favors a wake flame and also the slower heating of the droplets at the lower ambient temperature. The comparisons are also made for different ambient pressure ($p_\infty = 20$ and 10 atm) but the same ambient temperature ($T_\infty = 1500$ K), at $sp_0 = 2.4d_0$ and $5.9 \, d_0$. All the cases have the same initial relative stream velocity, with $Re_0 = 89$ and $Da_0 = 0.15$ for the cases at $p_\infty = 20$ atm, and $Re_0 = 45$ and $Da_0 = 0.09$ for the cases at $p_\infty = 10$ atm. The average surface temperature at the lower ambient pressure is much smaller due to a lower boiling point. The wake-to-envelope transition at the lower ambient pressure is also later due to a smaller initial Damkohler number which favors a wake flame. Therefore, the cases at the lower ambient pressure have smaller mass burning rate (with the same initial relative

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**Fig. 6.** Comparisons for different initial droplet spacing $sp_0$, at $Re_0 = 9$ and 45, respectively. (a) $Re_0 = 9$ ($Da_0 = 1.5$) (b) $Re_0 = 45$ ($Da_0 = 0.3$).
stream velocity) because of smaller forced convection, lower surface temperature, and later wake-to-envelope transition.

5. Concluding remarks

The transient convective burning of n-octane droplets within a periodic array in a hot air stream is simulated with considerations of droplet regression, deceleration of the stream flow, liquid motion, variable properties, non-uniform surface temperature and surface tension. The transient flame shape, surface temperature, relative stream velocity, and burning rate are investigated under different initial parameters and ambient conditions. The 3-D code benchmarks very well when compared to the axisymmetric results for an isolated droplet case [11].

The initial flame shape is either an envelope flame or a wake flame, and either a connected flame (group flame) or a separated flame, determined by the initial relative stream velocity and the initial droplet spacing. In the transient process, 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. An initially separated flame remains a separated flame and an initially connected flame remains a connected flame, if the initial flame is not too close to the critical state from a separated flame to a connected flame.

At intermediate initial droplet spacing, the decrease of the relative stream velocity becomes smaller as the initial droplet spacing is decreased; however, the relative velocity decrease becomes larger as the initial droplet spacing is further reduced and becomes comparable to the thickness of the velocity boundary layer. Similarly, for an initial wake flame, the wake-to-envelope transition time is advanced as the initial droplet spacing (intermediate) is decreased, but tends to be postponed as the initial droplet spacing is further reduced. The burning rate is influenced by the Reynolds number, the wake-to-envelope transition time (for an initial wake flame), and the interaction amongst droplets. Smaller initial droplet spacing or smaller initial Reynolds number may yield greater burning rate (for some period during the lifetime) because of an earlier wake-to-envelope transition. The curve of the instantaneous radius to three halves power is generally linear after the period of fast initial liquid heating due to the balance of the slower liquid heating and the decreasing Reynolds number, with a modest jump of the slope during the wake-to-envelope transition for an initial wake flame.

Lower ambient temperature yields smaller initial Damkohler number and slower heating of the droplets, and thus causes a later wake-to-envelope transition time and smaller mass burning rate. At the lower ambient pressure (with the same initial relative stream velocity), the initial Reynolds number is smaller, the average surface temperature is smaller due to a lower boiling point, and the wake-to-envelope transition is later due to a smaller initial Damkohler number which favors a wake flame. So, the mass burning rate at the lower ambient pressure is smaller.

References