Abstract

Three-dimensional unsteady Navier-Stokes computations have been performed for the ignition and flame propagation above a liquid fuel (propanol) pool in an airflow duct. Pulsating flame spread behavior occurs if the initial liquid temperature and/or the oxygen mass fraction in the incoming airflow is sufficiently low. The roles of surface-tension-driven flow, gas buoyancy, liquid buoyancy, and hot gas expansion are analyzed. The effects of oxygen mass fraction, pool depth, and pool width are evaluated. An extensive parameter survey determines the regimes of pulsating flame spread and uniform flame spread in the initial temperature/opposed air velocity, pool depth, pool width, or oxygen concentration plane. The two regimes are defined for both earth gravity and microgravity conditions. For narrow pools (2cm), the three-dimensional effects are focused near the poolside edges where the flame front wraps along the poolside edge but remains nearly two-dimensional over most of the pool. For a wider pool (8cm), three-dimensional variations in flame shape occur over much of the pool. The behavior of the flame along the poolside edges differs significantly for earth gravity and microgravity conditions. The supply of oxygen due to buoyancy at the edges is an important factor.

1 Introduction

Schiller, Ross, and Sirignano [1] studied ignition and flame spread above liquid fuels initially below the flashpoint temperature by using a two-dimensional computational fluid dynamics code that solves the coupled equations of both the gas and the liquid phases. Their computational studies and analysis identified the mechanisms for uniform and pulsating flame spread and studied the effects of gravity level, pool depth, fluid properties, and chemical kinetic coefficients on flame spread across liquid fuel pools. Pulsating flame spread was attributed to the establishment of a gas-phase recirculation cell that forms just ahead of the flame leading edge because of the opposing effect of buoyancy-driven flow in the gas phase and the thermocapillary-driven flow in the liquid phase. Schiller and Sirignano [2] extended the same study to include flame spread with forced opposed flow in the gas phase. A transitional flow velocity was found above which an originally uniform spreading flame becomes pulsating. The same type of gas-phase recirculation cell caused by the combination of forced opposed flow, buoyancy-driven flow, and thermocapillary-driven concurrent flow was found to be responsible for the pulsating flame spread. Ross and Miller [3] and Miller and Ross [4] performed experimental work that corroborates the computational findings of Schiller, Ross, and Sirignano [1] and Schiller and Sirignano [2].

Recently, Kim and Sirignano [5] extended the two-dimensional computations of [2] to include the effect of pool depth, initial pool temperatures. In addition, they computed the initial profiles of velocity and fuel vapor concentration of the gas flow over the pool surface before ignition instead of prescribing initial conditions of an artificial Blasius velocity profile and a fixed layer of constant fuel vapor concentration.
as was done in [2]. Their studies mapped out regions of uniform and pulsating flame spread for different opposed flow velocities, pool depths, initial pool temperatures, and gravity levels based on their two-dimensional model.

Cai, Liu, and Sirignano [6] developed a more comprehensive three-dimensional model and computer code for the flame spread problem over liquid fuel pools. Many improvements in modelling and numerical algorithms were incorporated in the three-dimensional code in addition to the improvement regarding the computation of the initial pre-ignition fields of velocity and fuel vapor concentration. The simple diffusion model using a single diffusion coefficient is replaced by a more realistic model using different diffusion coefficients for different species in the gaseous mixture. A second-order time-accurate numerical method with an approximate-factorization (AF) scheme and an adaptive grid method in three-dimensions significantly improve the computational accuracy and efficiency needed for the three-dimensional computations. Pools of finite width and length are studied in air channels of prescribed height and width. Instead of studying the fire spread with the pool placed in a wind-tunnel with an open top, computations are performed in a wind-tunnel with a closed top wall simulating the exact situation in the experiment. Three-dimensional effects of the flame are captured in the computation. The flame wraps around the pool edge and then trails along the edge. The flame extends beyond the edge of fuel pool to be attached to the wind-tunnel wall. Thermal expansion and buoyancy effects create a streamwise vortex near the two poolside edges of the liquid. Flame pulsation is found at both normal gravity and zero gravity for all three cases of initial fuel-air temperature with 30 cm/s opposed flow.

Results presented in [6], however, were restricted to conditions of single pool depth, pool width, and opposed air flow velocity. In this paper, the three-dimensional code developed in [6] is used to study in detail the effect of pool depth, pool width, opposed air flow velocity, and different levels of air oxygen concentration. Significant three-dimensional effects showing an unsteady wavy flame front for cases of wide pool width are found for the first time in computation. Regions of uniform and pulsating flame spread are mapped out for the flow conditions of pool depth, opposed flow velocity, initial pool temperature, and air oxygen concentration under both normal and micro gravity conditions. A detailed examination of the flow field is also done for the zero opposed flow case under normal gravity to compare with three-dimensional experimental data by Konishi et al. [7].

2 Computational Model and Boundary Conditions

The computational model and numerical method used in this study are the same as in [6]. Figure 1 shows the geometry of the three-dimensional model. A shallow pool of liquid n-propanol fuel is placed in a rectangular wind tunnel. The liquid pool surface is made flush to the wind tunnel floor to simplify the computation. Initially, the liquid and the air in the tunnel are assumed to be at the same temperature $T_0$. At the start of computation, air is forced to blow over the liquid fuel. Computation without reaction is performed for 1.0 second to establish the boundary layer and fuel vapor profiles in the gas phase before the igniter shown in Figure 1 is activated. The igniter is modelled as a hot pocket of gas with a temperature that increases linearly from $T_0$ to 1700 K in 0.01 s. The igniter temperature is kept constant until the flame has travelled 1 cm, after which the igniter is turned off. A symmetry about $z = 0$ is assumed. Some important assumptions are summarized below.

1. The gas/liquid interface remains flat and horizontal. Recession of the liquid surface is neglected;
2. All surfaces are assumed opaque and black, and gas radiation is neglected;
3. One-step, finite-rate chemical kinetics are assumed;
4. The energy equation is simplified by the following approximation: (i) low Mach number flow; (ii) work by body forces is neglected; (iii) time derivatives of hydrostatic pressure are neglected; and (iv) effects of concentration gradients on the diffusion of energy are neglected.
Details of the governing equations for the conservation of mass, species, momentum, and energy and the numerical method to solve them are described in [6]. A diffusion model based on [8] that accounts for the differences in diffusion speed of the different species in the mixture is used. Physical properties such as density, viscosity, heat conduction coefficient, and heat capacity \((\rho, \mu, k, c_p)\) for vapor-air mixtures are calculated using standard additive rules for an ideal gas.

The boundary conditions at the gas/liquid interface follow from a heat balance and balance of the shear stresses with surface tension; a continuity of the temperature and tangential velocity; no dissolution of air or combustion products into the liquid; and negligible recession of the liquid surface. The fuel vapor concentration at the liquid surface is assumed to be \(X_F = \frac{p_{sat}(T)}{p_a}\), where \(p_a\) is the ambient pressure and is set to 1 atm and \(p_{sat}(T)\) is obtained by a curve fit for the given fuel.

Zero normal gradient boundary conditions are used in the gas phase at the tunnel inlet while a uniform flow of velocity \(U\) is applied at the exit of the tunnel. No-slip boundary conditions are applied on the wind tunnel walls as well as the liquid pool walls. Adiabatic boundary conditions are used on all liquid pool walls. In three dimensions, the flame over the liquid pool curves around near the two edges of the pool on the sides. The ‘cold’ floor conditions is applied on the wind tunnel floor, in which the wind-tunnel wall is first assumed to be adiabatic until a certain temperature is reached. The maximum temperature of the wind-tunnel floor is limited by the boiling temperature of the liquid fuel.

The numerical method follows essentially the basic discretization steps of the SIMPLE algorithm [9] with SIMPLEC modification and the hybrid-differencing scheme [10] as detailed in Schiller et al. [1] and Schiller [11]. The method is, however, modified to have second-order time accuracy by using a two-step backward time differencing and an approximate factorization method to perform sub-iterations within each implicit time step. Details can be found in [6].

Only half of the wind tunnel is considered. Symmetry condition is applied at the symmetrical plane \(z = 0\). A non-uniform mesh of \(62 \times 42 \times 36\) in the gas phase with clustered grid points in the flame region is used. The mesh for the liquid phase has 20 grid points in depth and coincides with the mesh in the gas phase over the liquid surface. The grid lines in the streamwise direction and along the width of the tunnel are redistributed to concentrate in the flame region every time the flame front has moved.

Figure 1: Geometry for the three-dimensional liquid fuel pool in a wind-tunnel with forced flow.
1 mm. Linear interpolation is used to map each dependent variable from the old to the new grid.

3 Results and Discussion

3.1 Pulsating Spread without Opposed Flow

A recent three-dimensional experimental study by [7] presented transient three-dimensional structures of velocity and temperature created by a pulsating flame spread over n-propanol. The authors identified five distinct steps in a pulsating spread cycle: Onset of Pulsation, Formation of Cold Temperature Valley, Fuel Vapor Buildup, Flame Jumping, and Cessation of Spread. Computations at similar conditions have been performed in this study under both normal and zero-gravity. Figure 2 shows the History of flame position vs. time for initial pool temperatures at 11°C, 13°C, 15°C, and 17°C both at normal and micro gravities. The air flow is set to be zero and the pool depth is 1 mm. Pool width is 2 cm and air oxygen concentration is 21% by volume.

Under normal gravity, the flame pulsates at initial pool temperatures of 15°C or below. The flame spread faster and the pulsation amplitude decreases while its frequency increases as the initial pool temperature increases. When the initial pool temperature is at 17°C, the flame essentially propagates at a uniform speed.

Under microgravity the flames appear to always propagate at a steady speed without an opposed flow. They also start out faster than their counter parts under normal gravity. However, the flames propagate some short distances before they extinguish at later times when the initial pool temperatures are low. The higher the initial temperature is the longer the flame can persist before extinction. When the initial pool temperature reaches 17°C, the flame spreads at a uniform speed much in the same way as under normal gravity.

The temperature and velocity field are examined here of the case at 11°C initial pool temperature under normal gravity at four instants marked as A, B, C, and D at t = 1.507s, 1.793s, 2.002s, and 2.502s in Figure 2. These four instants roughly correspond to the fuel vapor build up (instants A and B), flame jumping (instant C), and onset of pulsation (instant D) steps, respectively. Figure 3 shows the side view of velocity vectors and temperature contours at the center of the pool (z = 0) at instant A. Figure 2
indicates that the flame has already entered some time into a stage of slow motion at this instant. The almost stationary flame heats the liquid surface causing significant convective motion of the liquid and the gas due to surface tension. On the other hand, buoyancy draws air towards the flame causing a recirculating zone in the air that can be clearly seen in Figure 3. Surface tension pulls the liquid on both sides near the maximum temperature point below the flame. Continuity of mass in the liquid contained in the tray then results in a pair of vortices centered around the maximum temperature point. Figure 3 shows that the vortex in front of the flame is significantly larger due to large temperature gradient and thus surface tension. Figure 4 shows the top view of velocity vectors and temperature contours at $y = 0.5 \ mm$ above the liquid surface at the same instant. The concurrent motion inside the circulation zone of the gas in front of the flame is clearly seen. Far upstream and also outside of the pool area, flow is drawn into the flame due to buoyancy. This results in a small vertical vortex near the edge of the pool as shown in Figure 4. This pattern of double vortices in the gas phase was depicted in the experimental measurement by Konishi et al. [7].

Figures 5 and 6 show the side and top views of the flame at the same locations as Figures 3 and 4.
but at instant B, which is at a later stage of the flame’s slow motion. The basic flow pattern remains the same. The vortices both in the liquid and in the gaseous phases are now of greater sizes in front of the flame.

Figure 5: Side view of velocity vector and temperature contours at \( z = 0 \ mm \) at instant B.

Figure 6: Top view of velocity vector and temperature contours at \( y = 0.5 \ mm \) at instant B.

The period between Instances A and B covers much of one slow motion phase of the flame spread as shown in Figure 2. During this period, the concurrent convection in both the liquid and gaseous phases help transport heat and fuel vapor upstream. Figures 7 and 8 show the temperature and fuel vapor mass fraction above the liquid surface near the flame front for the four instants. Both temperature and fuel vapor concentration are at elevated levels in a 1.5 cm region in front of the flame compared to instants C and D. This effectively creates a recirculating premixed zone. When the fuel vapor accumulates to a certain level, the flame will quickly enter the fast propagation phase characterized as the Flame Jumping state in [7].

Reference [7] identifies a temperature valley in front of the flame and attributes great significance
Figure 7: Liquid surface temperature distribution at instants A, B, C, and D.

Figure 8: Fuel vapor concentration above the liquid surface at instant A, B, C, and D.
of its existence to the slow ‘crawling’ motion of the flame. Although Figure 7 shows a flat portion of
the temperature distributions right before the flame front for the slow moving instants A and B, no real
temperature valley is observed. The current case has a pool depth of 1 mm while that reported in [7] has
a depth of 25 mm. It can be concluded that at least for shallow pools, the existence of a temperature
valley is not the mechanism responsible for the slow motion of the flame.

Instant C is at a time when the flame is propagating fast (see Figure 2), i.e., in the flame jumping state. Figures 9 and 10 show the side and top views of the velocity and temperature contours. At this instant, combustion is intense resulting in huge thermal expansion that destroys the gaseous recirculation zone in front of the flame. The vortex in the liquid is still obvious but now lags behind the flame, indicating that the flame has moved fast and quickly consumed the premixed recirculating gas mixture that is built up during the slow motion phase of the flame spread.

![Figure 9: Side view of velocity vector and temperature contours at $z = 0 \text{ mm}$ at instant C.](image)

![Figure 10: Top view of velocity vector and temperature contours at $y = 0.5 \text{ mm}$ at instant C.](image)

Instant $D$ is taken at a time when the flame has just completed its fast motion and is at the beginning
of a slow motion phase. Figures 11 and 12 show the side and top views of the velocity vectors and temperature contours at this instant. The flame is relatively weak. The vortex in the liquid is again a little ahead of the flame. The recirculation zone in the gas is being re-established again but is still rather small and thin. The motion in the bulk of the gas is dominated by buoyancy effect. The velocity vectors shown in Figure 12 does not show any concurrent flow because the plane at $y = 0.5 \text{ mm}$ is already outside the thin recirculation zone shown in Figure 11. The flow pattern shown here agrees closely with that observed in experiment at the Onset of Pulsation step in [7]. The temperature and fuel vapor mass fraction distributions shown in Figures 7 and 8 for instants C and D indicate no significant build-up of temperature and fuel vapor in front of the flame due to the lack of any significant recirculation zone in the gas.
3.2 Influence of Opposed Flow and Other Parameters

A large number of computations have been performed with the above three-dimensional computational model to determine the influences of pool depth, pool width, air oxygen concentration, and opposed flow velocity. Temperature regions of uniform and pulsating flame spread have been determined by varying those different parameters under both normal and zero gravity. A nominal standard case is chosen, which has a pool width of 2 cm, a pool depth of 2 mm, 21% oxygen concentration by volume, and an opposed air-speed of 30 cm/s. Variations of pool depth and width, air oxygen concentration, and opposed flow speed are each individually applied to the standard case while holding all other parameters constant.

![Figure 13: Temperature boundary of pulsating flame spread vs. pool depth](image)

![Figure 14: Temperature boundary of pulsating flame spread vs. air oxygen concentration.](image)

Figure 13 shows the critical initial pool temperature for pulsating flame spread vs. pool depth. Each point on the figure represents a computational run for the given initial pool temperature and pool depth. A solid circle indicates that the computation reveals a uniform flame propagation. On the other hand, an open circle is used to show that a regular pulsating flame spread pattern has been found in the computation. The temperature at which the solid circles changes to open circles is then the temperature at which the flame spread starts to pulsate as the initial pool temperature is decreased below this critical
temperature. It can be inferred from Figure 13 that this critical temperature decreases as the pool depth is increased for both 1-g and 0-g conditions. In addition, this critical temperature is higher under normal gravity than under 0-g condition. In other words, the flame is more likely to propagate in a uniform fashion with reduced gravity or increased pool depth. Figure 13 also shows that the critical temperature does not change anymore once the pool depth is over 13 mm. This is consistent with the results of Reference 5.

Figure 14 shows computations with varying air oxygen concentrations. The critical temperature for pulsating spread decreases fast as the oxygen level in the freestream air is increased. This is understandable since increased oxygen levels enhances combustion.

![Figure 15: Temperature boundary of pulsating flame spread vs. opposed air flow speed.](image1)

Figure 16 shows computations with varying air speed. As discussed earlier, the flame tends to extinguish at temperatures below the critical temperature without an opposed flow under zero gravity. Although the existence of an opposed flow is critical for sustained pulsating spread under microgravity, the critical temperature for pulsating spread does not depend significantly on the magnitude of the opposed flow velocity. It must also be recognized that the magnitude of the opposed flow does influence
the flame spread speed as was discussed in [2]. These conclusions agree qualitatively with the two-dimensional results presented in [5].

Figure 16 shows computations with varying width of the pool. Figure 17 shows the flame position vs. time for two wider pools, $w = 6$ cm and $w = 8$ cm. The critical temperature and also the average speed for pulsating spread do not depend significantly on the pool width under zero gravity. Under normal gravity, however, Figures 16 and 17 indicate that the critical temperature and the flame speed increase as the width increases. In other words, the flame tends to spread faster and more in a pulsating mode for wider pools. The next section will examine more details of the flame for wider pools.

### 3.3 Wavy Flame Structures for Wider Pools

Cai et al [6] studied the detailed flame structure for the $w = 2$ cm narrow pool case and reported significant three-dimensional edge effects as the flame front corners around the side edge of the pool and trails behind. It was also reported that the flame fronts at the center of the pool and near the pool edge alternately move past each other for the 2 mm width case, a phenomena that had been referred to as ‘fingering.’ Despite the curvature near the pool edge, the main flame front stayed more or less straight. As the pool width is increased, it is discovered in this study that the flame front becomes largely a wavy form that wiggles like ‘a snake laid across the pool’ while moving in the main direction of flame spread. This can be seen by looking at the contours of the fuel consumption rates at three consecutive time instants for the 6 cm wide pool at both 0-g and 1-g conditions as shown in Figures 18 and 19.

The amplitude of the wavy flame front is large and the wave length long at the low initial fuel temperature end. As the temperature increases, both the amplitude and wave length decreases and the flame also propagates faster as is shown in Figures 17, 18 and 19. As the temperature gets to 17°C for the 0-g case and 18°C for the 1-g case, the flame front becomes completely straight and the flame propagates uniformly. Figures 18 and 19 show that the general behavior of the flames under 0-g and 1-g are similar except that the flames in 1-g trails all the way along the pool side edge due to enhanced transport of oxygen by buoyancy effects discussed in [6].

There is a strong correlation between the wavy form of the flame front and the pulsation of the flame spread. The wavy flame front only appears in pulsating spread cases. Figures 20 and 21 show the same flame formation in the case of the 8 cm wide pool. Only pulsating flames are shown in these cases. With the larger width, more waves of the flame front can be seen across the pool. The fingering phenomena shown in the case of the narrow 2 cm wide pool in [6], which is reproduced here for the 1-g case in Figure 22, may be regarded as a one-wave exhibition of the general multi-wave flame front when the wave length and the pool width are comparable.

In order to examine in more detail the three-dimensional flame structures, velocity vector and tem-
Figure 18: Contours of fuel consumption rate at \( y = 1 \) mm and three different time instants for the 6 cm wide pool under 0-g. Initial pool temperature \( T_0 = 13^\circ C, 15^\circ C, \) and \( 17^\circ C \) from top to bottom.

Figure 23 shows the top view at the \( y = 1 \) mm plane. The peaks in the wavy flame front are propagating rapidly and cause large thermal expansions. If one cuts through this wavy front with a vertical plane at \( x/L = 0.56 \), one gets a front view of the flame shown in Figure 24, which clearly shows the lateral thermal expansion from the flame peaks. Velocity vectors and temperature contours are also plotted in two other vertical planes along the pool length at \( z/L = 0.043 \) and \( z/L = 0.059 \), corresponding to the peak and the trough of one of the waves. The flow is dominated by thermal expansion at the peak as shown in Figure 25. On the other hand, a recirculation zone is seen in front of the flame at the trough of the wavy flame shown in Figure 26.

Two movie clips are included in this CD ROM. Both of them are run for the 6 cm wide pool with an initial pool temperature of 13\(^\circ\)C. The flame is represented by a constant reaction rate surface. The colors on the pool surface represent temperature. The first movie shows the flame propagation under 0-g. The second movie shows the flame propagation under 1-g.

To see the first movie click here.

To see the second movie click here.
Figure 19: Contours of fuel consumption rate at \( y = 1 \) mm and three different time instants for the 6 cm wide pool under 1-g. Initial pool temperature \( T_0 = 13^\circ C, 15^\circ C, \) and \( 18^\circ C \) from top to bottom.
4 Conclusions

A three-dimensional computational code that solves the coupled reactive flow problem of forced gas-phase flow over liquid fuel is used to study ignition and flame propagation over liquid n-propanol fuel pools initially below flashpoint temperatures. A three-dimensional case with a narrow pool and zero opposed air flow velocity that has been studied experimentally by Konishi et al. [7] is examined computationally. Three-dimensional effects of the flame front and along the edge of the pool are captured in the computation. Vortices captured in both the liquid phase and the gaseous phases agree with those observed in the experiment for three distinct modes of the flame spread during pulsation: slow propagation and fuel vapor build-up, flame jumping, and cessation of spread. Unlike in the experiment, however, no temperature valley is observed in the computation despite the existence of flat temperature region in front of the flame when it is in its slow moving mode. Computations show that the mechanism of flame pulsation is due to the formation of a gas-phase recirculation zone resulting from the balance of buoyancy and thermo-capillary surface tension in the liquid fuel. This recirculation transports fuel-vapor upstream from below and behind an initially slow moving flame until it builds a sizable pre-mixed fuel-air mixture in front of the flame. The flame will then move fast and deplete the pre-mixed zone before it enters the slow moving phase again. No pulsation is observed in the computation due to lack of buoyancy under microgravity without an opposed flow. Flames started with initial pool temperatures below the flashpoint will eventually extinguish under zero gravity condition. Higher initial pool temperatures, however, make the flame persist longer before extinction.

A large number of computations have been performed to determine the regimes of pulsating flame spread and uniform flame spread in the initial temperature/opposed air velocity, pool depth, pool width, or oxygen concentration plane. Increasing pool depth decreases the critical initial fuel temperature for pulsation. Enhanced oxygen levels in the air also decreases the critical initial fuel temperature. Although opposed air flow is essential for pulsation under microgravity, its magnitude does not affect the critical fuel temperature for the cases studied. Pool width does not affect the critical fuel temperature for pulsation nor flame speed under microgravity. Under normal gravity, however, increasing pool width makes the flame more likely to pulsate and also spread faster.
Three-dimensional unsteady flame fronts consisting of ‘fingering’ multiple wave periods are computed for the first time for pools of wider width. Higher initial pool temperature decreases the wave length and amplitude of the wiggling flame front. There is a strong correlation between the waviness of the flame front and the pulsating flame propagation. The waviness of the flame disappears at higher temperatures when the flame starts to propagate in uniform speed.

Figure 21: Contours of fuel consumption rate at $y = 1$ mm and three different time instants for the 8 cm wide pool under 1-g. Initial pool temperature $T_0 = 13^\circ C$ and $15^\circ C$ from top to bottom.
Figure 22: Contours of fuel consumption rate at $y = 1\ mm$ and two different time instants for the 2 cm wide pool. Initial pool temperature $T_0 = 13^\circ C$. Top: 0-g; Bottom: 1-g.

Figure 23: Velocity vector and contours of temperature at $y = 1\ mm$ at $t = 1.6\ s$ for the 8 cm wide pool under 1-g. Initial pool temperature $T_0 = 15^\circ C$
Figure 24: Velocity vector and contours of temperature at $x/L = 0.56$ at $t = 1.6$ s for the 8 cm wide pool under 1-g. Initial pool temperature $T_0 = 15^\circ C$

Figure 25: Velocity vector and contours of temperature at $z/L = 0.043$ mm at $t = 1.6$ s for the 8 cm wide pool under 1-g. Initial pool temperature $T_0 = 15^\circ C$
Figure 26: Velocity vector and contours of temperature at $z/L = 0.059$ mm at $t = 1.6$ s for the 8 cm wide pool under 1-g. Initial pool temperature $T_0 = 15^\circ C$. 
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References


