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Temperature Field During Flame Spread over Alcohol Pools: Measurements and Modelling

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INTRODUCTION: A principal difference between flame spread over solid fuels and over liquid fuels is, in the latter case, the presence of liquid-phase convection ahead of the leading edge of the flame. The details of the fluid dynamics and heat transfer mechanisms in both the pulsating and uniform flame spread regimes [Akita] were heavily debated, without resolution, in the 1960s and 1970s; recently, research on flame spread over pools was reinvigorated by the advent of enhanced diagnostic techniques and computational power. Temperature fields in the liquid, which enable determination of the extent of preheating ahead of the flame, were determined previously by the use of thermocouples and repetitive tests [Glassman and Dryer], which suggested that the surface temperature does not decrease monotonically ahead of the pulsating flame front, but that there exists a surface temperature valley. Recent predictions support this suggestion [DiBlasi]. However, others' thermocouple measurements [Akita, Tsuji/Ozawa] and the recent field measurements [Ito et al] using holographic interferometry (HI) did not find a similar valley.

In this work we examine the temperature field using rainbow schlieren deflectometry (RSD), with a measurement threshold exceeding that of conventional interferometry by a factor of 20:1, for uniform and pulsating flame spread using propanol and butanol as fuels. This technique was not applied before to flame spread over liquid pools, except in some preliminary measurements reported earlier [Miller/Ross]. Noting that HI is sensitive to the refractive index while RSD responds to refractive index gradients, and that these two techniques might therefore be difficult to compare, we utilized a numerical simulation, described below, to predict and compare both types of field for the uniform and pulsating spread regimes. The experimental data also allows a validation of the model at a level of detail greater than has been attempted before.

EXPERIMENTAL APPARATUS: The fuel tray was 300 mm long, 20 mm wide, and 10 mm deep, and was placed inside a large chamber to avoid room drafts. The bottom and removable top of the tray were hollow, allowing a glycol-water solution to flow inside them to control the initial fuel temperature to within 0.1 °C, based on thermocouple measurements. The side walls were 1 cm thick, schlieren-quality quartz allowing the schlieren system a subsurface side view. Ignition was achieved with a hot wire stretched across one end of the tray 1 mm above the fuel surface.

A schematic of our RSD system is given in Fig. 1. The RSD technique, which involves replacing the standard schlieren knife edge with a colored filter, is explained in detail in Howes. A fiber-optic-coupled, xenon-arc lamp (ILC Model 131) is used as the light source and is collimated into a 100 mm diameter beam by an off-axis parabolic mirror. The beam traverses the tray test section and is refocussed onto a color filter. A lens behind the filter images the test section onto a camera. When there are no refractive index gradients in the tray, the light passes through a single color on the filter and the entire image appears that color. However, if light in part of the test section is refracted it undergoes a deflection in the filter plane and the image assumes a different color in that location. The color images, therefore, provide a reliable and accurate means of determining the uniformity of the preignition pool temperature, as well as the depth and surface position to which the temperature has been raised by the presence of the spreading flame.

Recent advances in RSD by Greenberg et al have laid the foundations for quantifying the technique by resolving the colors into RGB components and calculating the hue. The RSD filters are optimized to have a linear hue vs. position relationship. Depending on the orientation of the color bands to the fuel surface, either horizontal or vertical gradients can be detected; only vertical gradients are shown in this work. For our RSD system, estimates of the sensitivity are 7×10^{-2} °C/mm for propanol at room temperature.

NUMERICAL MODELLING: The unsteady, two-dimensional computational model, described in Schiller et al, uses primitive variables (u, v, p, h), the SIMPLE algorithm [Patankar], a staggered mesh, and the hybrid-differencing scheme. At the gas/liquid interface, Dirichlet-type boundary conditions from the solution of the liquid phase are used for the solution of the gas phase, while Neumann conditions from the gas phase are used for the upper boundary of the liquid phase. A no-slip bottom and end-wall is used in the liquid. Accurate modelling of the reaction zone requires a fine numerical mesh not only in the reaction zone itself, but also in the region between the reaction zone and the liquid surface to accurately predict the liquid surface heating ahead of the flame. In order to save computer time, a partially-adaptive gridding scheme is used to move the fine-mesh region along with the spreading flame in the axial direction.

The effects of surface tension, gravity level, variable density and thermophysical properties, vaporization, and one-step, first-order, finite-rate chemical kinetics are included in the computational model. Solutocapillary forces and recession of the liquid

surface due to vaporization are neglected. The solution domain consists of a 20 cm half-length pool 1 cm deep, with 3 cm in the gas phase, resolved with 112 points in the horizontal direction and 72 in each of the two phases vertically. The solution proceeds iteratively with time steps of 0.2 ms. The predictions of the model compared favorably to experimentally determined instantaneous flame spread rates for shallow propanol pools [Schiller et al] in both the uniform and pulsating spread regimes. Pulsation frequencies were well predicted over a range of temperatures. This work now provides a more detailed comparison of the predictions and experiment through an examination of the temperature field.

EXPERIMENTAL RESULTS/OBSERVATIONS: *Temperature Field Visualization Prior to Ignition:* Fig. 2a shows butanol equilibrated at 22.1 °C (a pool temperature in the pulsating spread regime) in the fuel tray covered with a lid. Figs. 2b, 2c, and 2d show the same fuel layer at various times after opening the lid, exposing it to the room environment. A thermal boundary layer immediately begins forming indicating cooling due to evaporation from the liquid surface. Quantification of Fig. 2c shows the surface temperature has dropped about 0.5 °C. Just prior to ignition in Fig. 2d evaporative cooling has affected the entire tray depth, and the surface is now about 0.9 °C below the bottom temperature. The highly wrinkled structure in the RSD image implies the existence of Rayleigh convection. The critical Rayleigh number (Ra_c) is 1100 for the case of a fluid layer that is warmer on the bottom and has a free surface which is cooler on the top [Gebhart]. For butanol (propanol), this corresponds to $\Delta T_c = 0.06$ (0.05) °C, respectively so that for greater temperature differences, the layer is unstable and any disturbance will cause liquid motion to begin. The RSD image for 1-propanol at 23.7 °C (uniform spread regime) shows a similar surface boundary layer, as well as cooler liquid which has sunk to the tray bottom (fig. 3a). When propanol was cooled to 14.2 °C (bottom of tray) and then exposed to air at about 23 °C, the surface becomes more than 2 °C warmer than the bulk liquid, as shown in fig. 3b. These variations were unreported in previous flame spread studies and reveal that neither isothermal nor quiescent conditions really exist in uncovered pools (as they are always assumed modelled) prior to ignition.

Temperature Field Visualization in the Uniform Regime: Fig. 4a corresponds to fig. 3a, with uniform flame spread over propanol nominally at 23.7 °C. Little if any change in the surface can be seen ahead of the flame; the darkening under and behind the flame is due to the schlieren system being driven off scale. Tests probing the field for horizontal gradients also produced little evidence of heating ahead of the flame. Thus, the RSD suggests elevated liquid temperatures only penetrate very small distances (1 mm or less) both into the pool depth and ahead of the flame. In fact, the RSD by itself offered no evidence from which we could infer flow ahead of the uniformly spreading flame for the 10 mm deep propanol pool. In contrast to the very detailed HI data reported in Ito et al for the uniform spread case, our RSD images resembled those of Akita's and Tsuji/Ozawa's shadowgraph and standard schlieren pictures.

It is not readily apparent why our RSD yielded results so different from HI for the same fuel, temperature, pool depths and lengths. These differences include the presence under the flame leading edge of a heated layer approximately 4.5 mm deep for HI vs. < 1mm for RSD, and a clearly defined vortex in the HI vs. no vortex in the RSD. The temperature differences between the surface and 10 mm pool depth as reported in Ito et al are greater than 10 °C. As noted above, the demonstrated RSD sensitivity easily discerned gradients 50-100 times smaller that developed from fuel evaporation prior to ignition. The spatial resolution of HI is probably better than RSD since it employs black and white rather than color film as the final recording medium (the exact resolution depends on the film type, developing process, and details of the two optical systems), but in any case the RSD resolution is on the order of 50 μ m for our system which is entirely adequate to image subsurface phenomena. The RSD should have identified a temperature rise into the depth and it should have shown a vortex like HI if one really existed.

We offer four possible reasons for the differences between our work and Ito et al: (a) our or their fuel might have been contaminated so surface-tension-driven flow was altered (e.g., a flame spreading over pure fuel may slow upon reaching contamination allowing a vortex to form); (b) differences in tray widths (our 2 cm compared to Tsuji/Ozawa's 4.4 cm compared to Ito et al's 1 cm) may change the existence and nature of the convective field in the liquid or the temperature of the sidewalls and therefore the temperature profile of the fuel ahead of the flame; (c) HI reveals temperatures while RSD reveals temperature gradients (this difference was investigated and discounted via numerical simulation, described below); and (d) the uniformity of the initial pool temperature, both axially and in depth, of their and our experiments was different. We believe (d) to be the predominant cause of the different experimental observations. We base this conclusion on our preliminary experiments in which we found erratic flame spread and occasionally more extensive liquid-phase convection if the initial temperature in the pool was not uniform. When the flame drew near a cooler pocket of liquid fuel, the flame slowed momentarily then accelerated due to an increase of liquid-phase convection. During the slowing period, a flow vortex develops and extends into the depth much more than in the initially isothermal pool. Our review of the raw video-recorded HI data, kindly provided by those authors, suggests that this also was the case in their experiments.

Temperature Field Visualization in the Pulsating Regime: Fig. 4b, which may be compared to fig. 3b, shows the RSD image for a flame spreading over 1-propanol at 14.2 °C; the tray lid was opened 2 minutes prior to ignition, so that the yellow region had penetrated to the bottom of the pool. In this case one vortex is seen fully developed ahead of the flame, visibly penetrating about 4-5 mm into the pool depth. Its general shape is consistent with the HI image of Ito et al. Behind the flame front, vortices formed in earlier pulsations have merged. Being directly under the trailing diffusion flame, the near-surface gradient at the top of these merged vortices has risen to such an extent that it is off-scale and appears black. A similar black region appears in the liquid ahead of the spreading flame, seen with the filter positioned to detect either horizontal or vertical gradients. The depth of the black region is greater at 10 mm than it is at say 5 mm ahead of the flame. This might indicate the existence of the surface temperature valley, or it might indicate a physical pool surface deformation, as occurs in thermocapillary-driven flow. There is no simple means to distinguish between the two possible sources. Fig. 5 shows a corresponding picture for 1-butanol. The flame induces a vertical gradient at least 40 mm ahead of the flame; the larger extent of the temperature affected region is owed to 1-butanol being further below the flash point, and the flame therefore spreading across the surface more slowly. Behind the leading edge, the merged vortices extend deeper into the pool for the same reason. In this case, the depth of the off-scale region ahead of the flame decreases monotonically with distance ahead of the flame, but there appear to be a few on-scale areas -- near the surface at about 10 mm ahead of the flame and also at a depth of 2 mm and about 5 mm ahead of the flame -- surrounded by off-scale areas. It is not clear why these should exist, though we speculate it may have to do with flame-front curvature and side-wall heat losses producing non-uniform heating across the width of the flame front.

COMPARISON WITH NUMERICAL MODEL PREDICTIONS: No attempt was made to predict the pre-ignition flow cells or temperature variations described earlier. Instead, the traditional assumptions of isothermicity and quiescence were invoked. Fig. 6a shows the predicted temperature gradient field (dT/dx) for flame spread over propanol in the uniform regime, and can be compared to the experimental result in fig. 4a. Color coding of the model's liquid-phase predictions have been chosen to correspond to those of the experiments. Note that the code correctly predicts the depth of heated layer ahead of the flame front. Fig. 6b shows the predicted temperature fringes for the same conditions, corresponding to what would appear with an HI image. The code shows that the HI and RSD should reveal a similar extent of heating ahead of and under the flame's leading edge.

Fig. 7a shows the model's predictions of gradients for flame spread over 1-propanol in the pulsating regime. These may be compared to fig. 4b. It is interesting to note the predicted vortex size, shape, and even its interior structure, show excellent agreement with the experiments. Fig. 7b, shows the predicted fringes as they would appear in an HI image. Again the general shape of the heated region using either HI or RSD should be similar, and in this case, all -- model, HI, and RSD -- are in agreement. Fig. 8 shows the calculated liquid surface temperature and does not show a temperature valley.

CONCLUSIONS: RSD provides a useful tool to visualize temperature gradients for flame spread over liquids. It has superb sensitivity -- note especially the clear visualization of the pool temperature variations prior to ignition, which has not previously been reported using other techniques -- and the color patterns are easily discernible to the eye as compared to grey-scale variations. The numerical model is in excellent qualitative agreement with the experiments, and the matched coloring suggests good quantitative agreement as well, though a more thorough analysis of the experimental data is required. The model correctly predicts the depth and distance ahead of the flame of the liquid-phase vortex in the pulsating regime and, in agreement with the RSD results, predicts no vortex ahead of the flame in the uniform regime. The model and the RSD show good agreement with the HI experimental results in the pulsating regime, but not in the uniform regime.

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