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Flow Circulation within a Methanol Droplet: Effects of Surface Tension

A methanol droplet of 0.43 mm initial diameter burning in air at an ambient temperature of 300 K and 1 atm is presented. Combustion takes place within a weak convective environment (initial Reynolds number is 0.01). Ignition is achieved by applying an external ignition source. The code is executed without the ignition source for a short period of time so that, due to evaporation, a fuel/vapor air mixture builds up around the droplet. Then, an energy source is added to a small axisymmetric region upstream of the droplet until ignition takes place.

Before Ignition:

During the pure evaporation phase in dry air, the numerical results with and without surface tension are nearly identical. The only result that is noticeably affected when surface tension effects are included is the droplet circulation. At the start of the simulation, a weak clockwise circulation is induced within the droplet due to the slow convective flow surrounding the droplet. The weak clockwise circulation remains throughout the evaporation phase when surface tension is neglected. When surface tension effects are included, the weak clockwise circulation eventually reverses direction. The cause of this flow reversal is the variation of the surface tension along the droplet surface. The gradient of the surface tension (σ) along the droplet surface can be expressed in terms of the surface temperature and surface water mass fraction (Y_{ws}) gradients, as follows:

$$\frac{\partial \sigma}{\partial \theta} = \frac{\partial \sigma}{\partial T_s} \frac{\partial T_s}{\partial \theta} + \frac{\partial \sigma}{\partial Y_{ws}} \frac{\partial Y_{ws}}{\partial \theta}$$

The first term in the above equation represents the thermal Marangoni effect, which moves liquid from hot to cold regions along the gas-liquid interface. The second term represents the solutal Marangoni effect, which moves liquid from low to high water mass fractions along the gas-liquid interface. During evaporation, since there is no water formation, the solutal Marangoni effect is absent. Due to the convective field, enhanced evaporative cooling occurs at the front portion of the droplet when compared to the rear. As a result of this small temperature gradient along the droplet surface, the thermal Marangoni effect comes into play when the surface tension effects are included and the weak clockwise circulation eventually reverses its direction.

During Ignition:

The external ignition source is added to a small axisymmetric region upstream of the droplet at 1.5 ms after the start of the simulation. The ignition source causes a drastic change in the circulation pattern, due to the volumetric gas expansion that takes place near the front of the droplet. For the case that neglects surface tension, this volumetric gas expansion enhances the clockwise circulation already present within the droplet. The effect of the external ignition source on circulation is even more pronounced when surface tension effects are included. The high temperature region in the gas phase causes heating of the front portion of the droplet and water vapor produced in the gas phase condenses on the droplet surface from front to rear. The volumetric expansion near the front of the droplet and the thermal Marangoni effect due to the negative temperature gradient together overcome the solutal Marangoni effect. Thus, the very weak counter-clockwise flow that is present near the end of the evaporation phase changes to a strong clockwise flow shortly after the application of the ignition source.

Envelope Flame Formation:

The addition of energy is terminated when the maximum gas-phase temperature reaches 2000 K, at which point, combustion becomes self sustaining. As a result, energy addition is terminated at approximately t = 16.4 ms and t = 12.7 ms when surface tension effects are included and neglected, respectively. At this point, the flame begins to surround the droplet. A clockwise circulation is seen when surface tension effects are included, due to the thermal Marangoni effect. The flame continues to engulf the droplet, eventually forming an envelope flame. The volumetric gas expansion of the gas phase along the trailing half of the droplet causes a back pressure on the droplet. This backpressure is insufficient to overcome the strong clockwise circulation induced by the thermal Marangoni effect. However, when surface tension effects are neglected, the backpressure is sufficient to initiate a counter-clockwise flow in the trailing half of the droplet.

Envelope Flame (non-spherical):

An envelope flame is formed around the droplet at approximately t = 19.2 ms and t = 17.4 ms when surface tension effects are included and neglected, respectively. At this moment, the flame is closer to the droplet surface at the rear of the droplet. During the formation of the

envelope flame, the volumetric expansion of the gas phase near the rear of the droplet is violent enough to cause counter-clockwise circulation when surface tension effects are neglected. When surface tension effects are included, this same volumetric gas expansion contributes to the formation of a small region of counter-clockwise circulation near the trailing edge of the droplet. The appearance of the envelope flame allows for heating of the entire droplet surface and creates a "source" of water vapor that surrounds the droplet. Therefore, the case that includes surface tension effects shows a decrease in the magnitude of the temperature difference along the droplet. The resulting decrease in the temperature gradient along the droplet surface lessens the thermal Marangoni effect. Detailed analysis of the numerical results indicates that when the envelope flame forms, the solutal and thermal Marangoni effects are of the same order. The closeness of the flame to the rear of the droplet causes an increased rate of water condensation along the trailing edge (between $\theta = 130^{\circ}$ and 150°). However, water mass fraction along the droplet surface slightly decreases between $\theta = 150^{\circ}$ and 180°. This negative gradient of Y_{ws} near $\theta = 180^{\circ}$ also contributes to the region of counter-clockwise circulation near the trailing edge of the droplet. When surface tension effects are neglected, due to the counter-rotating flow along the droplet surface, the water mass fraction is higher at the front of the droplet.

Envelope Flame (nearly spherical):

As the time progresses, the envelope flame tends to become spherically symmetric. For the case that neglects surface tension effects, when the flame is nearly spherically symmetric, the major impetus for droplet circulation is the weak convective flow in the gas phase. Thus, flow within the droplet is largely characterized by a weak clockwise circulation superimposed on a strong radial flow caused by rapid vaporization during the majority of the active combustion period. The flow within the droplet does not alter much during the active combustion period.

However, for the case with surface tension effects, the flow within the droplet consists of several strongly counter-rotating cells which are rapidly changing in number, size, and direction of rotation. This happens over the entire period of the active combustion.

A more detailed description is available in the following article:

V. Raghavan, D.N. Pope, D. Howard and G. Gogos, "Surface Tension Effects during Low Reynolds Number Methanol Droplet Combustion," Combustion and Flame, 2006, In Press.