MULTIPLE NUMERICAL SOLUTIONS OF STRUCTURES OF COUNTERFLOWING SPRAY FLAMES

E. Gutheil

Interdisziplinäres Zentrum für Wissenschaftliches Rechnen,
Universität Heidelberg
Im Neuenheimer Feld 368, 69120 Heidelberg, Germany
e-mail: gutheil@iwr.uni-heidelberg.de
Phone: +49-6221-546114, Fax: +49-6221-546111

Counterflow spray flames have been investigated in the last years both by means of experiment, numerical simulations as well as asymptotics. Numerical simulations often are performed in a one-dimensional physical space that result from the application of a similarity transformation of the two-dimensional, governing conservation equations of the gas phase. The dilute spray then is included in a Lagrangian way accouting for droplet heating, vaporization, and combustion as well as droplet motion.

The present paper reports two different spray flame structures in the low-strain regime for liquid fuel sprays in air for identical boundary conditions. One flame structure comprises two chemical reaction zones where one flame resides in the primary vaporization regime on the spray side of the flame whereas the second chemical reaction zone occurs on the gas side of the counterflow configuration. In the second flame structure, the gas-side flame is extinguished and the spray flame structure consists of a single reaction zone on the spray side of the configuration. These multiple solutions of the governing equations have been postulated before, but this is the first report of multiple solutions of counterflowing spray flames.

1 Introduction

Counterflow spray flames have been investigated in the last years both by means of experiment [1, 2, 3, 4], numerical simulations [5, 6, 7, 8] as well as asymptotics [9, 10]. The counterflow configuration is convenient for the investigation of both reacting and non-reacting (spray) flows since the flow field is well defined and boundary conditions can easily be modified. For numerical studies, a similarity transformation [5] is suitable that transfers the two-dimensional governing gas phase equations into one-dimensional form which accesses the use of detailed gas-phase processes such as chemical reactions and detailed transport modeling [6, 7].

Continillo and Sirignano [5] postulate that there may be multiple solutions of structures of counterflowing spray flames. It is known that for gas flames, there is a solution with and without a flame, the second one presents the cold solution. For spray flames, the same situation exists, and typically the solution with a flame is presented. For spray flames in the counterflow configuration, there may be two reactions zones where one resides on the spray side of the configuration and the second one on the gas side. At elevated strain, the flame may extinguish due to the low residence time of reactants associated with high strain. The present paper presents structures of methanol/air spray flames with multiple solutions of low strained spray flames that have not been reported in the literature so far.

2 Mathematical Model and Numerical Solution Procedure

The mathematical model is identical to the formulation in previous papers [6, 7] and is not reported here. The multiple solutions are found using a somewhat different numerical approach.

The procedure to obtain structures of counterflowing spray flames is as follows. Typically, the computations are initiated at a low strain rate of 55/s for the gas on the fuel side of the configuration. After having obtained a converged solution for this case, the strain rate is increased to 100/s and then either by one or some hundreds depending on the purpose which may be investigation of the extinction strain rate or to obtain structures at specified values of strain rate. At low strain rates, it has been found that there are two reactions zones for a variety of fuel sprays in air [5]–[7] as well as for the LOX (liquid oxygen) – hydrogen system [11]. At a certain value of strain rate, the gas-side reaction zone extinguishs and a single reaction zone is obtained for the spray configuration. Starting the computation for a low value of strain using an initial profile of a high-strain result with one reaction zone, there is no ignition on the gas side of the configuration and a solution with one single chemical reaction zone is obtained.

3 Results and Discussion

The paper concerns a methanol spray in air where air is injected on both sides of the axisymmetric counterflow configuration and one stream (on the LHS in the figures) is laden with a monodisperse spray. The initial gas and droplet temperatures are 300 K, and the initial droplet radius, r_0, is 25 μm. The equivalence ratio at the fuel boundary is 3. Figures 1 and 2 show two flame structures with identical initial conditions at a gas-strain rate on the fuel side of the configuration of $a = 300/\mathrm{s}$. In Fig. 1, two reaction zones exist whereas in Fig. 2 a structure with a single reaction zone is displayed. The latter case corresponds to the cold solution of the gas flame structure.

The figures reveal that the reaction zones on the spray side of the flame essentially are the same: this appies to the gas temperature profile as well as to the concentrations and spray characteristics. The differences occur on the gas side of the configuration where the gas-side reaction zone is absent or present, respectively. In Fig. 1, the droplet vaporization is enhanced due to the high gas phase temperature in the second reaction zone which stongly affects droplet vaporization. The vaporization in turn enhances the chemical reactions, and the chemical species profiles considerably differ for both cases. Thus, different outer flame structures are obtained for identical boundary conditions.

The present findings raise two questions that are addressed in the next few paragraphs. One question concerns the differences between the gas side flame of the spray configuration and a pure gas flame. The second one arises in the connection with the use of the flamelet model of turbulent spray flames where laminar spray flames may be used [12]. The flamelet model requires a one-to-one correspondence between conditions in the turbulent spray flame and a laminar flamelet.

For clarification of the first item, the gas-side reaction zone may be compared to pure gas-phase combustion. The boundary conditions for a representative gas flame are identified from the spray flame shown in Fig. 1. It is assumed that the two reaction zones of the spray flame shown are separated at the point of the lowest gas temperature occuring roughly at the stagnation plane at $z = 0$ mm.

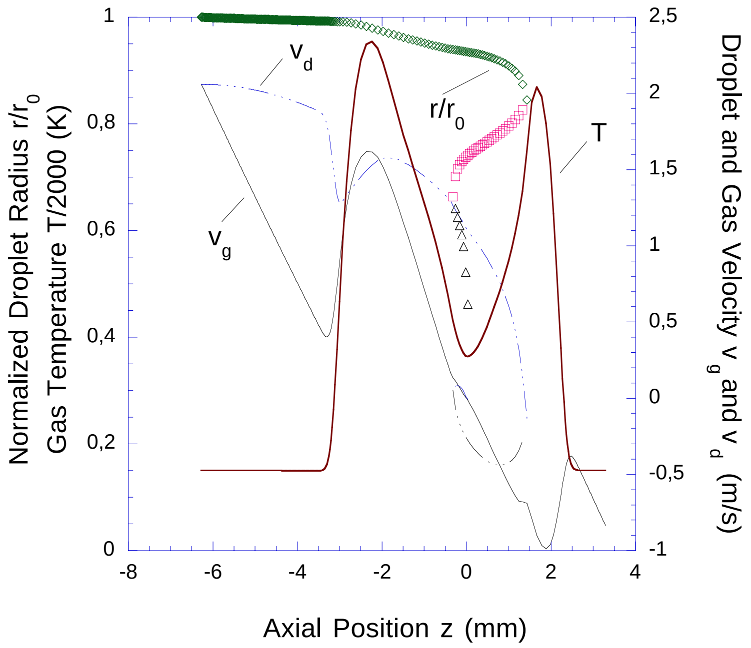

Figure 1: Structure of a methanol/air spray flame with two reaction zones, $a = 300/\text{s}$.

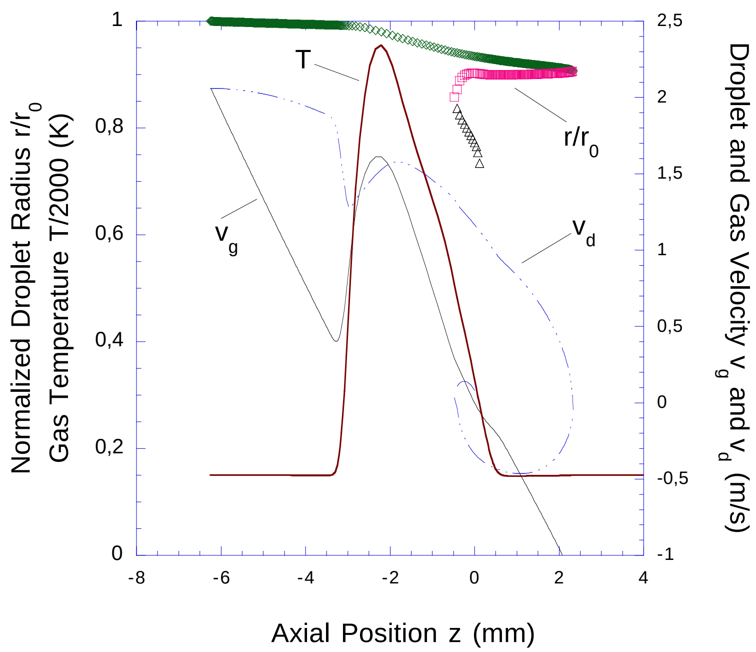

Figure 2: Structure of a methanol/air spray flame with one reaction zone, $a = 300/\text{s}$.

At this position the initial gas temperature for the pure gas-flame computation is evaluated to be 729 K, the initial composition of the gaseous reactants are taken to be 0.448, 0.088, 0.057, 0.067, and 0.34 for the mass fractions of the species CH_3OH, H_2O, CO_2, CO, and N_2, respectively. All other values are set to zero. The resulting gas flame structure is shown in Fig. 4 and compared to the gas-side flame of the spray flame that has been discussed in Fig. 1 and which is displayed in more detail in Fig. 3. It can be seen that the flame structure for both cases is almost identical except for minor differences in the profile of HO_2 near the fuel side of the configuration. The agreement for all other species is excellent. This result motivates the discussion of the second question raised above.

In the context of the flamelet model for turbulent spray flames, the laminar spray flame structures may be used for the generation of a laminar flamelet libaray [12]. The present finding raises the question how a spray flamelet may be chosen in the situation of multiple structures.

The procedure followed by Hollmann *et al.* [12] includes a splitting of the flame structure with two reaction zones into a spray part and a gas part. If there is spray in the computational cell of the turbulent flow field, the spray part is chosen and in case of a pure gas cell, the gas part of the reaction zone is taken. The present result shows that this procedure may be changed by replacing the gas-phase side of the spray flame by a flamelet resulting from a pure gas flame since the flamelets shown in Figs. 3 and 4 do not differ considerably. The result of the present study simplifies the use of the flamelet model in spray flames since gas flames only depend on strain rate and inlet composition and temperature whereas the spray flames need to account for differences in initial droplet size and velocity in addition to the gas-flame inlet conditions. Therefore, this study is not only interesting in terms of a basic finding, but it also strongly simplifies the formulation and use of a laminar spray flame library in turbulent spray combustion.

The multiple flame structures discussed in the paper for the present conditions persist up to a straim rate of 400/s; at $a = 500$/s, the gas-side flame is extinguished. On the lower side we find structures with both one and two reaction zones for a strain rates down to $a = 55$/s which is the lowest studied here. In summary, the multiple solutions persist for strain rates of up to 400/s.

Figure 5 displays the maximum flame temperature versus strain rate for the conditions of the spray flames shown in Figs. 1 and 2. It can be seen that the spray-sided reaction

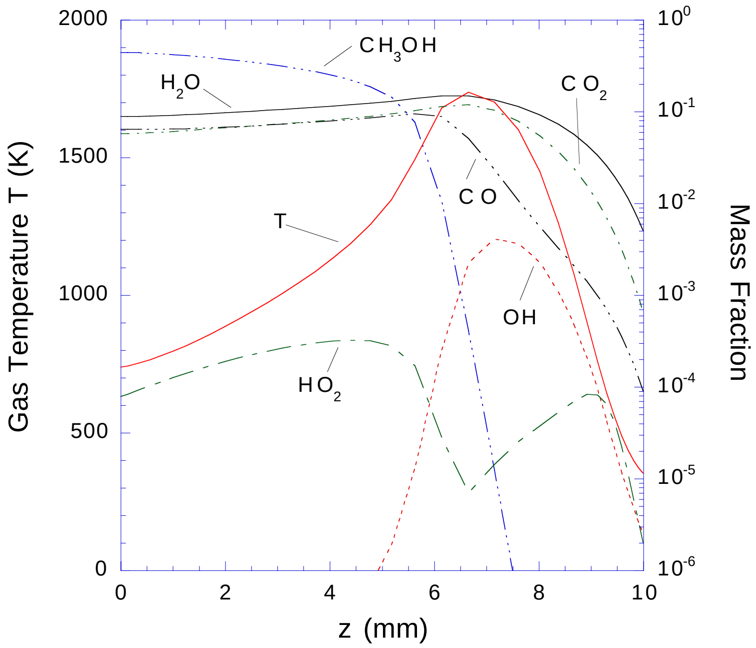

Figure 3: Gas-side flame structure of a methanol/air spray flame, $a = 300/\mathrm{s}$.

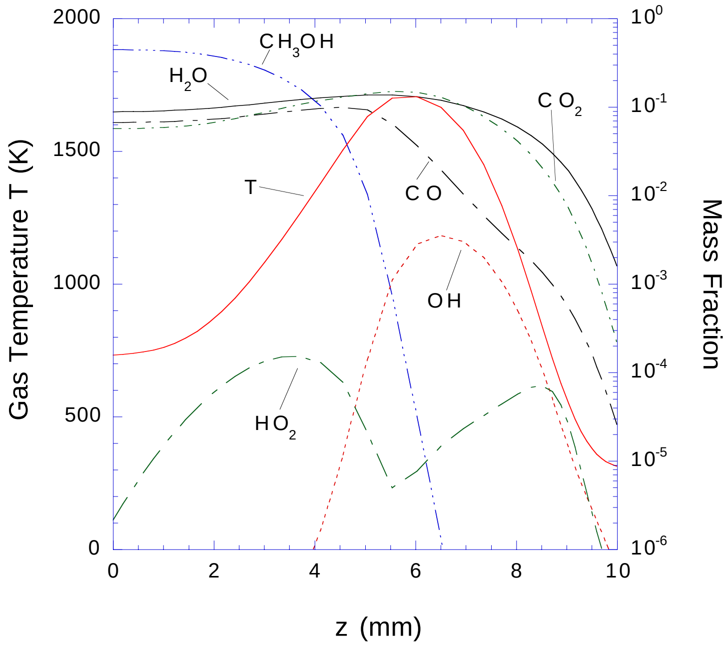

Figure 4: Flame structure of a methanol/air gas flame, $a = 300/\mathrm{s}$.

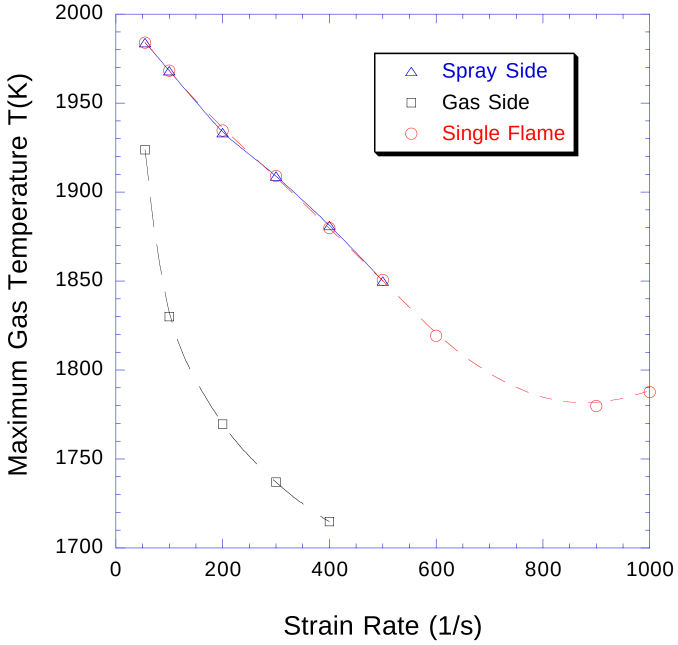

Figure 5: Maximum flame temperature of methanol/air spray flames with two and with one reaction zones, resp., versus strain rate.

zone (triangles) and the single spray flame solution (circles) coincide within the range of existence between strain rates of 55/s through 400/s. Squares show the maximum gas temperature of the gas-side reaction zone of the double-flame structure which typically lies below the spray-sided reaction zone. As strain rate is increased above a certain value, the spray oscillates between the opposed jets as discussed in Refs. [6]-[7], and the flame temperature may increase again as shown in Fig. 5. The current computation has not been carried to extinction.

The present findings of multiple flame structures are also found for planar flame structures and for different liquid fuels such as ethanol, and the range of strain rate in which they occur is similar as for the conditions shown in this paper.

The question may arise if the set of structures found in this paper is complete or if it is possible to find even more different structures for the same inlet conditions. The third possibility of a potential structure where the spray-side flame is extinguished and the gas-side flame persists may not be physical at low strain since this situation does not allow for enough fuel vapor to sustain a flame since evaporation is reduced if no flame exists. At elevated strain, the gas-side flame does not exist which leads to the conclusion that there may not be other numerical solutions.

4 Summary and Conclusions

The present paper identifies multiple flame structures for spray flames in the counterflow configuration at low strain rates. Multiple solutions exist between a range of $a = 55/\text{s}$ and 400/s. At higher strain, the reaction zone on the gas side of the configuration breaks down due to short residence time of the reactants. The study also reveals that the gas-side reaction zone of the spray flame and the reaction zone of a pure gas flame with the same inlet conditions hardly differ.
The paper also addresses the consequences of the present finding for the use of laminar spray flame structures in the flamelet of turbulent combustion. In particular, the multiple flame structures do not question the model but lead to a simplification: The spray-side structures do not differ and are used in areas of the turbulent spray flames where droplets exist, and pure gas flame structures may be used where no droplets are present.

REFERENCES

[1] Chen Z H, Liu T H and Sohrab, S H 1988 *Combust. Sci. and Tech.* **60** 63-77

[2] Gomez A and Chen G 1994 *Combust. Sci. and Tech.* **96** 47-59

[3] Li S C 1997 *Prog. Energy Combust. Sci.* **23** 303-347

[4] Santoro V S and Gomez A 2002 *Proc. Combust. Inst.* **29** to appear

[5] Continillo G and Sirignano W A 1990 *Combust. Flame* **81** 325-340

[6] Gutheil E Sirignano W A 1998 *Combust. Flame* **113/2** 92

[7] Gutheil E 2001 *Combustion Theory and Modeling* **5** 131-145

[8] Chen N-H, Rogg B and Bray K N C 1992 *Proc. Combust. Inst.* **24** 1513-152

[9] Greenberg J B and Sarig N 1996 *Combust. Flame* **104** 431-459

[10] Greenberg J B and Sarig N 1998 *Combust. Sci. and Tech.* **131** 277

[11] Schlotz D and Gutheil E 2000 *Combust. Sci. and Tech.* **158** 195-210

[12] Hollmann C and Gutheil E 1998 *Combust. Sci. and Tech.* **135** 1-6, 175