Fall Technical Meeting of the Eastern States Section of the Combustion Institute
Hosted by the Clemson University, Clemson, SC
Oct 13-16, 2013

On the Uncertainty of Extrapolation of Laminar Flame Speed and Markstein Length from Expanding Spherical Flames

Fujia Wu[1], Wenkai Liang[1], Chung K. Law[1] and Zheng Chen[2]

[1]Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA

[2]Department of Mechanics and Aerospace Engineering Peking University, Beijing 100871, China

Expanding spherical flames are frequently used to determine laminar flame speeds. One of the largest errors associated with this technique is the extrapolation of the experimental data to remove the influence of flame stretch, using a linear or nonlinear relation between the local flame speed and stretch. The present work investigated the uncertainties of various extrapolation equations based on the computation results of the 1-D planar flame and the expanding spherical flame. Computation of the expanding spherical flame starts from ignition to a sufficiently large radius (~50 cm), thereby providing the relation between the local flame speed and stretch for a wide range. It is shown that the computed flame speeds of expanding flames at large radii agree closely with the results of the 1-D planar flame, and that the uncertainties of flame extrapolation largely depend on the Lewis number, *Le*. While the uncertainties for large *Le* or near-unity *Le* flames fall within 5%, those for small *Le* flames can be as high as 50%. It is suggested that previous measurements at small *Le* need to be re-analyzed, and that future measurements for such flames need to be conducted with great care. The present work also investigated the effect of pressure on the uncertainties of extrapolation.

1. Introduction

One of the most important global parameters of a combustion mixture is the propagation speed of the steady, one-dimensional, planar, adiabatic flame, namely the laminar flame speed, S_u^0. The expanding spherical flame is proven to be an effective method to measure S_u^0. In the measurement, stretch effect needs to be eliminated by extrapolating the measured flame speed to zero stretch. It is believed that the extrapolation procedure and the selection of experimental data for extrapolation is one of the major contributions of uncertainties [1]. Recognizing that the extrapolation equations currently in use were all derived from asymptomatic analysis based on various assumptions, such as one-step chemistry scheme, weak stretch, etc., it is necessary to quantify the uncertainty of these extrapolation relations.

Different extrapolation relations and procedures have been used and disagreements in the preferences as well as the extrapolated results still exist [2–7]. Most commonly used are the linear extrapolation, such as [3],

$$S_b = S_b^0 - L_b K \tag{1}$$

where S_b^0 and L_b are the unstretched laminar flame speed and the Markstein length with respect to the burned mixture, $S_b = dR_f / dt$ and $K = \left(2/R_f\right) dR_f / dt$ are the stretched flame speed with respect to the burned mixture and the stretch rate of an expanding spherical flame, and R_f is the measured flame radius. Since the model assumes linear relation between flame speed and stretch, we denote it as LMS in this study. Kelley and Law [4] suggested using a nonlinear relation for the extrapolation involving expanding spherical flames,

$$\left(\frac{S_b}{S_b^0}\right)^2 \ln\left(\frac{S_b}{S_b^0}\right)^2 = -\frac{2L_b K}{S_b^0} \tag{2}$$

This relation was derived by Ronney and Sivashinsky [8] and Bechtold *et al*. [9], assuming quasi-steady flame propagation and large flame radius relative to the flame thickness. For the past few years, this model has been used extensively for extrapolating laminar flame speeds from expanding spherical flames, such as [10–13] and many others. Since the nonlinear model is based on quasi-steady flame propagation, we denote it as NMQ in this study. Chen [5] suggested another nonlinear extrapolation equation,

$$S_b = S_b^0 - L_b \kappa = S_b^0 - \frac{2L_b}{R_f} \tag{3}$$

where $\kappa = 2/R_f$ is the curvature of the flame surface. It was demonstrated in [5] that the difference between the extrapolated laminar flame speeds using Equation (3) and NMQ is large for mixtures with $Le > 1$ while they gives almost the same results for mixtures with $Le < 1$. Since the model is actually a linear relation between flame speed and curvature, we denote it as LMC in this study. To explain the apparent improved accuracy of LMC over NMQ, Kelley et al. [7] noted that in the analysis of Ronney and Sivashinsky [8] and Bechtold et al. [9], if the unsteady term is retained and the expansion in inverse powers of R_f gives,

$$\frac{S_b}{S_b^0}\left[1 + \frac{2L_b}{R} + \frac{4L_b^2}{R^2} + \frac{16L_b^3}{3R^3} + o^4\left(\frac{L_b}{R}\right)\right] = 1 \tag{4}$$

This relation has been used in [14–16]. Since Equation (4) comes from expansion, it is denoted as NME in this study.

Despite of the effort in seeking extrapolation models with high accuracy, the analysis that leads to these models still invoke some essential assumptions, such as one-step chemistry, weak stretch rate (small flame thickness compared to flame radius), quasi-steady propagation, and/or zero thermal expansion. The validity and systematic uncertainties of these models under different conditions have not been adequately examined.

Another influence of stretch that is frequently neglected is the change of burnt gas density due to the change in the flame temperature. The issue was recently raised in [17], in which it was shown that the local displacement flame speed and consumption flame speed can differ noticeably for non-unity *Le* at small radii (large stretch). Recognizing that the stretch effect decreases as an expanding spherical flame grows,, the burnt gas density would approach the equilibrium value. Consequently the burnt gas density effect will modify the relation between local flame speed and stretch, and as a result the extrapolation will be modified and the induced uncertainty needs to be quantified.

The present work aims to investigate the uncertainties of different extrapolation relations for flame speed measurement using the constant-pressure spherical flame method. The focus is on the extrapolation of stretched displacement and consumption flame speed to zero stretch. In the present study, the uncertainty quantification is based on the computation results of both the 1-D planar flame and the expanding spherical flame using detailed chemistry without radiation loss.

2. Numerical and Experimental Methods

The one-dimensional expanding spherical flame is simulated using the A-SURF code [18,19], which has been successfully used in a serious of studies on spherical flame initiation and propagation [20–22]. A-SURF solves the conservation equations of one-dimensional, multi-component, reactive flow in a spherical coordinate using the finite volume method. The chemical reaction rates as well as thermodynamic and transport properties are evaluated using the CHEMKIN and TRANSPORT packages [23] interfaced with A-SURF. We have ensured the confinement effect is negligible by using a large chamber wall radius and only considering flame radius that is less than a fraction of the wall radius [20,22]. The one-dimensional planar steady adiabatic flame is simulated using the PREMIX Code, which is part of the CHEMKIN package [23]. To be consistent, simulations with PREMIX and A-SURF both do not include radiation model to eliminate the effects of radiation heat loss. Both simulations used multi-component formulation for transport properties and allowed Soret diffusion.

Experiments reported in this study were conducted in a dual-chamber, constant-pressure vessel. Detailed specification of the experimental apparatus, procedure and data analysis were reported previously [24,25]. The dual-chamber design allows the flame radius to grow independent of ignition and compression effects from 1.0 cm to 2.0 cm for typical flames.

3. Results

H_2-O_2 system is selected for the uncertainty quantification. Figure 1 (left) plots $S_{b,d}^0 \big/ S_{b,\mathrm{Premix}}^0$ versus $Ka = K\delta_L \big/ S_{b,\mathrm{Premix}}^0$ (δ_L is flame thickness) for various equivalence ratios for H_2/air at 1 atm. As expected, for lean mixtures the stretched flame speeds, calculated by A-SURF, start from high values at small radii and large stretch rate, while that for rich mixtures start from low values. As the flame grows and the stretch rate decreases, the flame speed calculated by A-SURF for lean and rich mixtures decreases and increases, respectively, approaching the solution of PREMIX for all equivalence ratios. Figure 1 (left) also shows the performance of the extrapolation relations. It is seen while the extrapolated flame speeds for rich mixtures ($Le > 1$, $L_b > 0$) typically differ by less than 5% from the PREMIX solutions using all relations, those for lean mixtures ($Le < 1$, $L_b < 0$) for $\phi < 0.7$ are substantially higher than the PREMIX solutions. This means none of the models are valid for mixtures with negative Markstein lengths and will cause significant over prediction. In addition, for very rich mixtures, for example $\phi = 5.0$, LMS turns out to be more accurate than the other three nonlinear relations, which under-predicts by 5-10%.

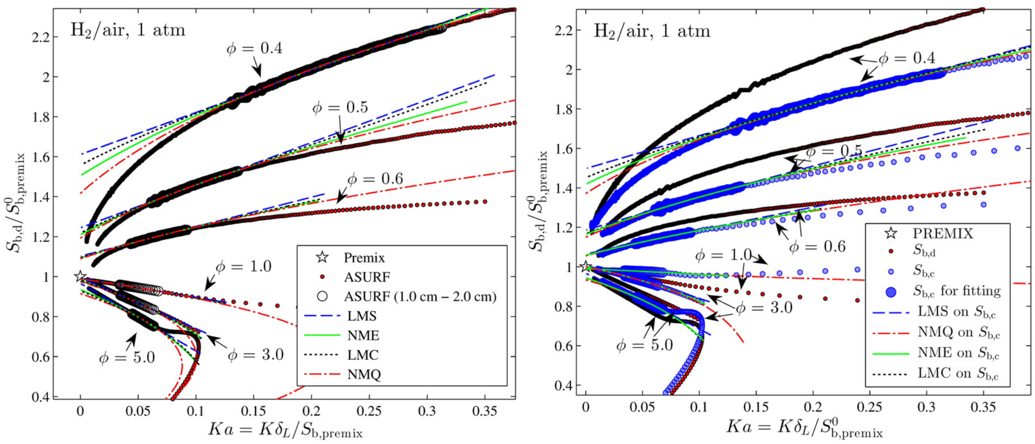

Figure 1: Comparison between results of various extrapolation models with numerical simulation for various equivalence ratios of H_2/air at 1 atm based on displacement and consumption speed

To quantify the effect of burned gas density on the local stretched flame speed as well as the extrapolation, the instantaneous consumption flame speeds are calculated from A-SURF simulations and extrapolations based on consumption flame speeds $S_{b,c}$ are performed. The results are shown in Figure 1 (right). The consumption flame speed is calculated based on the formulations in [17]. First, it is seen that for very lean or very rich mixtures, the displacement and consumption flame speeds do differ significantly at small radii and large stretch. As expected, the consumption flame speed is lower and higher than the displacement flame speed at rich and lean conditions, respectively. The difference at $\phi = 0.4$, for example, is about 20% of the PREMIX solution for flame radius from 1 cm to 2 cm. However, despite the difference, extrapolations based on the consumption flame speed do not have much improvement compared to those based on the displacement flame speeds. The results are similar, i.e., while the extrapolations for rich mixtures ($Le > 1$, $L_b > 0$) are reasonably accurate, those for lean mixtures ($Le < 1$, $L_b > 0$) are significantly over-predicted.

Figure 2 (left) plots the experimental data in comparison to the A-SURF simulations and the extrapolation results based on the experimental data. It is seen that the experimental data agree closely with the simulated displacement flame speed at $\phi = 0.5$, 0.6, 1.0 and 3.0. Such agreement is much smaller than the difference between the extrapolated flame speeds and the PREMIX solutions. This supports the validity of both the A-SURF simulations, experiments as well as the kinetic model. At $\phi = 0.4$, the experimental data is slightly lower than the simulated flame speed, indicating influencing factors, such as radiation or chemistry. The extrapolation results based on the experimental data are similar to those based on the displacement flame speeds from A-SURF simulations. The difference with the PREMIX solutions for rich mixtures is small; however, the results for lean mixtures are still largely over predicted.

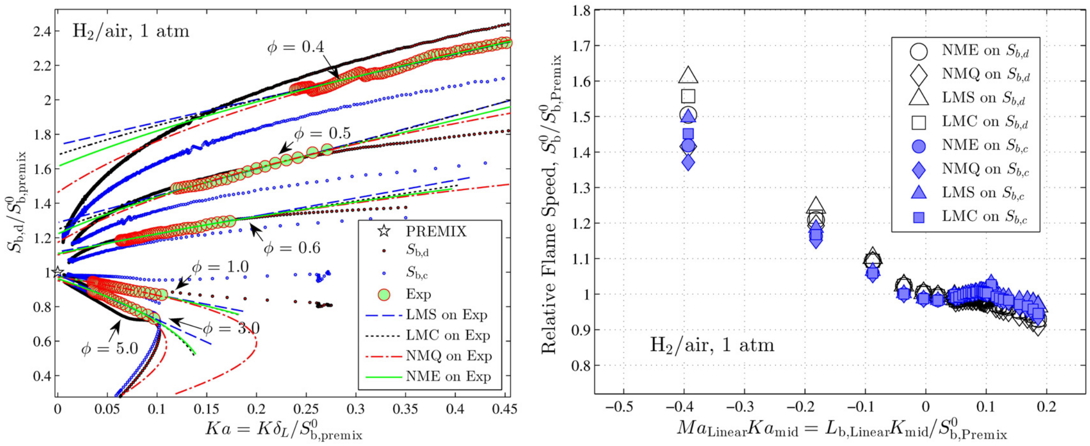

Figure 2: Comparison between results of various extrapolation models with numerical simulation for various equivalence ratios of H_2/air at 1 atm based on displacement and consumption speed

Fundamentally, the variation of flame speeds on stretch comes from two sources [26]: the first one is the non-unity *Le*, which manifests the effect in terms of the Markstein number, $Ma = L_b / \delta_L$, while the second source is the normalized stretch rate, i.e., the Karlovitz number $Ka = K\delta_L / S_{b,\mathrm{Premix}}^0$. The combined effect is the product of the two, $MaKa$. It is important to recognize that the nonlinearity of the relation between flame speed and stretch not only depends on the *Le*, but also on *Ka*. This means that for data at different *Ka*, the nonlinearity is different. For example, although we can access the flame radius history experimentally from 1 to 2 cm for all equivalence ratios, they correspond to different *Ka* at different equivalence ratios. The data we can obtain at $\phi = 0.4$ is at high *Ka* due to larger flame thickness, while the data we obtained at $\phi = 1.0$ is at small *Ka* due to small flame thickness. To generalize the uncertainties of different relations, we plot the error versus $MaKa$. Such a relation is expected to be universal even for non-H_2 flame as well as H_2 flames at different levels of dilutions. For a set of experimental data, the slope of the flame speed on stretch is directly accessible, which is the Markstein length corresponding to LMS, Ma_{Linear}. The averaged *Ka* is approximately the value at the middle point, Ka_{mid}, for example, for a data set from 1 to 2 cm, $Ka_{\mathrm{mid}} = Ka_{R_f=1.5\mathrm{cm}}$. Figure 2 (left) plots the extrapolated flame speeds as a function of $Ma_{\mathrm{Linear}}Ka_{\mathrm{mid}}$. It is seen that for $Ma_{\mathrm{Linear}}Ka_{\mathrm{mid}} < -0.1$, the extrapolations have significant over-prediction, while for $Ma_{\mathrm{Linear}}Ka_{\mathrm{mid}} > 0.1$, the extrapolations also have slight under-predictions. Such a relation will be useful to guide further measurements and quantify the uncertainties of existing measurements. For example, future measurements should be conducted in the range of $-0.1 < Ma_{\mathrm{Linear}}Ka_{\mathrm{mid}} < 0.1$ to get the most accurate results.

5. Concluding Remarks

The present study aims to quantify the systematic uncertainties associated with the extrapolation process of flame speed measurements using expanding spherical flames. Results show that the uncertainties of extrapolation largely depend on the Lewis number (or Markstein number) and the Karlovitz number. For H_2-air, it is found that all the existing models have large over-predictions for $\phi < 0.4$ and slight under prediction for $\phi > 3.0$, with the over-predictions for $\phi < 0.4$ conditions can be as large as 60%. The reason is that none of the existing relations were able to capture the strong nonlinear trends between stretch flame speed and stretch rate for $Ma <$ 1. The dependence of uncertainties on a controlling parameter $Ma_{\mathrm{Linear}}Ka_{\mathrm{mid}}$, which is easily accessible, is given. It is suggested future measurements should be in the range $\left|Ma_{\mathrm{Linear}}Ka_{\mathrm{mid}}\right| < 0.1$ to ensure accuracy. The consumption flame speeds of expanding flame speeds are also calculated. It is shown that they indeed differ substantially from the displacement flame speeds at small radii and large stretch. However, the difference of the two decreases as the flame size increases. The extrapolations based on consumption flame speeds show slight improvements but the error is still large for very lean and rich mixtures. The experimental data agree closely with the simulated displacement flame speeds on expanding spherical flames. The extrapolations based on the experimental data show similar uncertainty dependence on equivalence ratio as those based on simulation data, even though they both differ substantially from the calculated flame speeds of planar flames. This indicates that extrapolation is the largest source of error, compared to the uncertainties in the kinetic model and other factors such as radiation.

Acknowledgments

This work was supported by the Combustion Energy Frontier Research Center, an Energy Frontier Research Center funded by the US Department of Energy, Office of Basic Energy Sciences under Award Number DESC0001198.

References

[1] A.P. Kelley, Dynamics of Expanding Flames, 2011.
[2] C.K. Wu, C.K. Law, Proceedings of the Combustion Institute 20 (1984) 1941.
[3] D.R. Dowdy, D.B. Smith, A. Williams, Combustion and Flame 23 (1990) 325.
[4] A.P. Kelley, C.K. Law, Combustion and Flame 156 (2009) 1844.
[5] Z. Chen, Combustion and Flame 158 (2011) 291.
[6] F. Halter, T. Tahtouh, C. Mounaïm-Rousselle, Combustion and Flame 157 (2010) 1825.
[7] A.P. Kelley, J.K. Bechtold, C.K. Law, Journal of Fluid Mechanics 691 (2011) 26.
[8] P.D. Ronney, G.I. Sivashinsky, SIAM 49 (1989) 1029.
[9] J.K. Bechtold, C. Cui, M. Matalon, Proceedings of the Combustion Institute 30 (2005) 177.
[10] B. Galmiche, F. Halter, F. Foucher, Combustion and Flame 159 (2012) 3286.
[11] D.G. Pugh, T. O'Doherty, A.J. Griffiths, P.J. Bowen, A.P. Crayford, R. Marsh, International Journal of Hydrogen Energy 38 (2013) 3459.
[12] G. Broustail, F. Halter, P. Seers, G. Moréac, C. Mounaïm-Rousselle, Fuel 106 (2013) 310.
[13] N. Bouvet, F. Halter, C. Chauveau, Y. Yoon, International Journal of Hydrogen Energy 38 (2013) 5949.
[14] F. Wu, A.P. Kelley, C. Tang, D. Zhu, C.K. Law, International Journal of Hydrogen Energy 36 (2011) 13171.
[15] F. Wu, A.P. Kelley, C.K. Law, Combustion and Flame 159 (2012) 1417.
[16] F. Wu, C.K. Law, Combustion and Flame in Press (2013).
[17] A. Bonhomme, L. Selle, T. Poinsot, Combustion and Flame 160 (2013) 1208.
[18] Z. Chen, M.P. Burke, Y. Ju, Proceedings of the Combustion Institute 32 (2009) 1253.
[19] Z. Chen, Combustion and Flame 157 (2010) 2267.
[20] Z. Chen, M.P. Burke, Y. Ju, Combustion Theory and Modelling 13 (2009) 343.
[21] Z. Chen, X. Qin, B. Xu, Y. Ju, F. Liu, Proceedings of the Combustion Institute 31 (2007) 2693.
[22] M.P. Burke, Z. Chen, Y. Ju, F.L. Dryer, Combustion and Flame 156 (2009) 771.
[23] R.J. Kee, F.M. Rupley, J.A. Miller, M.E. Coltrin, J.F. Grcar, E. Meeks, H.K. Moffat, A.E. Lutz, G. DixonLewis, M.D. Smooke, J. Warnatz, G.H. Evans, R.S. Larson, R.E. Mitchell, L.R. Petzold, W.C. Reynolds, M. Caracotsios, W.E. Stewart, P. Glarborg, C. Wang, A. O., CHEMKIN Collection, Release 3.6, Reaction Design, Inc., San Diego, CA, 2000.
[24] A.P. Kelley, A.J. Smallbone, D.L. Zhu, C.K. Law, 6th U.S. National Combustion Meeting (2009).
[25] A.P. Kelley, A.J. Smallbone, D.L. Zhu, C.K. Law, Proceedings of the Combustion Institute 33 (2011) 963.
[26] C.K. Law, Combustion Physics, Cambridge University Press, New York, 2006.