# Simplified correlations for burning velocity of gaseous fuel-air mixtures

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# Introduction

- Measurement of burning velocities of gaseous fuel-air mixtures has been the subject of study for over five decades and a recent review by Konnov et al (2018) that has covered 500 references on the subject. More than thousand researchers have been involved.
- The above review and several other papers contain data comparisons for many fuel-air mixtures from various sources using a number of different techniques.
- Also are contained predictions using premixed flame code (at least three codes) with reaction kinetics from different sources.
- The dependences on initial temperature and pressure are extracted for the exponents of initial temperature and pressure.
- There are many correlations for each of the fuels including straight chain hydrocarbons.
- What appears clear from this paper is that the data show differences arising out of different researchers, different apparatus and schemes used for deduction for most fuels – the differences being about ± 5 % for standard fuels and more close to ± 10 % for most other fuels.
- While it is not obvious why the subject has received (or should receive) such an enhanced degree of interest on the part of researchers (and journals), this feature was what drew our attention

### ...Motivation

Burning velocity(cm/s)



- As can be noted, the scatter in the experimental data and the differences in the predictions by various authors (with different mechanisms and codes) is about ± 7 %.
- It is not easy to swear by theory (with complex chemistry and diffusion models) or experiment easily.
- In view of these, it was thought:



CH4	H <sub>2</sub>	со	CO2	N <sub>2</sub>
%	%	%	%	%
9.8	47.2	27	16	0
8.33	40.12	22.95	13.6	15
6.37	30.68	17.55	10.4	35
4.9	23.6	13.5	8	50

...the numerical simulation was conducted with GR-3 mechanism through using s premix code CHEMKIN-PRO to predict the burning velocity.....

The calculations seem to under-predict significantly for nearly all compositions at lower equivalence ratios.

Would it be useful if <u>simpler correlations</u> can be developed for a range of fuels together by examining the basic causes for the variations with equivalence ratio ( $\phi$ ), and initial temperature ( $T_{ini}$ )? Influence of pressure effects could also be simplified

### No other correlations? Curvefits?

#### Dong et al (2010) have set out a correlation as follows.

Basing on the experimental data, fitting curves of laminar flame speeds for  $H_2/air$  mixtures and NG/air mixtures are drawn in Figs. 5 and 6. The formulas for calculating laminar flame speed of  $H_2/air$  and NG/air mixtures are given in Eqs. (4) and (5):

$$\begin{split} S_{\rm H_2} &= -1.11019 + 4.65167 \phi - 1.44347 \phi^2 + 0.04868 \phi^3, \\ &(\varphi = 0.8 - 2.1), \, R^2 = 0.993; \end{split} \label{eq:generalized_states}$$

$$S_{\rm NG} = -0.00075 + \frac{0.1352}{4 \times (\phi - 1.04072)^2 + 0.34623},$$
  
(\varphi = 0.8-2.1), R<sup>2</sup> = 0.983. (5)

To calculate the laminar flame speed of H<sub>2</sub>/NG/air mixtures, we define  $(S_x - S_{NG})/(S_{H_2} - S_{NG})$  as laminar flame speed increment. Here,  $S_x$  denotes the laminar flame speed at x% volumetric fraction of H<sub>2</sub>. Figure 7 illustrates the

increments of the laminar flame speed against volumetric fraction of  $\rm H_2$  for  $\rm H_2/NG/air$  mixtures. The correlation

between the increment of laminar flame speed and volumetric fraction of  $H_2$  can be fitted as formula (6):

$$\frac{S_x - S_{\rm NG}}{S_{\rm H_2} - S_{\rm NG}} = 0.00221 + 0.009 \exp\left(\frac{\phi}{21.30807}\right),$$

$$R^2 = 0.996.$$
(6)

Using Eqs. (4)–(6), the laminar flame speed at different volumetric fraction of  $H_2$  and given equivalence ratio can be easily calculated.

The number of significant digits following the decimal point in the curve fits for a quantity that is about 5 to 10 % accurate is worrisome. - also too specific



Fig. 6 Fitting curve of laminar flame speed versus equivalence ratio for NG



### Methodology for the simplified correlation - 1

- Burning rate depends on the adiabatic flame temperature  $(T_{f,ad})$  and so, the crucial dependence of the burn rate variation with equivalence ratio ( $\phi$ ) is related to the variation of  $T_{f,ad}$  with  $\phi$ .
- This is equilibrium thermochemistry dependent and not rate dependent.
- It was thought that if this could be factored in, simpler correlations of greater generality can be obtained.
- Seeking a dimensionless dependence between Su/Su( $\phi = 1$ ) and T<sub>f</sub>/T<sub>f</sub>( $\phi = 1$ ) was thought first appropriate.



- The dependence is linear
- The constant slope is different for lean and rich cases.
- It is inferred that the effect of flame temperature for rich cases can be different from the lean as the role of chemistry is more involved in rich mixtures.
- The fact that the behavior is linear, but with different slopes is factored into the correlation.
- It is noted that the burning velocity peaks at a richer equivalence ratio and hence may bring in some inaccuracy with the simplified correlation.
- Such a behavior is taken valid for all hydrocarbons & alcohols

## Methodology for the simplified correlation - 2

Initial temperature dependence is treated by plotting the burning velocity at  $\phi = 1$  as a function of initial temperature (T<sub>ini</sub>).



- This behavior is linear and can be described by a simple relationship.
- It is inferred that the relationship of Su with  $\mathsf{T}_{f,\mathsf{ad}}$  reduces to this relationship after suitable linearization
- The dependence on pressure has been presented in Konnov et al (2018) for a number of fuel-air mixtures (see for instance Fig. 40 of their paper).
- The variation set out here from different sources has a complex variation over the equivalence ratio.
- It appears that for the present purposes of getting an overall correlation, it is appropriate to choose a single value for the pressure index.
- The pressure index of 0.3 is chosen for all straight-chain HCs after checking out the value for minimum error.

### Therefore the correlation is set out as

Su (cm/s) = 35.6 p<sup>-0.3</sup> (T<sub>f</sub>/T<sub>f,max</sub> - C)/(1-C) [(T<sub>ini</sub>-150)/150] [1 + 0.3(M<sub>f</sub>/16-1) exp{- 0.8\*(M<sub>f</sub>/16-1)}]  
Dependences on 
$$p \phi T_{ini}$$
 Fuel

with **p** = pressure (atm), T<sub>f</sub> and T<sub>f, max</sub> are the adiabatic flame temperatures at any  $\phi$  and at  $\phi$  = 1 (K), and **C** = constant = 0.65 for  $\phi$  < 1 and 0.8 for  $\phi$  > 1.

- The stoichiometric burning velocity of CH<sub>4</sub>-air is taken as 35.6 cm/s. This is the basic burn rate of all straight chain hydrocarbons considered here (Acetylene excluded)
- The dependence with respect to equivalence ratio is obtained through the dependence on the adiabatic flame temperature (that can easily be obtained online from NASA CEA code for any condition of relevance here).
- From an examination of the data of peak burning velocities of higher hydrocarbons it is found that it increases for ethane, propane and butane to about 40 cm/s and settles down for octane at 35 cm/s. While once can argue that these differences are small, the term within the flower brackets accounts for this observation.
- All predictions depend on the above equation (No other constants introduced).

Predictions and comparisons Hydrocarbons & Alcohols

The basis of experimental data is: Konov et al, 2018









Comparisons considered satisfactory



1.3 1.4 1.5

1.3

1.4













Φ





Comparisons are better at lean conditions Than under rich conditions

0.5

0.6

0.7

0.8

0.9

Φ

1.0 1.1 1.2 1.3 1.4 1.5

1.6



Φ



Heptane and Octane at different conditions for which data are set out in Konnov et al

Comparisons reasonable









#### Ethyl Alcohol as extrapolated from Methane seems to behave very differently

 $CH_3OH$  even if treated as related to  $CH_4$  in its combustion behavior with the oxygen atom integrated into the molecule allows higher reaction rates, no simple hypothesis can explain the complex behavior -

At 300 K, the burning velocity at the peak And under rich conditions are seriously under-predicted Also, at 373 K, lean flames are over-predicted

At 400 K, predictions seem reasonable!

No simple explanation seems possible for the observations.





# Predictions and comparisons for Hydrogen and Syngas compositions

- Experimental data are obtained from Li et al, 2016; Wu, et al, 2018; Kannov et al, 2018; Verghese et al, 2019
- It is clearly noted that the peak in burning velocity occurs at very rich equivalence ratios
- This means the approach chosen for hydrocarbons seeking relationship with adiabatic flame temperature variation alone will not work because stronger diffusional effects -of H2 come into play.
- Fortunately, the variation with equivalence ratio alone would be adequate, as is seen to follow......

### Syngas compositions considered

		CO, % v	H2 % v	CH4 <i>,</i> % v	CO2 %v	N2, % v	Mol wt		Sources
Г	SG1	15	15	0	15	55	26.5	21	Konnov et al, 2018
Close to Producer gas from air gasification of biomass	SG2	15	15	5	15	50	25.9	22.5	same
	SG3	15	20	5	10	50	23.8	34	same
	SG4	20	15	0	15	50	26.5	26	same
	SG5	20	15	5	10	50	25.1	31.5	same
	SG6	20	20	5	10	45	23.8	41	same
	SG7	20	20	5	15	40	24.6	35	same
	SG8	25	20	5	10	40	23.8	46	same
	SG9	25	15	0	15	45	26.5	30	same
	SG10	13.5	23.6	4.9	8	50	22.6	46	Wu, et al, 2018
	SG11	17.5	30.7	6.4	10.4	35	20.9	70	same
	SG12	23	40.1	8.3	13.6	15	18.8	85	same
	SG13	27	47.2	9.8	16	0	17.1	97	same
Largely CO	SG14	95	5	0	0	0	26.7	60	Natarajan et al, 2007
	SG15	50	50	0	0	0	15.0	160	Same
	SG16	41.70	41.7	0	16.6	0	17.36	91.3	same
H <sub>2</sub>	SG17	0	100	0	0	0	2.0	270	Konnov et al, 2018







P1 = [100 (%H2) + 36.5 (%CH4) + 35 (%CO)]

### Syngas compositions

Two approaches have been made for correlating the burning velocity Out of which the more successful one is set out here.

A parameter, P1 is constructed such that it has the features of summation on mixture composition with individual burning velocities

 $\mathsf{P1} = (100 f_{H2} + 36.5 f_{CH4} + 35 f_{CO})$ 

Su, max = 2 (P1 - 9) cm/s for P1 <62 up to  $\phi$  = 1.05 = 2.4 (P1 - 20) cm/s for P1 > 62

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Su,min (\phi = 0.6) = 1.1 (P1-11)
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(Su - Su,min)/(Su,max - Su,min) = (\phi - 0.6)/(1.05 - 0.6)
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Su = 1.1 (P1 - 11) + (2 P1 - 13) (φ - 0.6) for P1 < 62

= 1.1 (P1 - 11) + (2.5 P1 - 50) (φ - 0.6) for P1 > 62

where  $f_i$ 's are mole fractions of individual species in the composition.

This correlation does not distinguish between  $CO_2$  and  $N_2$ This is not consistent with experimental data.











20

10

0

0.4





0.8

1

φ

1.2

1.4

except for SG10. It appears that computational results favor the simpler expectation!

20

0

0.4

0.6

Comparisons







#### Observation:

The correlation seems to be able to distinguish between close but differently performing compositions











Su  $(C_2H_2) = 100 \phi + 25 cm/s, \phi < 1.2$ = 145 cm/s, 1.8 >  $\phi > 1.2$ 

This is just a curve fit since relating to simple hydrocarbons is tortuous, if not impossible. It is because the reactivity of acetylene arises from its triple bond

#### Overall performance of the correlations



# Summary

- Premixed flame burning behavior of 45+ compositions of hydrocarbons + alcohols + hydrogen and syngas have been considered for study
- Simplified correlations the burning velocity of hydrocarbons + alcohols and hydrogen and syngas as three sets have been attempted.
- For hydrocarbons and alcohols for various initial temperatures and pressures (CH $_3$ OH needs more study):

Su (cm/s) = 35.6  $p^{-0.3}$  (T<sub>f</sub>/T<sub>f,max</sub> - C)/(1-C) [(T<sub>ini</sub>-150)/150] [1 + 0.3(M<sub>f</sub>/16-1) exp{- 0.8\*(M<sub>f</sub>/16-1)}], T<sub>f</sub> to be obtained from NASA CEC code

- For Hydrogen: Su (H<sub>2</sub>, cm/s) = 230 ( $\phi$  0.2) (1-1.9 $f_{N2}$ ) (T<sub>ini</sub>-150)/150 cm/s for 0.2 <  $\phi$  < 1.4, = 276 (1-1.9 $f_{N2}$ ) (Tini-150)/150 cm/s for 2.2 >  $\phi$  > 1.4
- For Syngas: P1 =  $(100f_{H2}+36.5f_{CH4}+35f_{CO})$  Su, max = 2 (P1 9) cm/s for P1 <62 = 2.4 (P1 20) cm/s for P1 > 62, up to  $\phi = 1.05$ , Su,min ( $\phi = 0.6$ ) = 1.1 (P1-11) (Su - Su,min)/(Su,max - Su,min) = ( $\phi - 0.6$ )/(1.05 - 0.6); Therefore, Su = 1.1 (P1 - 11) + (2 P1 - 13) ( $\phi - 0.6$ ) for P1 < 62 = 1.1 (P1 - 11) + (2.5 P1 - 50) ( $\phi - 0.6$ ) for P1 > 62, where  $f_i$ 's are mole fractions of individual species in the composition.
- Several alternate, somewhat more involved correlations did not do as well as the above.
- If experiments are beset with inaccuracies of measurement, calculations are beset with issues of kinetic schemes and other thermochemical details. The final outcome from these efforts do not point to any of them being superior at this stage (accuracies  $\sim \pm 7$  to 10 %).
- If these data are intended for calculating for complex turbulent combusting premixed flows simpler correlations may as well do except close to flammability limits where detailed chemistry matters

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Thank you.





Comparisons of maximum Su are reasonable for 10 of the 16 cases considered here.

The comparisons are not good for some, but bad for SG14. High CO cases have an issue in this format. Su (H<sub>2</sub>) = 225 ( $\phi$  - 0.2) (T<sub>ini</sub>-150)/150, for  $\phi$  < 1.4, 270 (T<sub>ini</sub>-150)/150 f<sub>H2</sub> for all  $\phi$  > 1.4 Su(CH<sub>4</sub>) = 36.5\*(1.71 $\phi$ -0.71) (Tini-150)/150 for  $\phi$  < 1.0 Su(CO) = 60 ( $\phi$  -0.33) (Tini-150)/150 f<sub>CO</sub> for  $\phi$  < 1.0 Su = [Su (H<sub>2</sub>) f<sub>H2</sub> + Su(CH<sub>4</sub>) f<sub>CH4</sub> + Su(CO) f<sub>CO</sub>] (1-1.3 f<sub>CO2</sub>-0.45 f<sub>N2</sub>) for  $\phi$  < 1 where f<sub>i</sub>'s are mole fractions of individual species







The poor comparison of composition SG14 cannot be understood because any simple modification is inconsistent with some good comparisons like of SG15

For SG16, it appears that computational results compare better with simple predictions compared to experiments. CO has been known to burn very slowly without  $H_2O$  (moisture); CO + OH  $\longrightarrow$  CO<sub>2</sub> + H is supposedly the most dominant reaction.

CO problem remains to be resolved.