implified correlations for burning velocity gaseous fuel-air mixtures

Introduction and Motivation
Methodology for the simplified correlation
Predictions and comparisons for HCs and alcohols
Predictions and comparisons for Hydrogen and Syngas compositions
Issues related to inadequate "performance" of correlations
Summary

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FCRC, Jain (Deemed-to-be-University)
@Seventh PJP memorial Workshop, IIT Bombay

Introduction

easurement of burning velocities of gaseous fuel-air mixtures has been the subject o udy for over five decades and a recent review by Konnov et al (2018) that has covere ferences on the subject. More than thousand researchers have been involved.

ne above review and several other papers contain data comparisons for many fuel-air ixtures from various sources using a number of different techniques.

lso are contained predictions using premixed flame code (at least three codes) with action kinetics from different sources.

ne dependences on initial temperature and pressure are extracted for the exponents itial temperature and pressure.

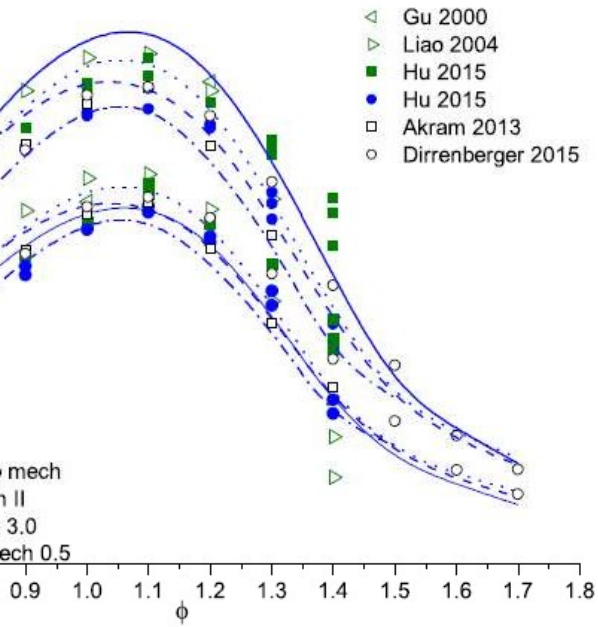
here are many correlations for each of the fuels including straight chain hydrocarbon

/hat appears clear from this paper is that the data show differences arising out of fferent researchers, different apparatus and schemes used for deduction for most f ne differences being about ± 5 % for standard fuels and more close to ± 10 % for mos her fuels.

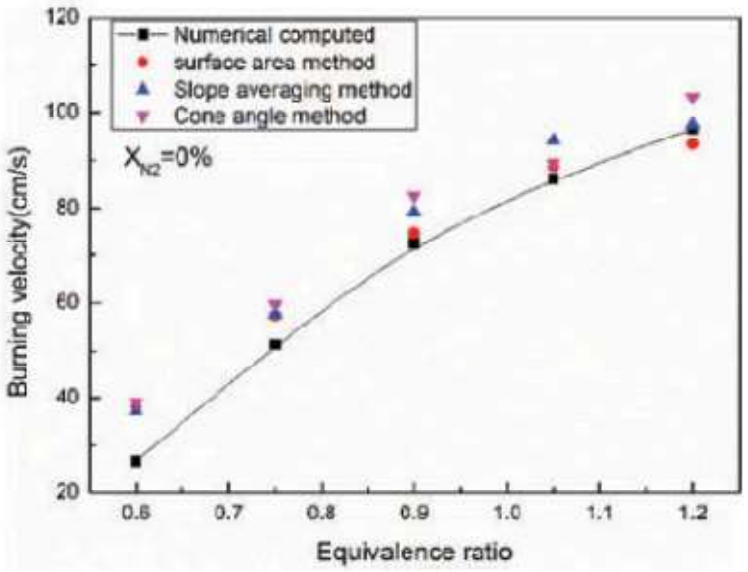
/hile it is not obvious why the subject has received (or should receive) such an enhanc egree of interest on the part of researchers (and journals), this feature was what dr ttention

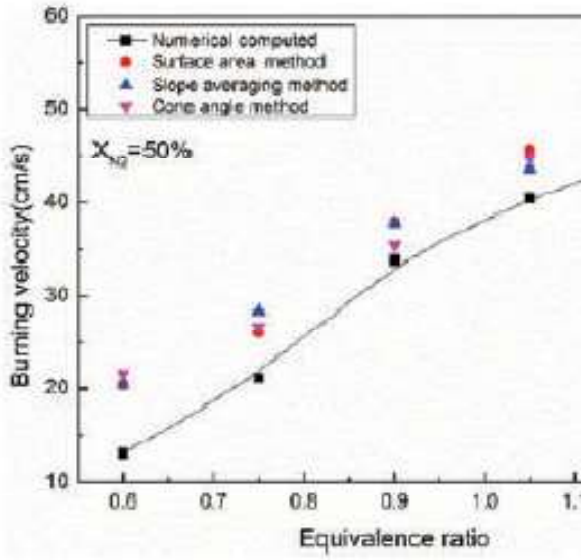
...Motivation

From Konnov, et al, 2018



From: Wu et al, 2018





be noted, the scatter in the experimental data
differences in the predictions by various
(with different mechanisms and codes) is
7 %.

t easy to swear by theory (with complex
try and diffusion models) or experiment easily.

of these, it was thought:

CH_4	H_2	CO	CO_2	N_2
%	%	%	%	%
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 w
conducted with GR-3 mecha
through using s premix code
PRO to predict the burning v

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

it be useful if simpler correlations can be developed for a range of fuels together by examining the basic
for the variations with equivalence ratio (ϕ), and initial temperature (T_{ini})?
nce 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):

$$S_{H_2} = -1.11019 + 4.65167\phi - 1.44347\phi^2 + 0.04868\phi^3, \quad (\varphi = 0.8-2.1),\ R^2 = 0.993; \tag{4}$$

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

To calculate the laminar flame speed of H_2/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_2. Figure 7 illustrates the increments of the laminar flame speed against volumetric fraction of H_2 for 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):

$$\frac{S_x - S_{NG}}{S_{H_2} - S_{NG}} = 0.00221 + 0.009\exp\left(\frac{\phi}{21.30807}\right), \quad R^2 = 0.996. \tag{6}$$

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

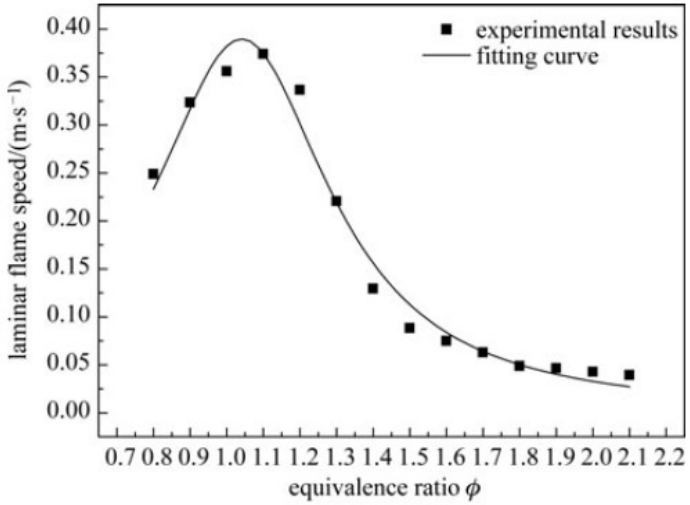
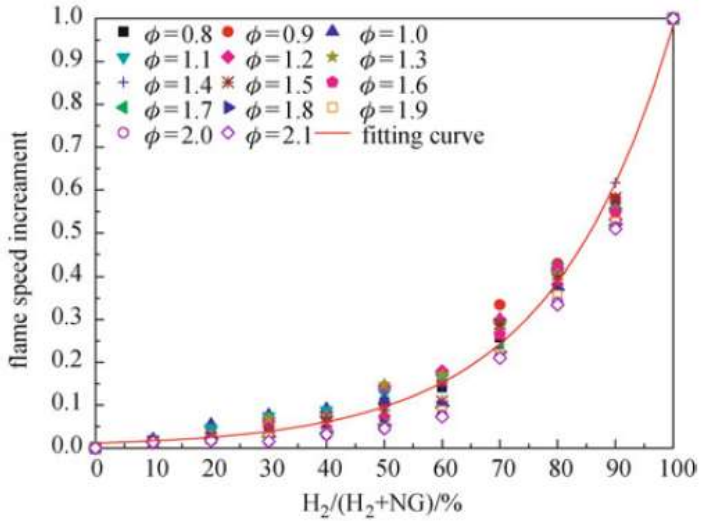
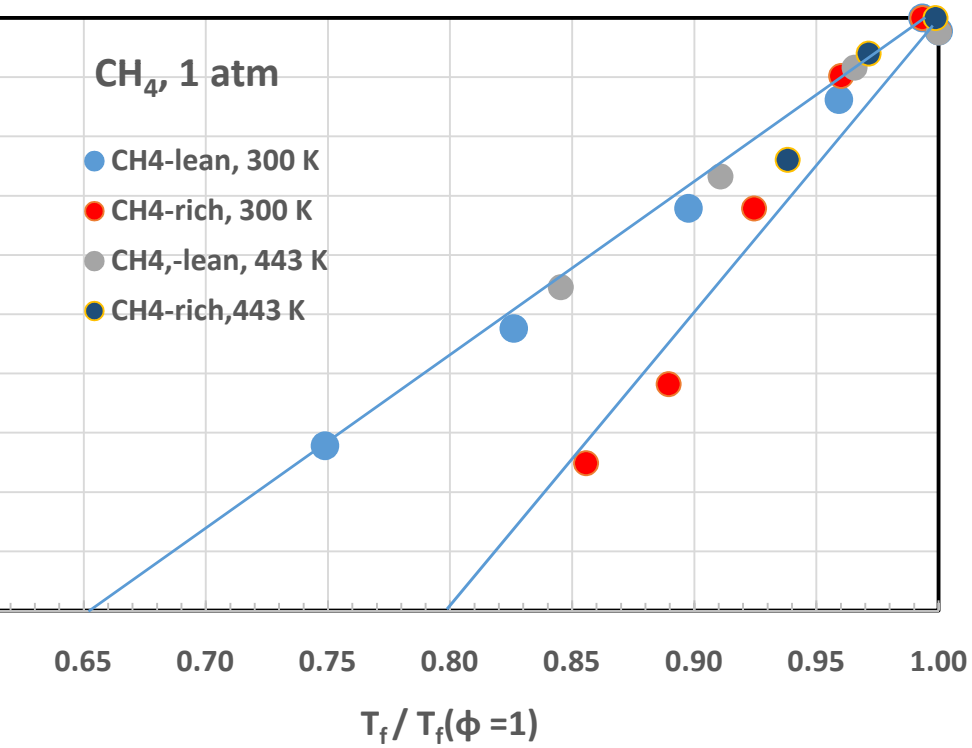


Fig. 6 Fitting curve of laminar flame speed versus equivalence ratio for NG



Methodology for the simplified correlation - 1

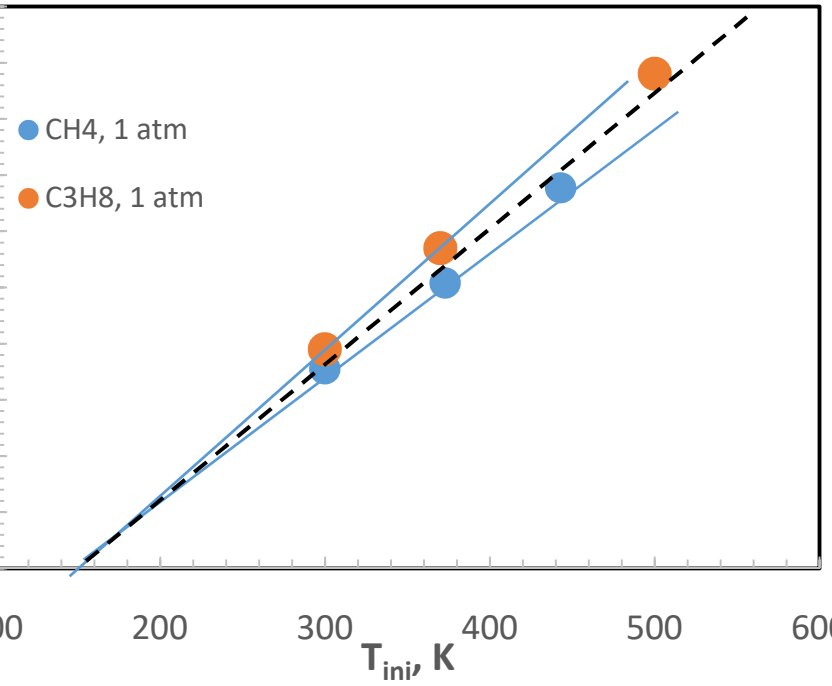
ng rate depends on the adiabatic flame temperature ($T_{f,ad}$) and so, the crucial dependence of t
variation with equivalence ratio (ϕ) is related to the variation of $T_{f,ad}$ with ϕ.
is equilibrium thermochemistry dependent and not rate dependent.
s thought that if this could be factored in, simpler correlations of *greater generality* can be ob
ing a dimensionless dependence between $Su/Su(\phi = 1)$ and $T_f/T_f(\phi = 1)$ was thought first approp



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

Methodology for the simplified correlation - 2

mperature dependence is treated by plotting the burning velocity at ϕ = 1 as a function of initial temperature



- This behavior is linear and can be described by a s relationship.
- It is inferred that the relationship of Su with $T_{f,o}$ reduces to this relationship after suitable lineariz
- The dependence on pressure has been presented i Konnov et al (2018) for a number of fuel-air mixtu (see for instance Fig. 40 of their paper).
- The variation set out here from different sources complex variation over the equivalence ratio.

ars that for the present purposes of getting an overall correlation, it is appropriate to choose a sing r the pressure index.

ssure index of - 0.3 is chosen <u>for all straight-chain HCs</u> after checking out the value for minimum er

Therefore the correlation is set out as

$$Su\ (cm/s) = 35.6\ p^{-0.3}\ (T_f/T_{f,max} - C)/(1-C)\ \ [(T_{ini}-150)/150]\ \ [1 + 0.3(M_f/16-1)\ \exp\{-0.8*(M_f/16-1)\}]$$

ndences on → p, ϕ, T_{ini}, *Fuel*

= pressure (atm), T_f and $T_{f,\,max}$ are the adiabatic flame temperatures at any ϕ and at ϕ = 1 (K), and

stant = 0.65 for ϕ < 1 and 0.8 for ϕ > 1.

stoichiometric burning velocity of CH_4-air is taken as 35.6 cm/s. This is the basic burn rate of all straight rocarbons considered here (Acetylene excluded)

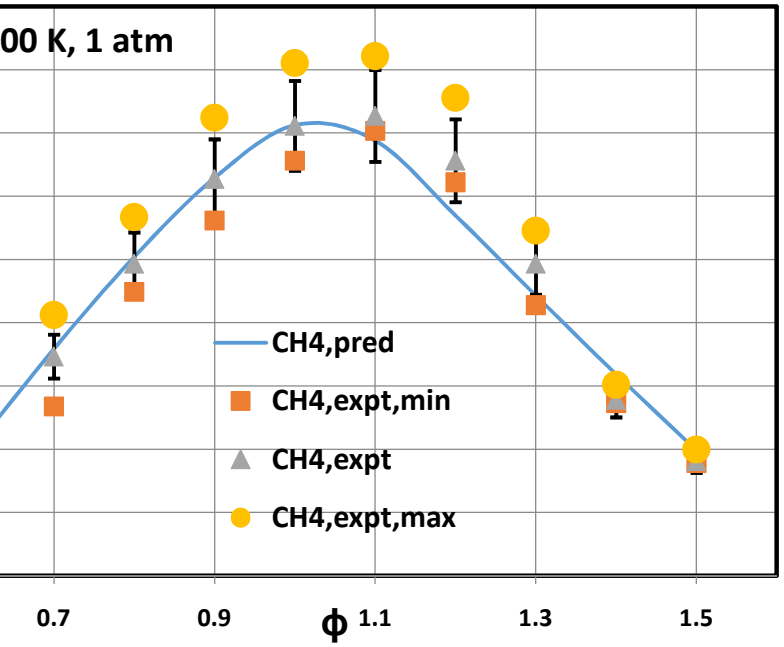
dependence with respect to equivalence ratio is obtained through the dependence on the adiabatic flame perature (that can easily be obtained online from NASA CEA code for any condition of relevance here).

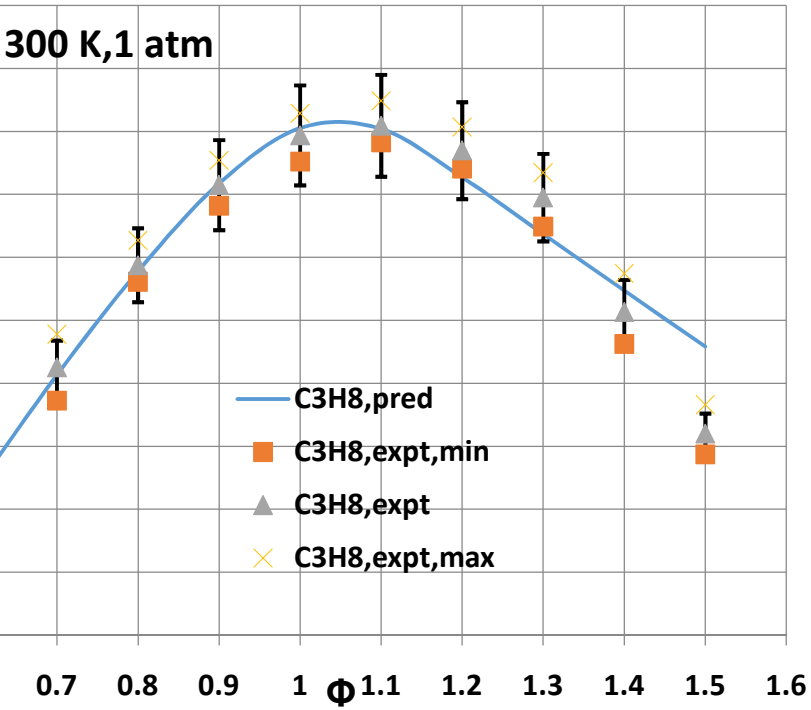
n an examination of the data of peak burning velocities of higher hydrocarbons it is found that it increases ane, propane and butane to about 40 cm/s and settles down for octane at 35 cm/s. While once can argue th e differences are small, the term within the flower brackets accounts for this observation.

predictions depend on the above equation (No other constants introduced).

Predictions and comparisons Hydrocarbons & Alcohols

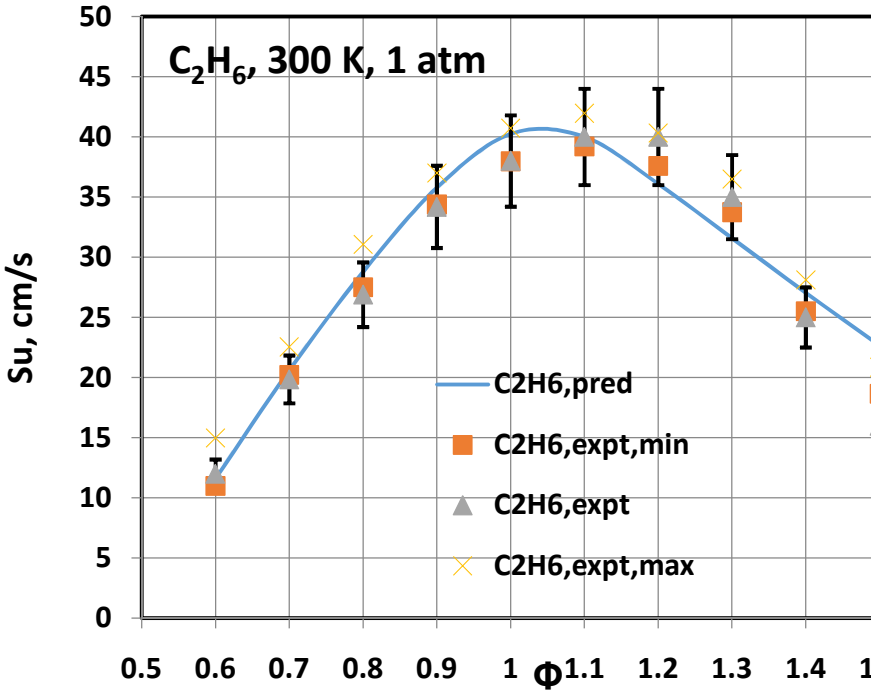
The basis of experimental data is: Konov et al, 2018

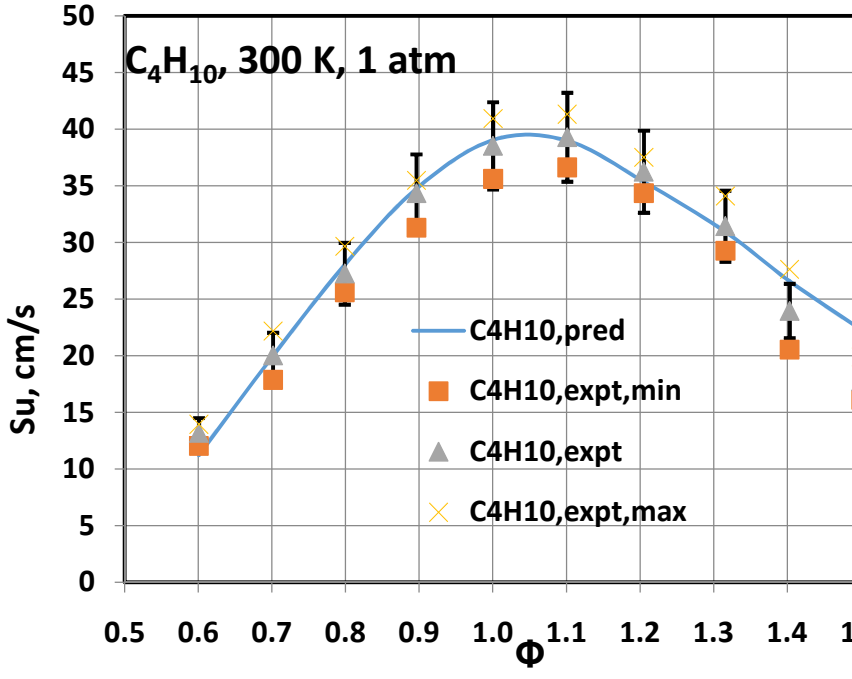


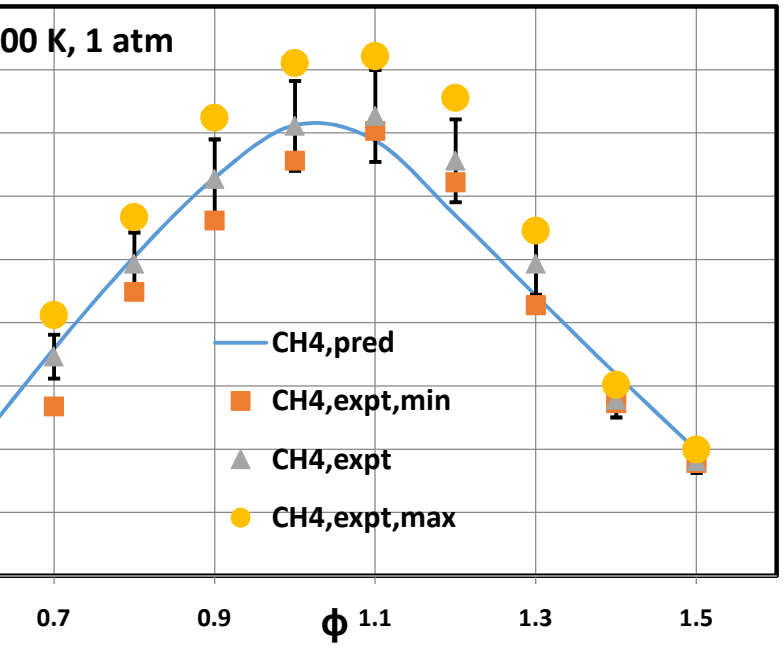


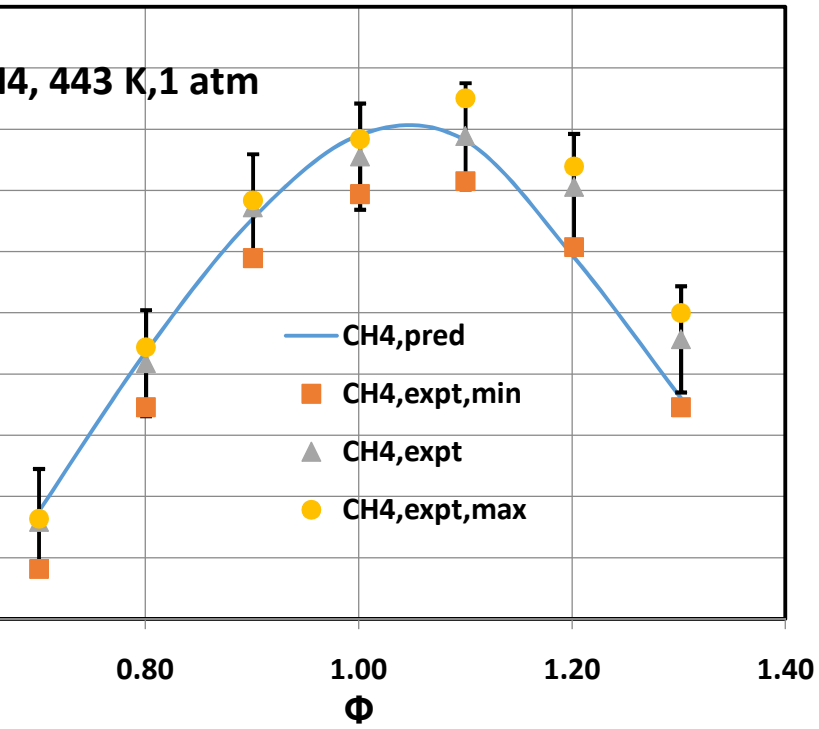
Hydrocarbons at $P = 1$ atm, $T_{ini} = 300$ K

Comparisons considered satisfactory



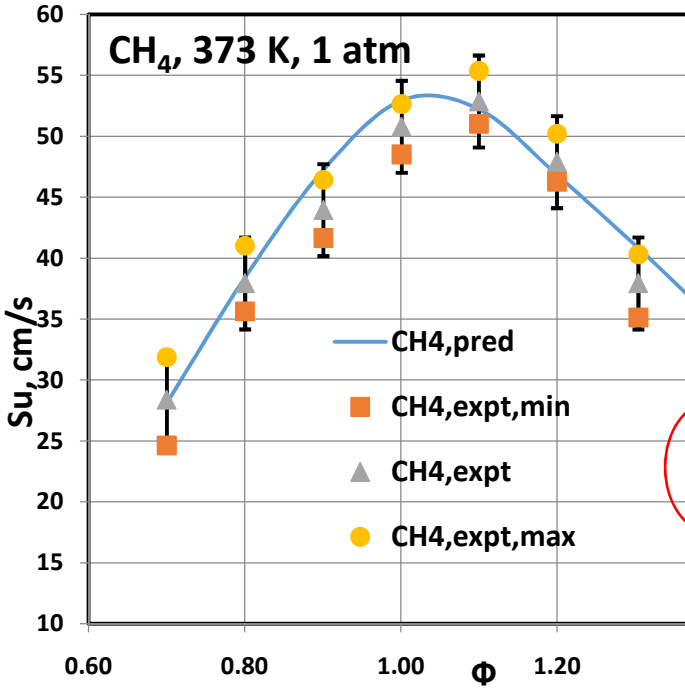


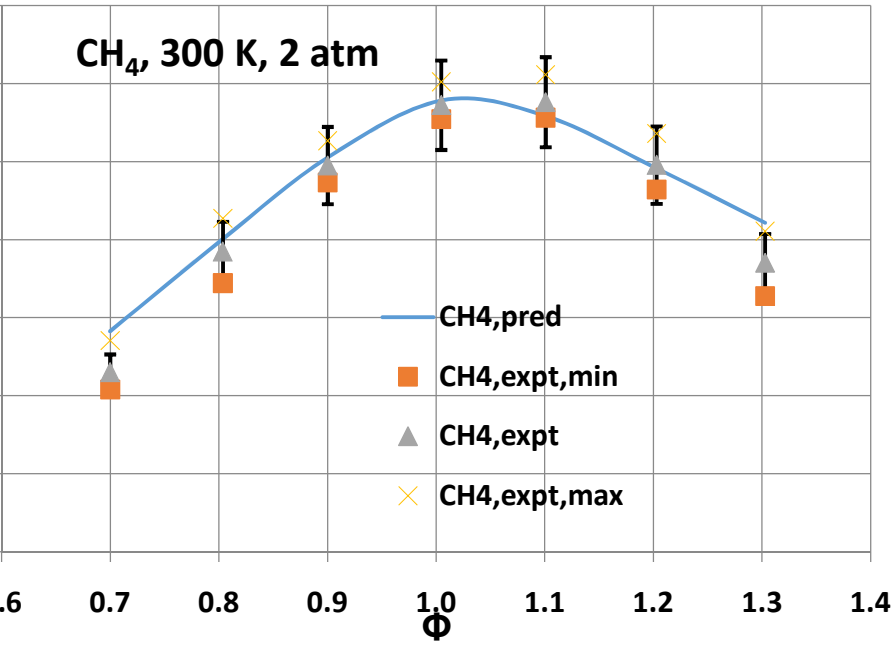


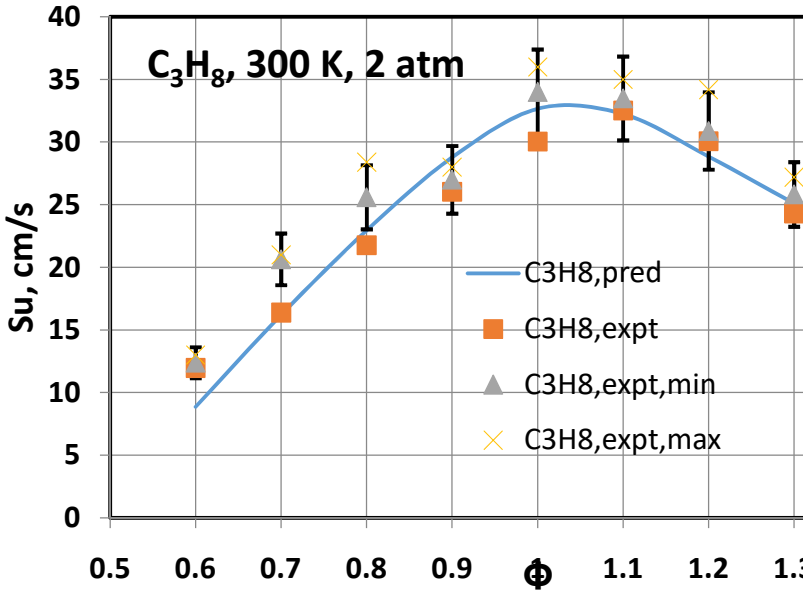


CH_4 at
p = 1 atm
but increasing T_{ini}

Comparisons considered satisfactory

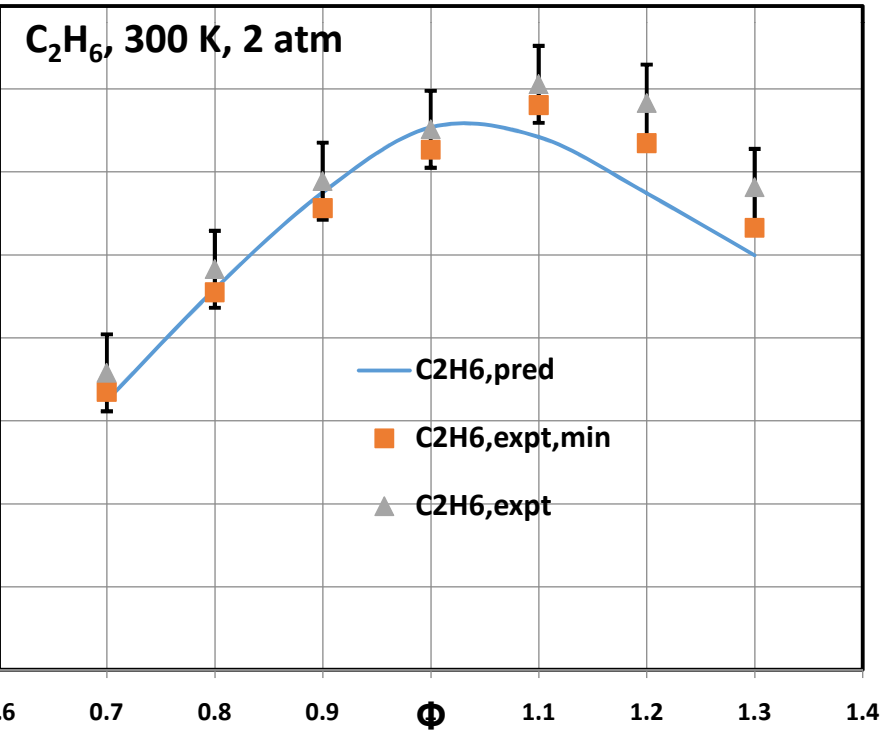






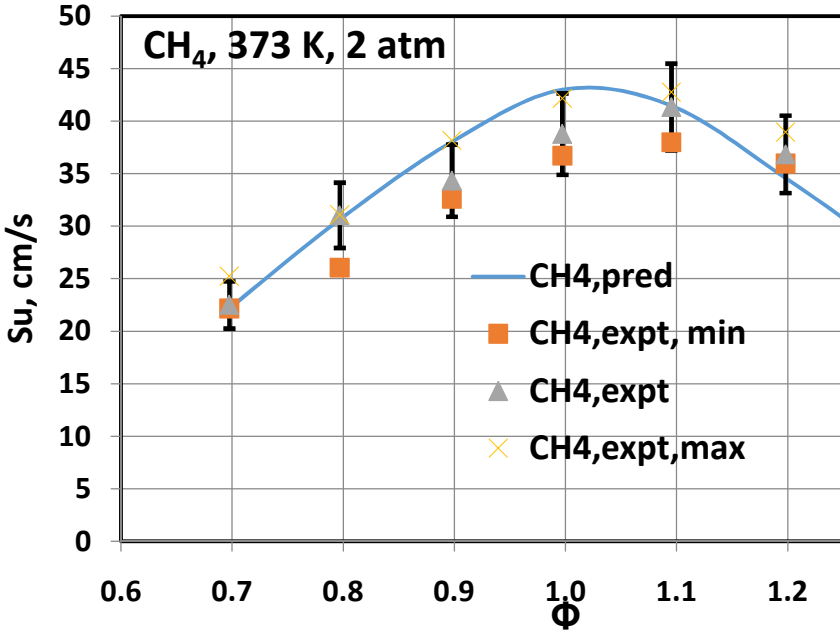
Hydrocarbons
p = 2 atm,

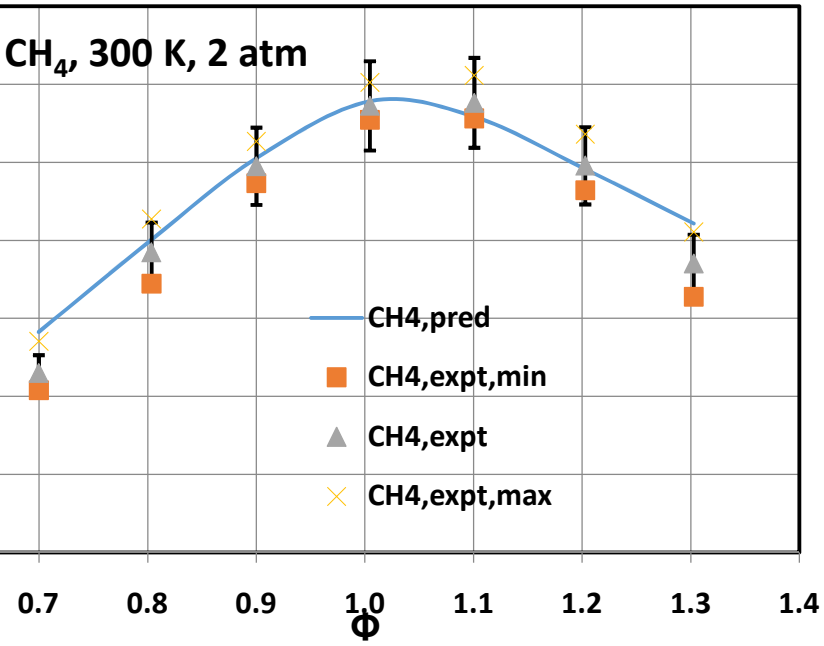
T_{ini} = 300 K
(& 373 K)

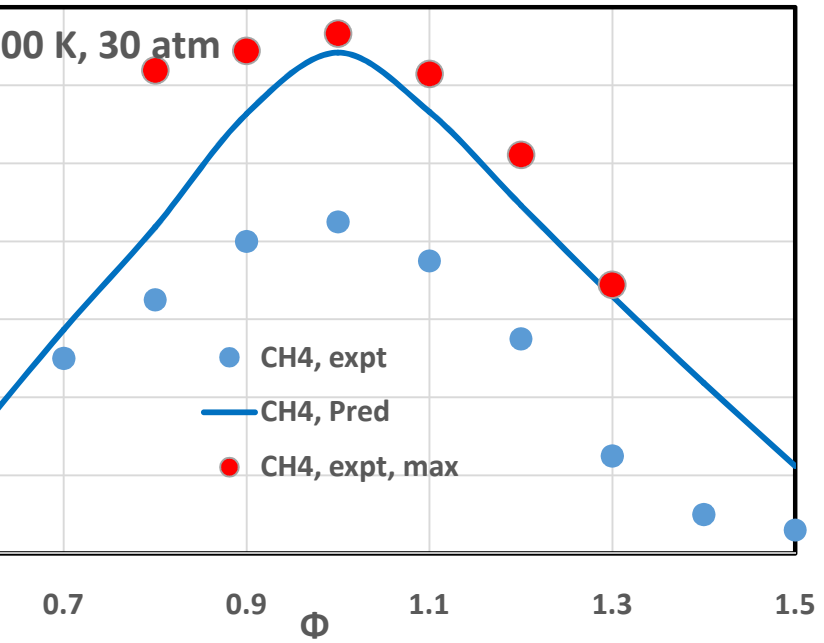


C_2H_6 predictions on the rich side are not all that good

Is experimental data good?



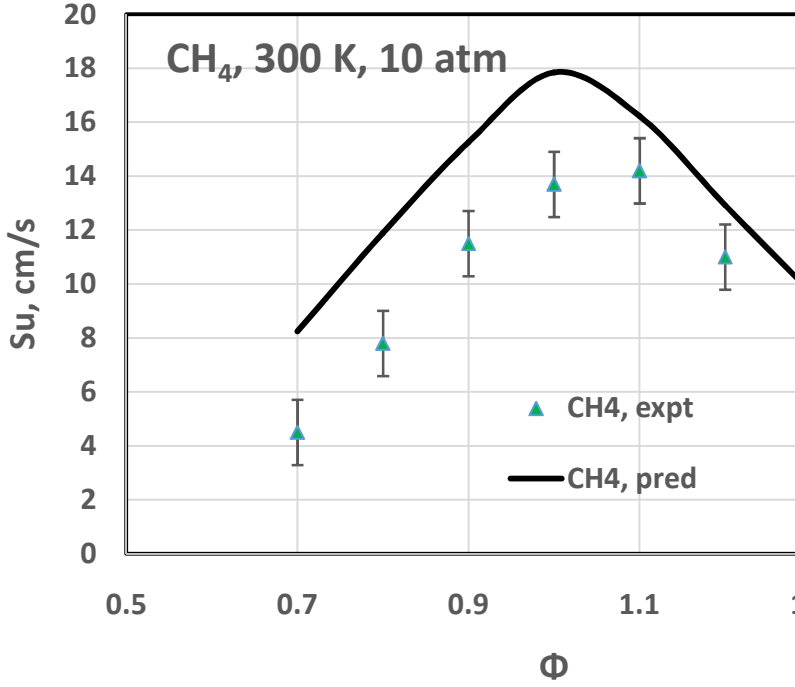


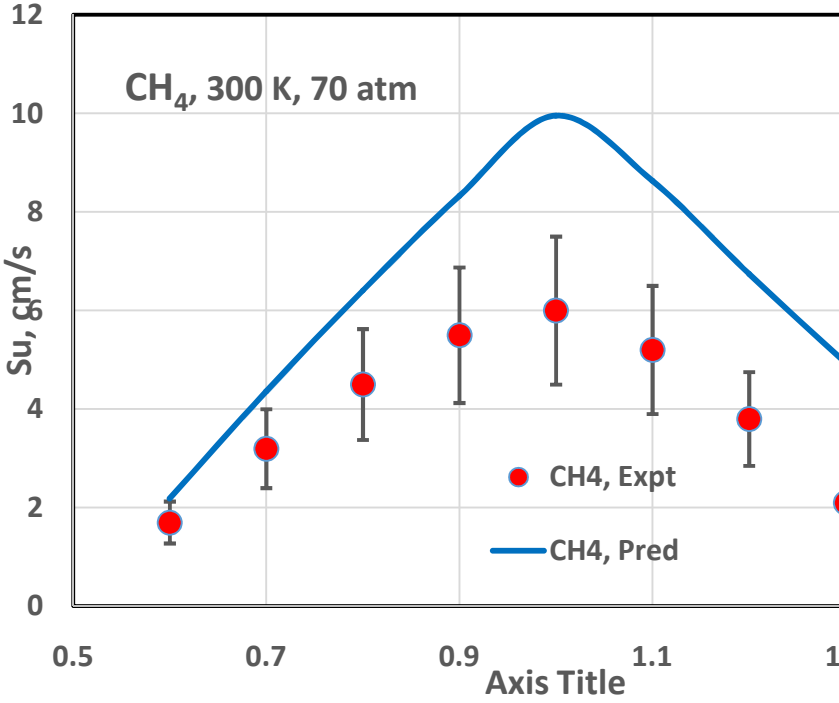


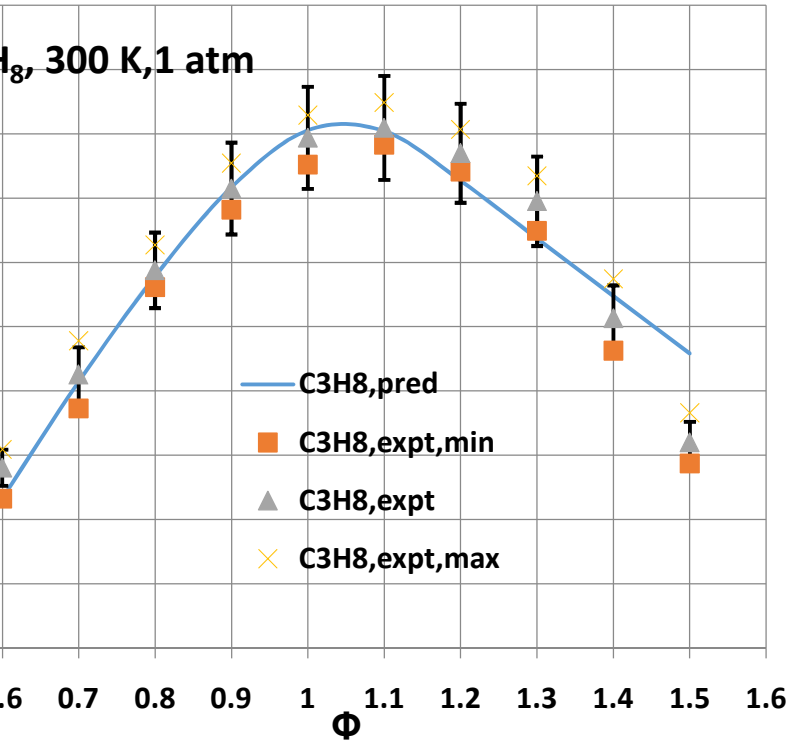
Methane
T_{ini} = 300 K
P = 2 to 70 atm

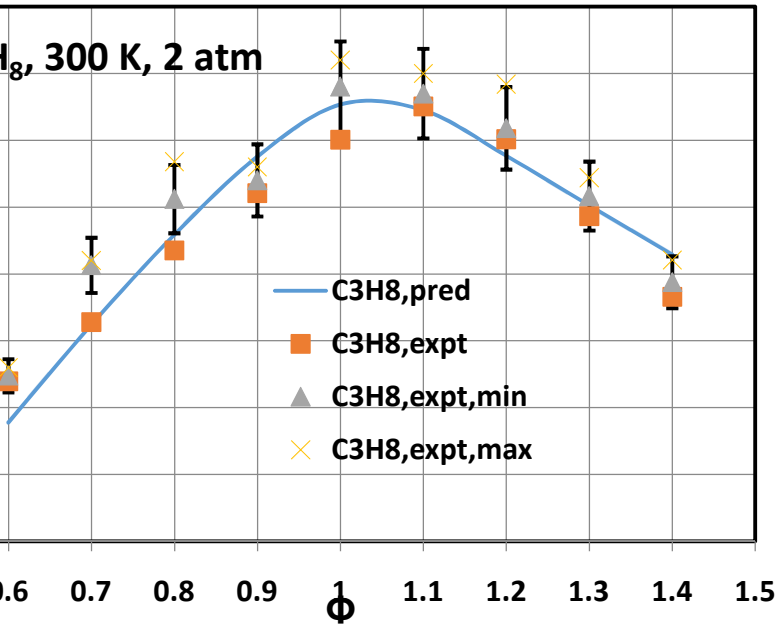
Predictions at higher pressures do not seem good. But the data quality also does not seem good.

Perhaps these measurements have inherent difficulties





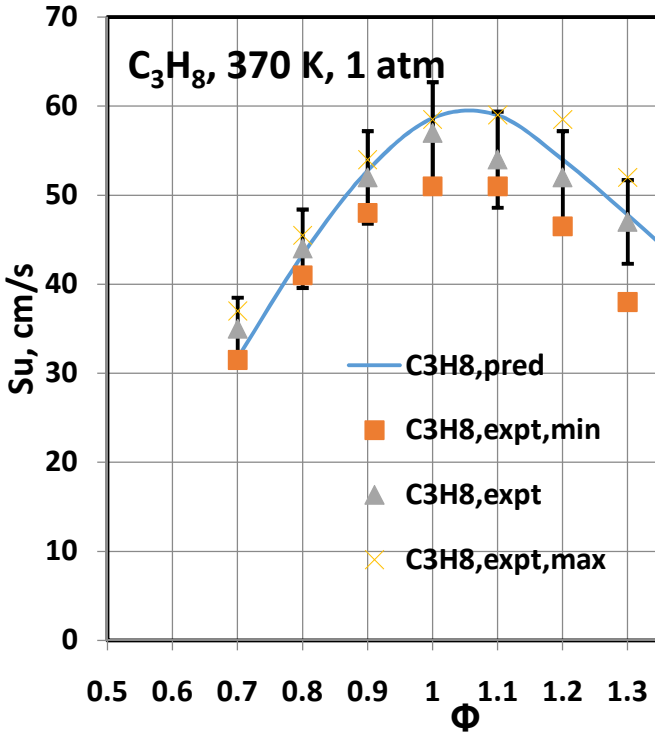


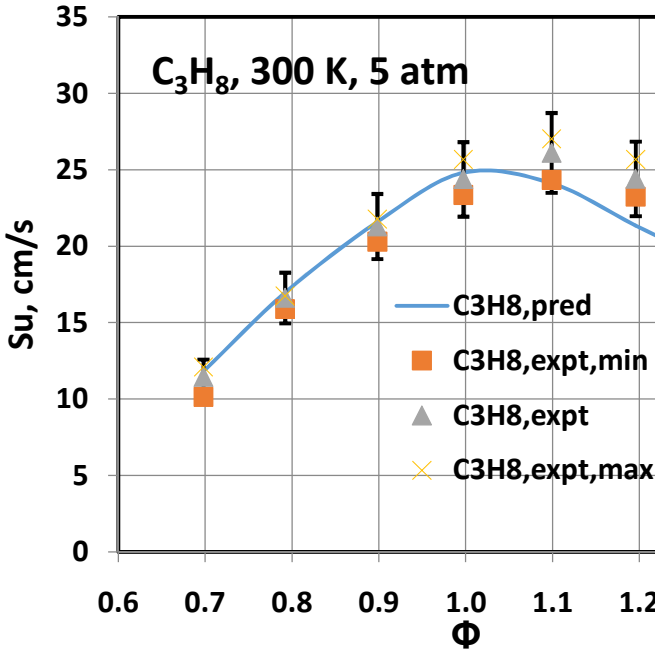


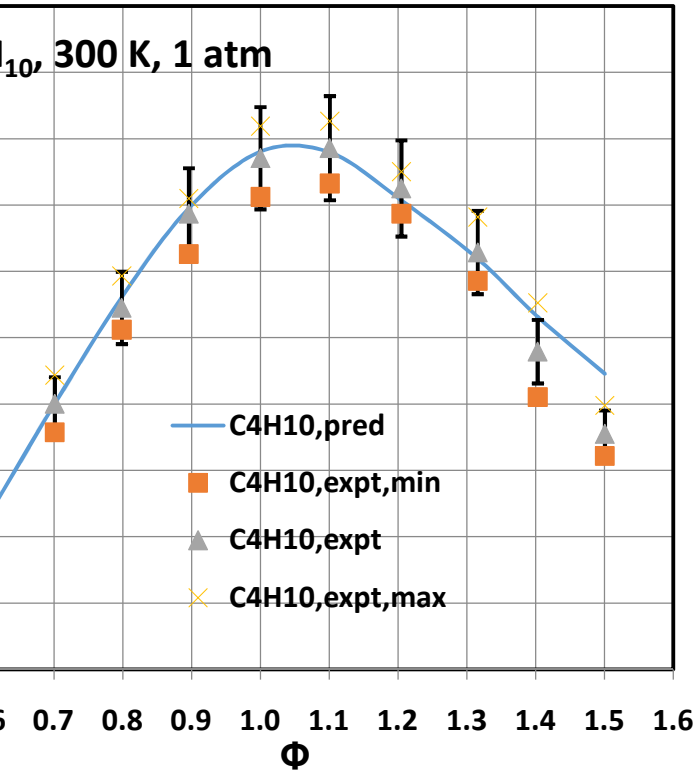
Propane at 300, 370 K, 1 atm

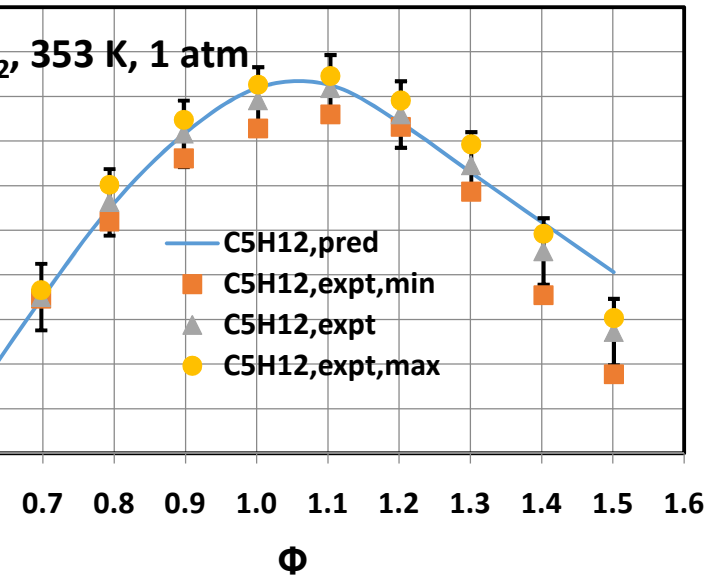
300 K, 2 and 5 atm

Comparisons are satisfactory



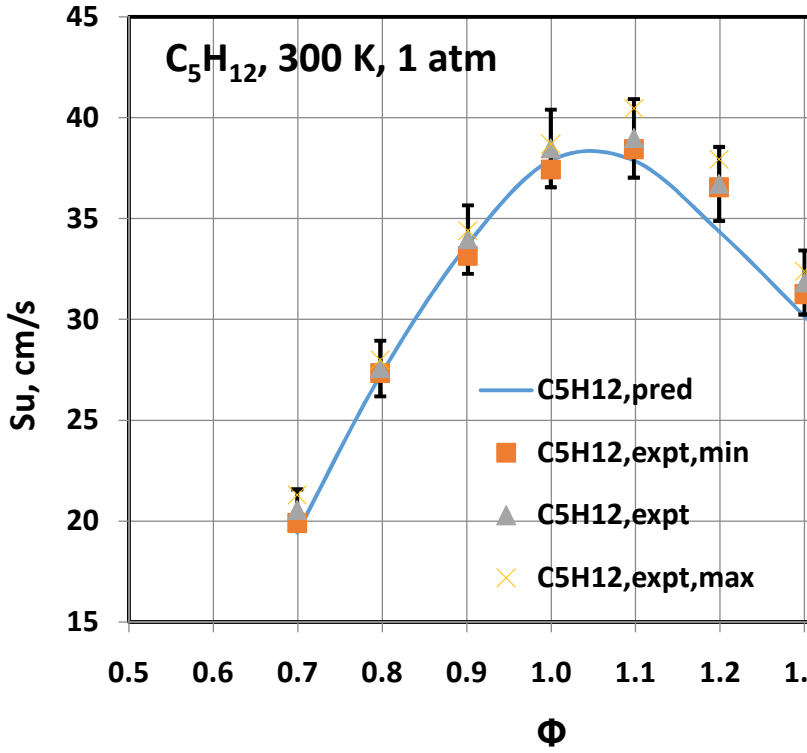


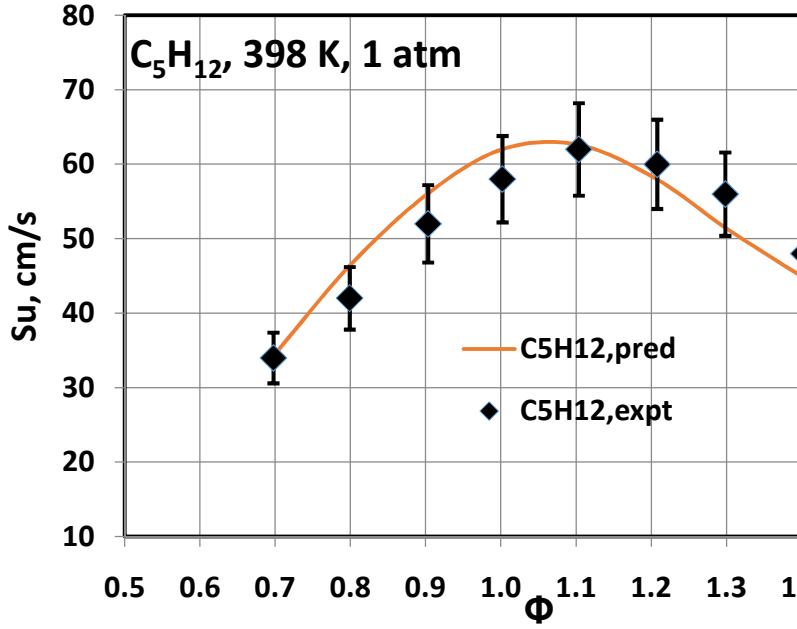


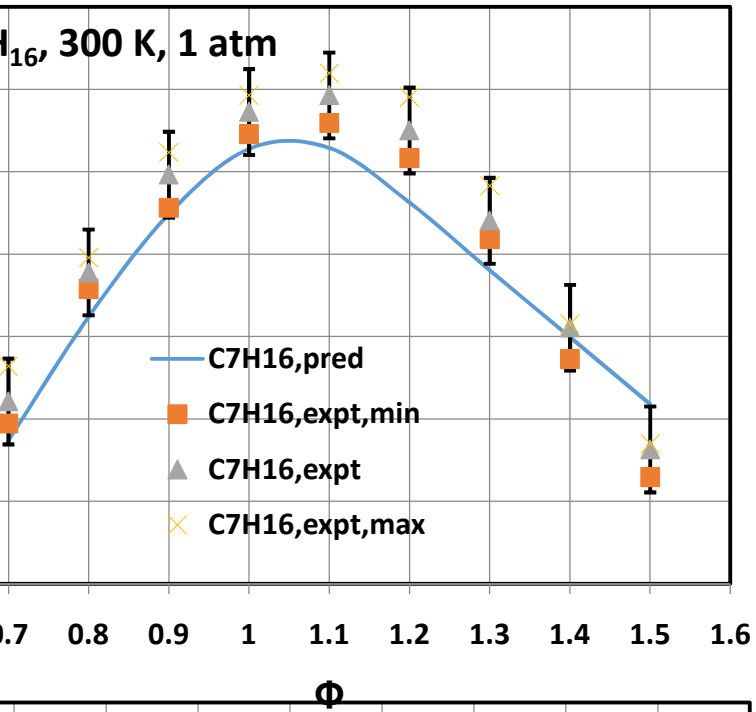


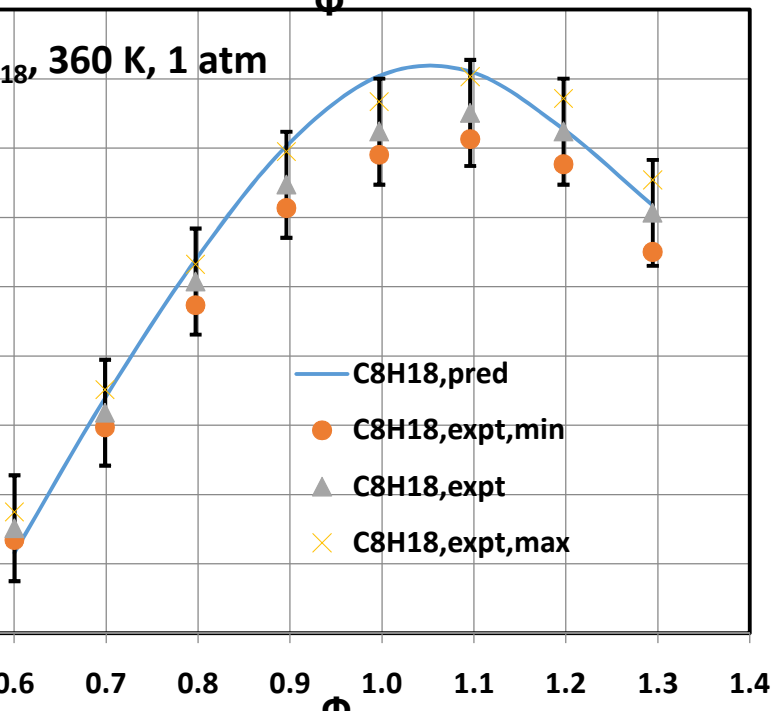
Butane and Pentane at 1 atm different T_{ini}

Comparisons are better at lean conditions Than under rich conditions



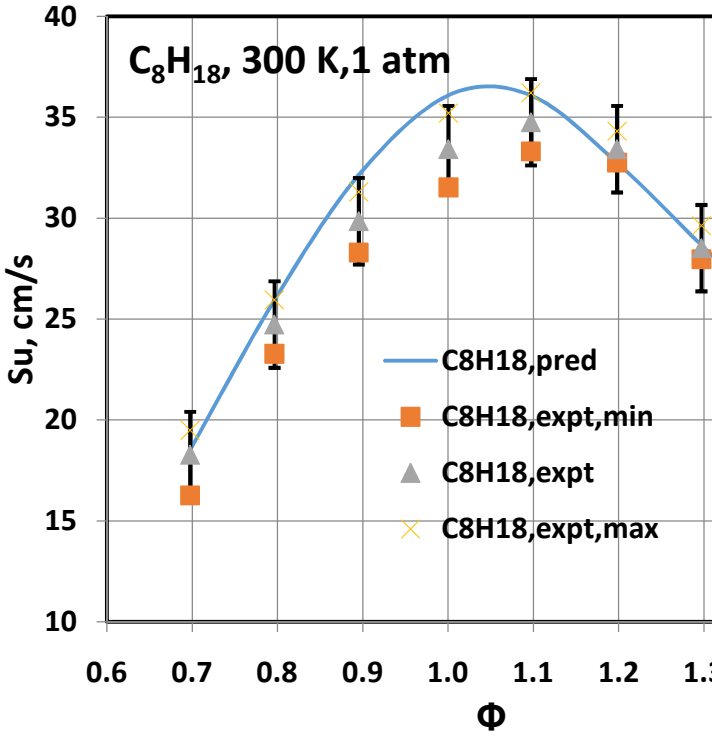


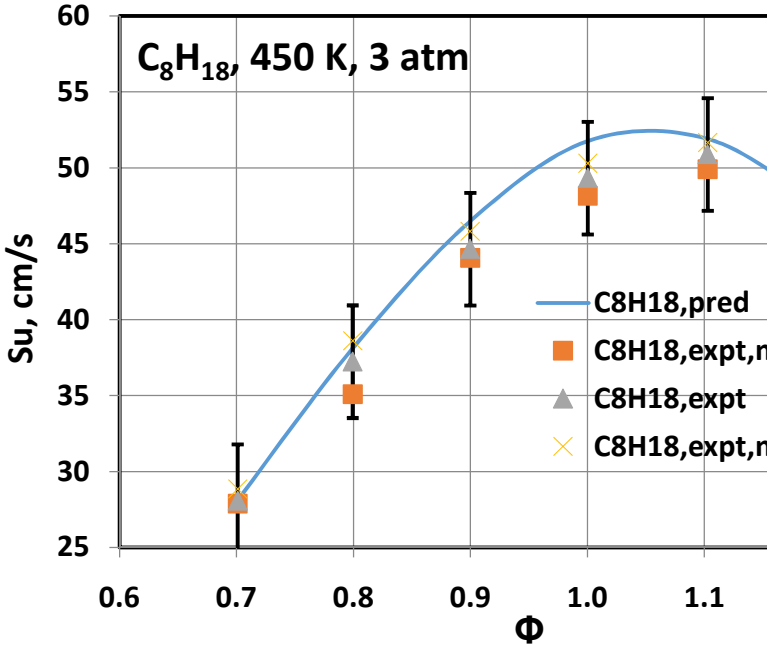


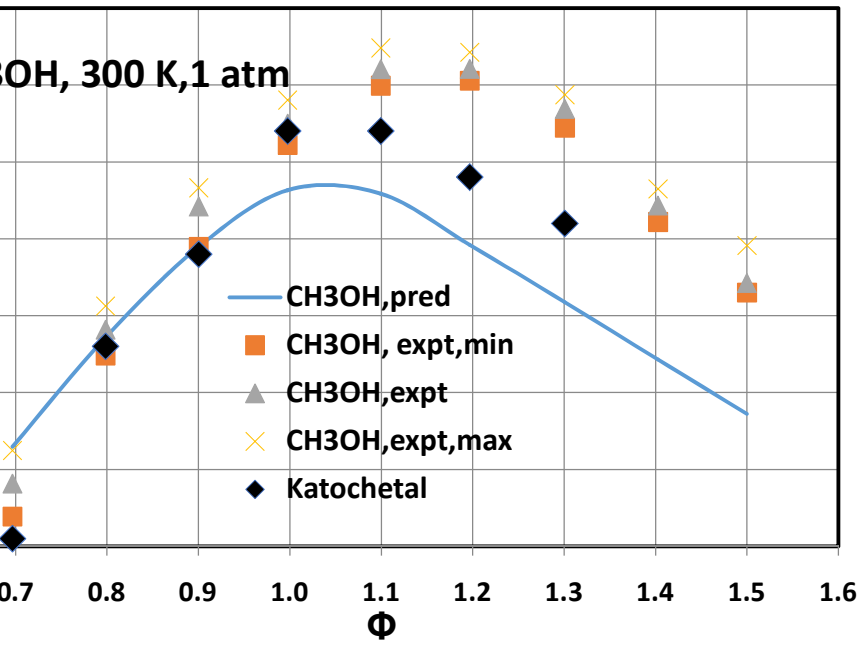


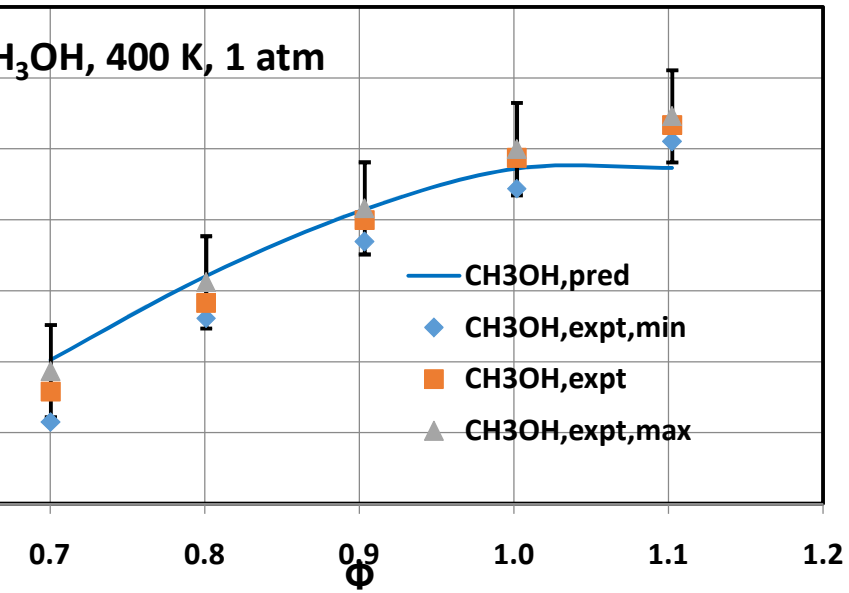
Heptane and Octane at different conditions for which data are set out in Konnov et al

Comparisons reasonable









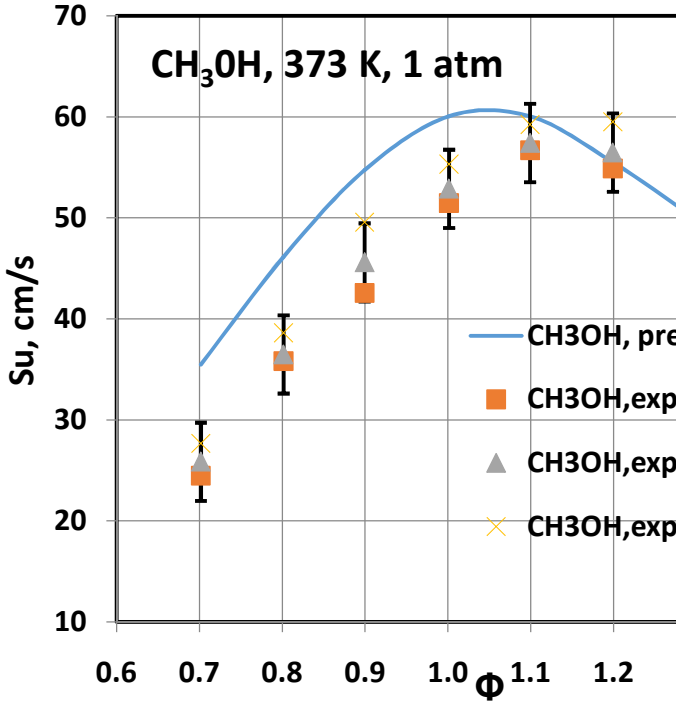
Ethyl Alcohol as extrapolated from Methane seems to behave very differently

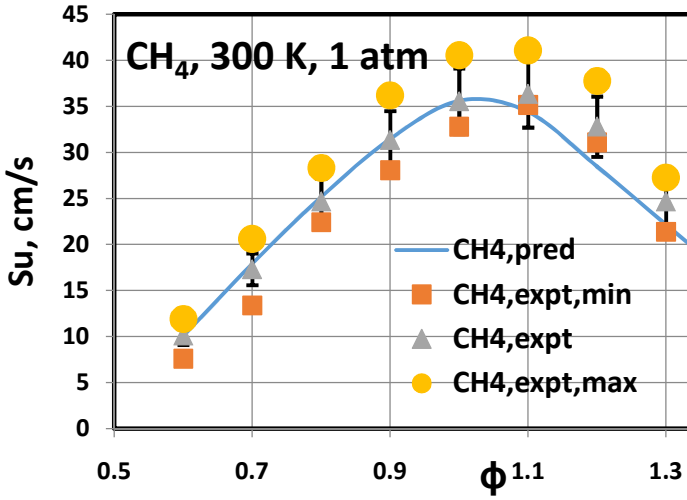
CH_3OH even if treated as related to CH_4 in its combustion behavior with the oxygen atom integrated into the molecule allows higher reaction rates, no simple hypothesis can explain the complex behavior –

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

rimental data are obtained from Li et al, 2016; Wu, et al, 2018; Kannov et al, 2018; hese et al, 2019

clearly noted that the peak in burning velocity occurs at very rich equivalence ratios

means the approach chosen for hydrocarbons seeking relationship with adiabatic flame erature variation alone will not work – because stronger diffusional effects –of H2 come play.

unately, the variation with equivalence ratio alone would be adequate, as is seen to w…….

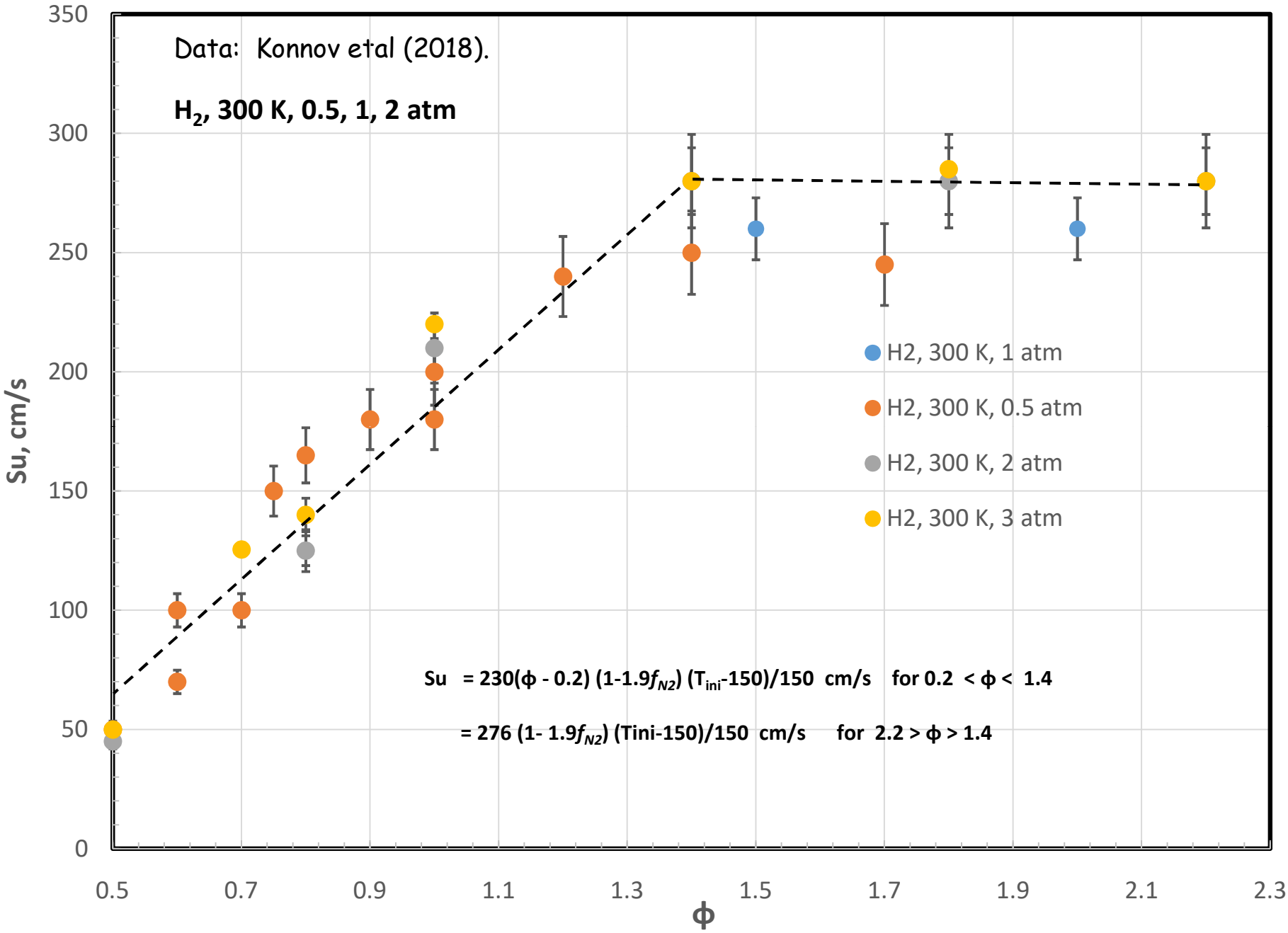
Syngas compositions considered

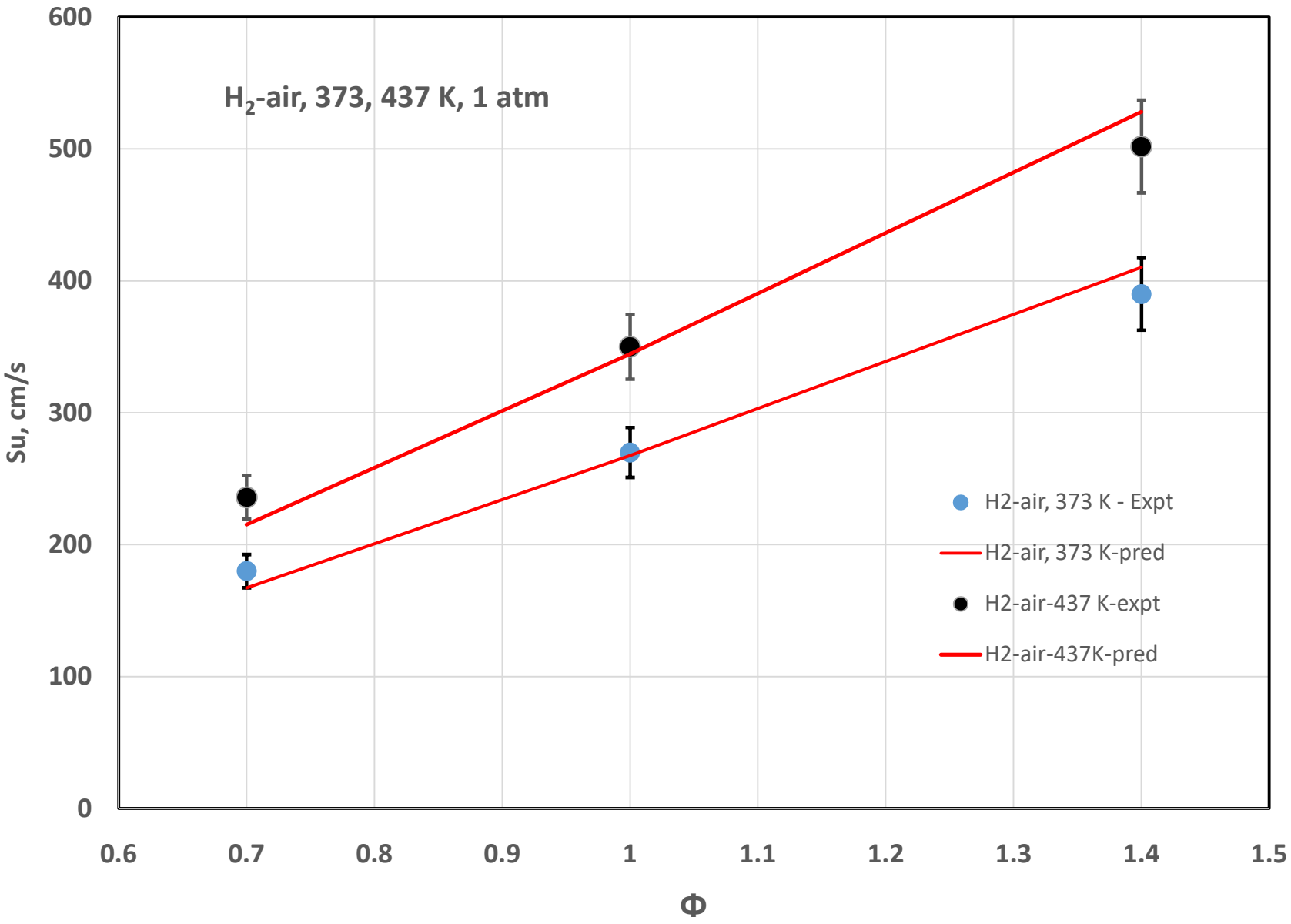
to
cer
rom air
cation
mass

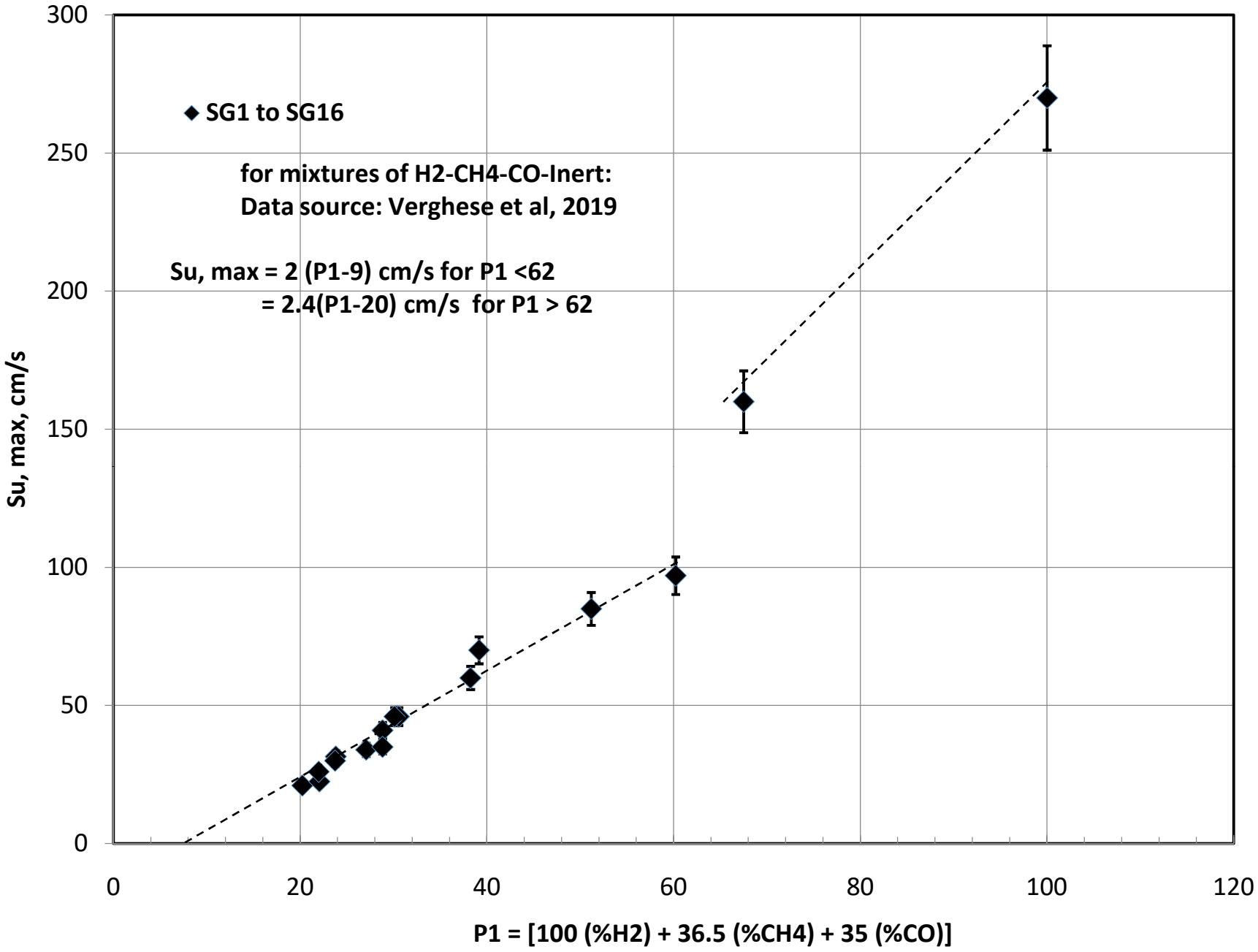
Largely CO

H_2

	CO, % v	H2 % v	CH4, % v	CO2 %v	N2, % v	Mol wt		Sources
SG1	15	15	0	15	55	26.5	21	Verghese et al, 2019
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
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
SG17	0	100	0	0	0	2.0	270	Konnov et al, 2018


Data: Konnov etal (2018).
H2, 300 K, 0.5, 1, 2 atm
H2, 300 K, 1 atm
H2, 300 K, 0.5 atm
H2, 300 K, 2 atm
H2, 300 K, 3 atm
Su = 230(ϕ - 0.2) (1-1.9f_{N2}) (T_{ini}-150)/150 cm/s for 0.2 < ϕ < 1.4
= 276 (1- 1.9f_{N2}) (Tini-150)/150 cm/s for 2.2 > ϕ > 1.4
Su, cm/s
ϕ
0
50
100
150
200
250
300
350
0.5
0.7
0.9
1.1
1.3
1.5
1.7
1.9
2.1
2.3


H2-air, 373, 437 K, 1 atm
Su, cm/s
Φ
600
500
400
300
200
100
0
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
H2-air, 373 K - Expt
H2-air, 373 K-pred
H2-air-437 K-expt
H2-air-437K-pred


SG1 to SG16
for mixtures of H2-CH4-CO-Inert:
Data source: Verghese et al, 2019
Su, max = 2 (P1-9) cm/s for P1 <62
= 2.4(P1-20) cm/s for P1 > 62
Su, max, cm/s
P1 = [100 (%H2) + 36.5 (%CH4) + 35 (%CO)]
0
50
100
150
200
250
300
0
20
40
60
80
100
120

Syngas compositions

oaches have been made for correlating the burning velocity
nich the more successful one is set out here.

ter, P1 is constructed such that it
eatures of summation on mixture composition with
burning velocities

+36.5f_{CH4}+35f_{CO})

2 (P1 - 9) cm/s for P1 <62 up to ϕ = 1.05
2.4 (P1 - 20) cm/s for P1 > 62

= 0.6) = 1.1 (P1-11)

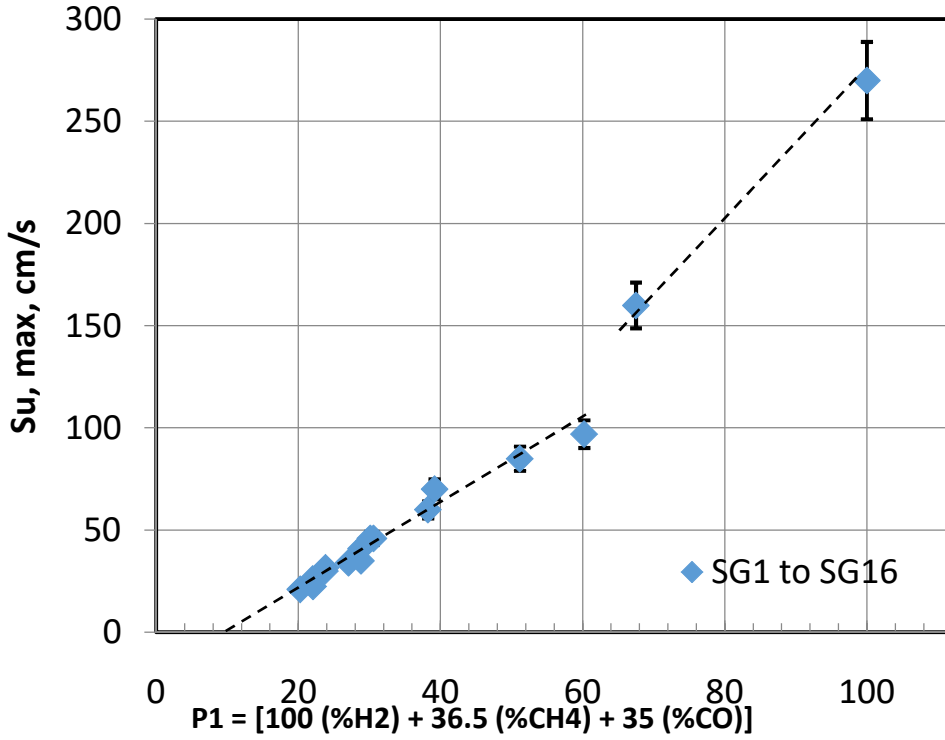
in)/(Su,max – Su,min) = (ϕ – 0.6)/(1.05 – 0.6)

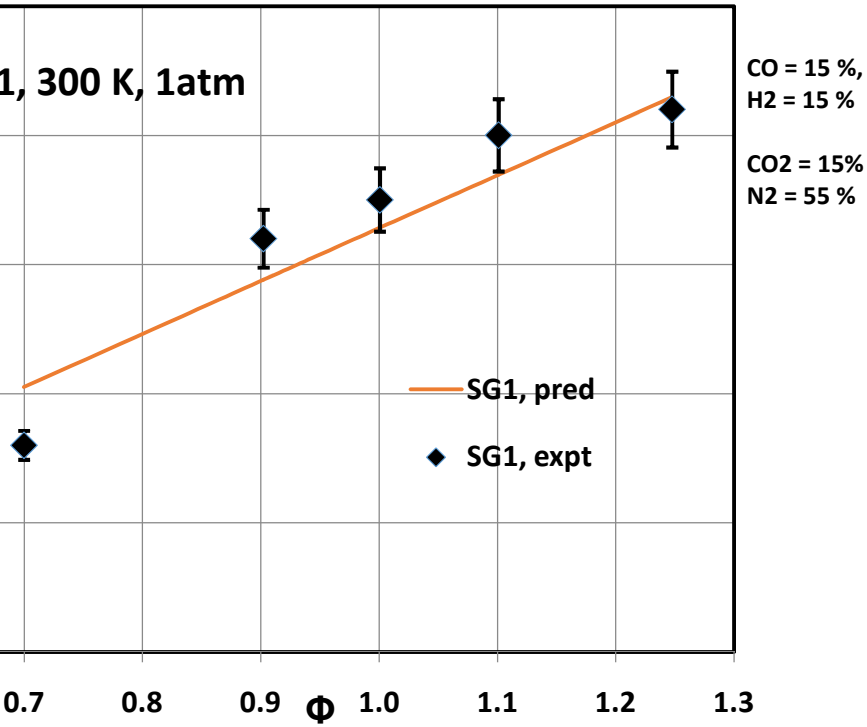
P1 - 11) + (2 P1 - 13) (ϕ - 0.6) for P1 < 62

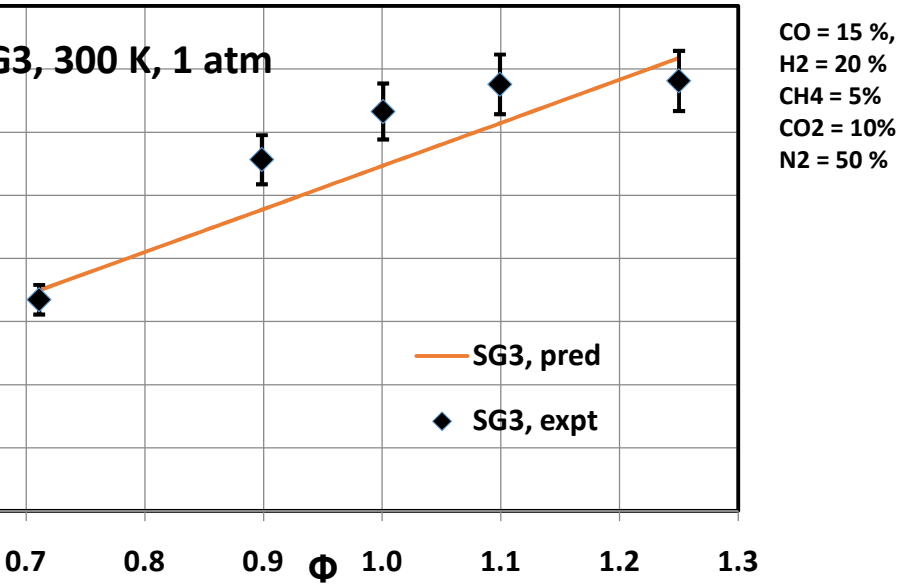
1 - 11) + (2.5 P1 - 50) (ϕ - 0.6) for P1 > 62

re mole fractions of individual species in the
n.

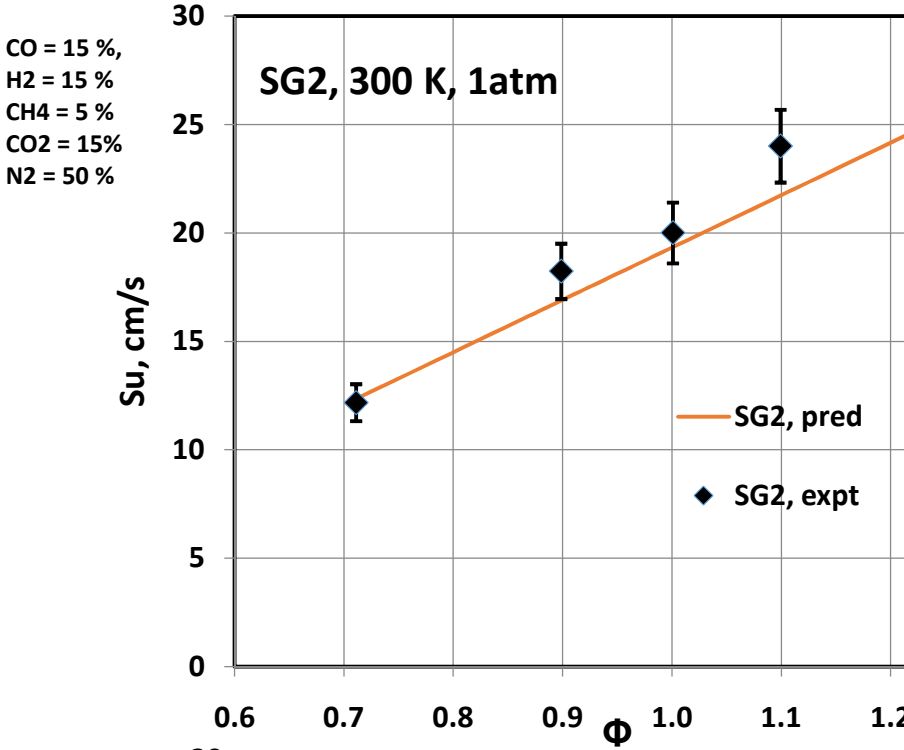
ation does not distinguish between CO_2 and N_2
consistent with experimental data.

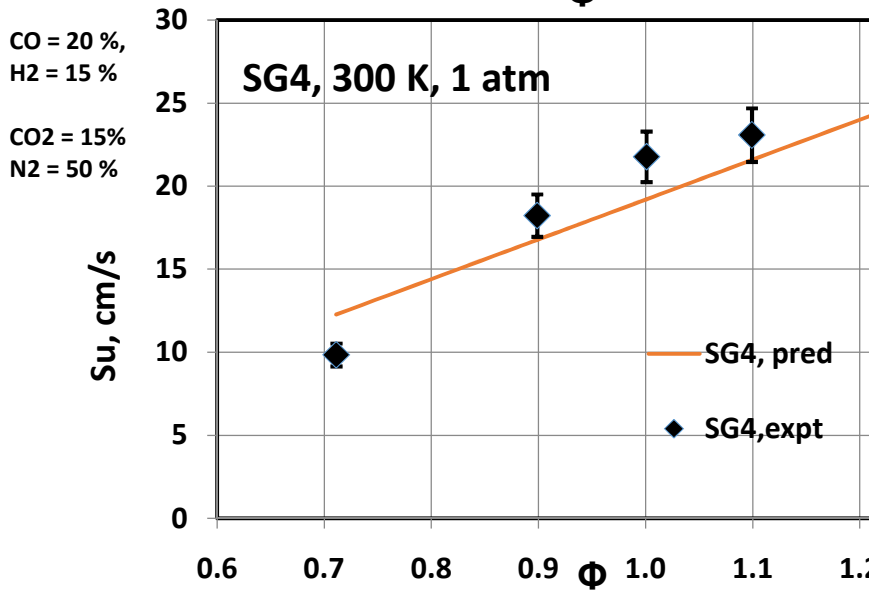


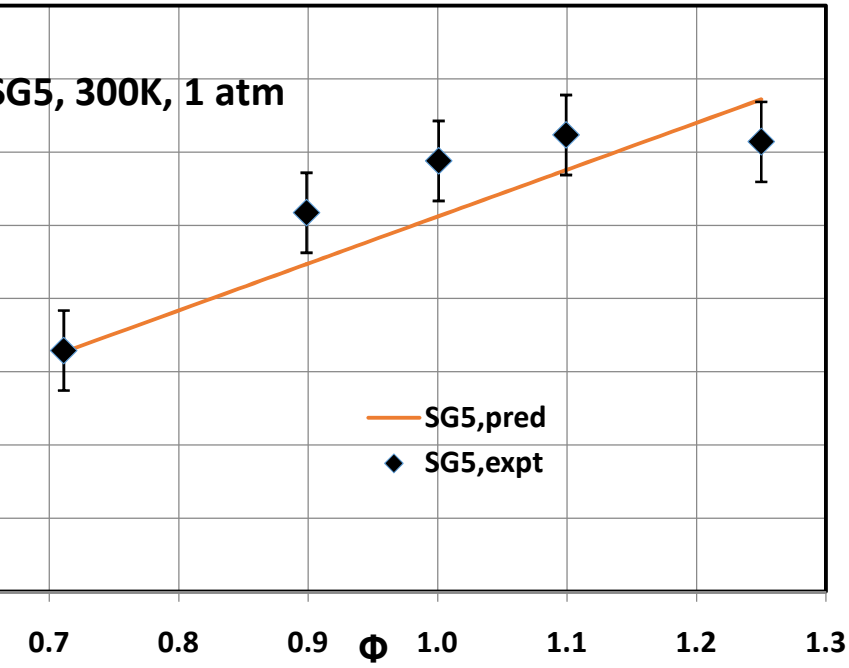




Comparisons appear good.

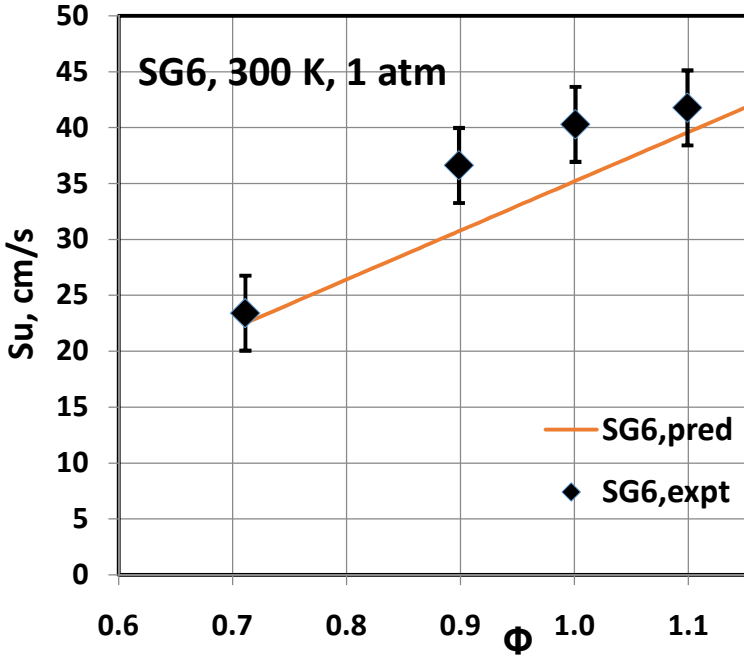


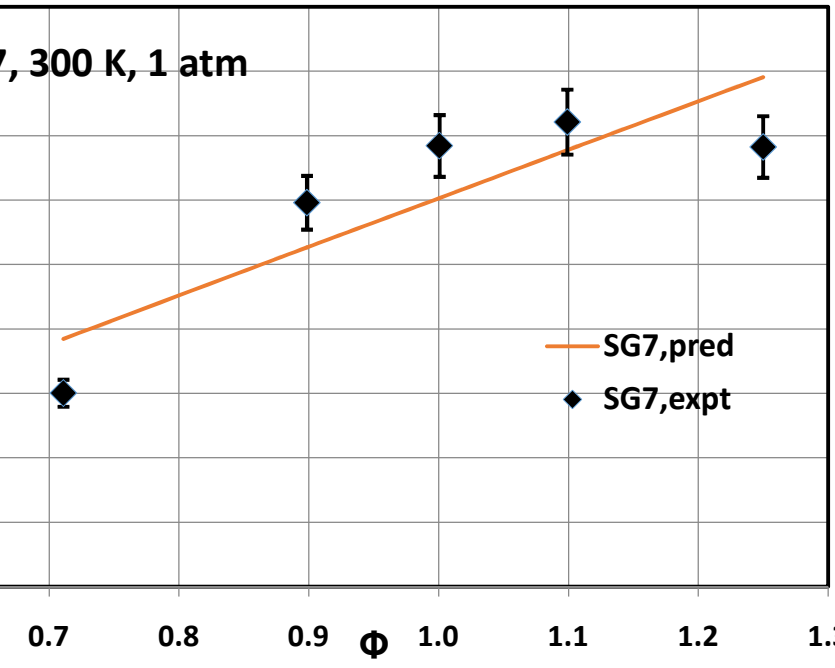




CO = 20 %,
H2 = 15 %
CH4 = 5 %
CO2 = 10%
N2 = 50 %

CO = 20 %,
H2 = 20 %
CH4 = 5 %
CO2 = 10%
N2 = 45 %

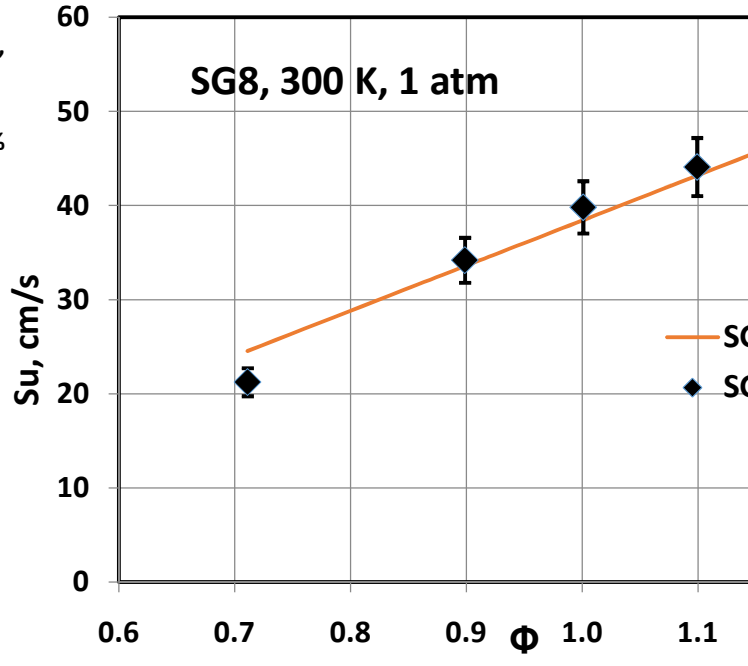


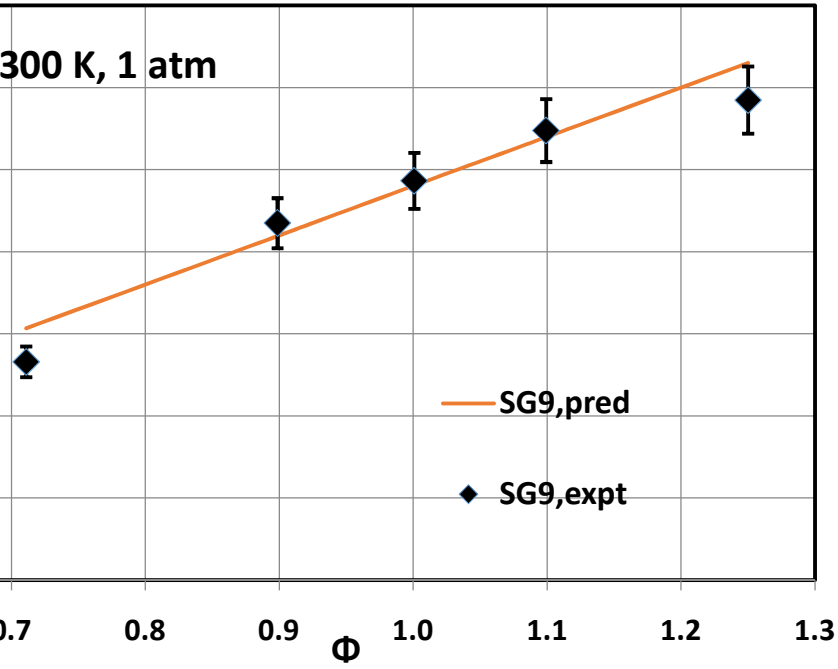


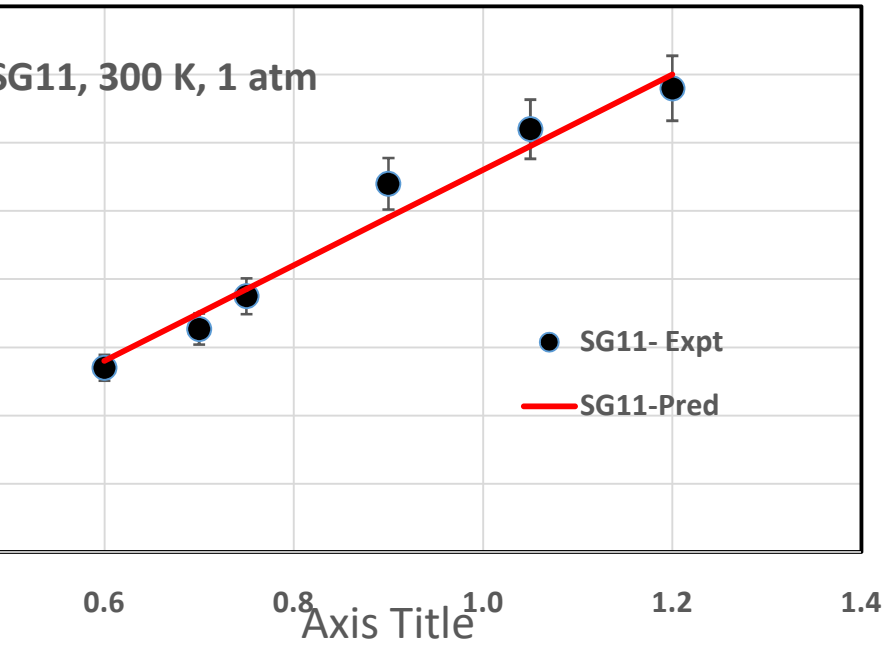
CO = 20 %,
H2 = 20 %
CH4 = 5 %
CO2 = 15%
N2 = 40 %

Comparisons are reasonably good

CO = 25 %,
H2 = 20 %
CH4 = 5 %
CO2 = 10%
N2 = 40 %

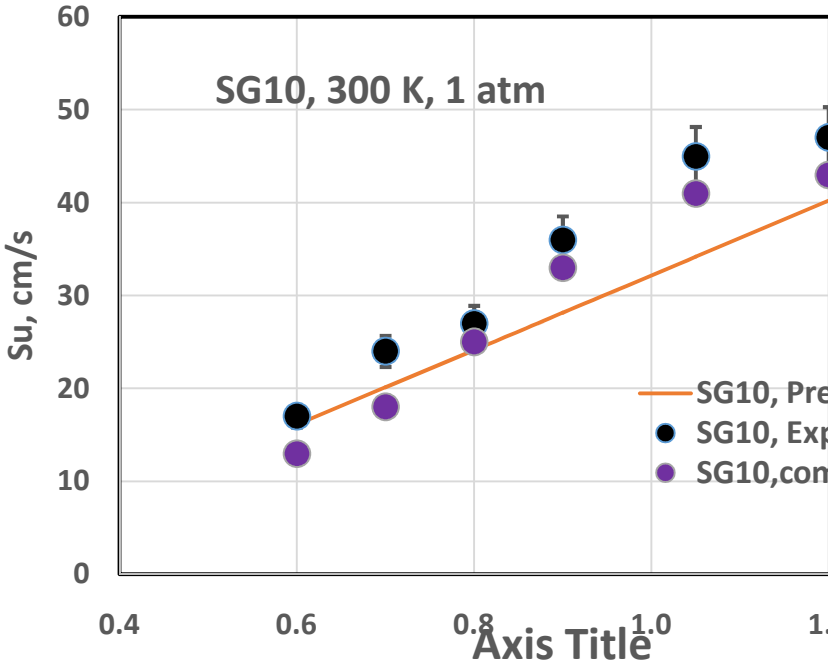


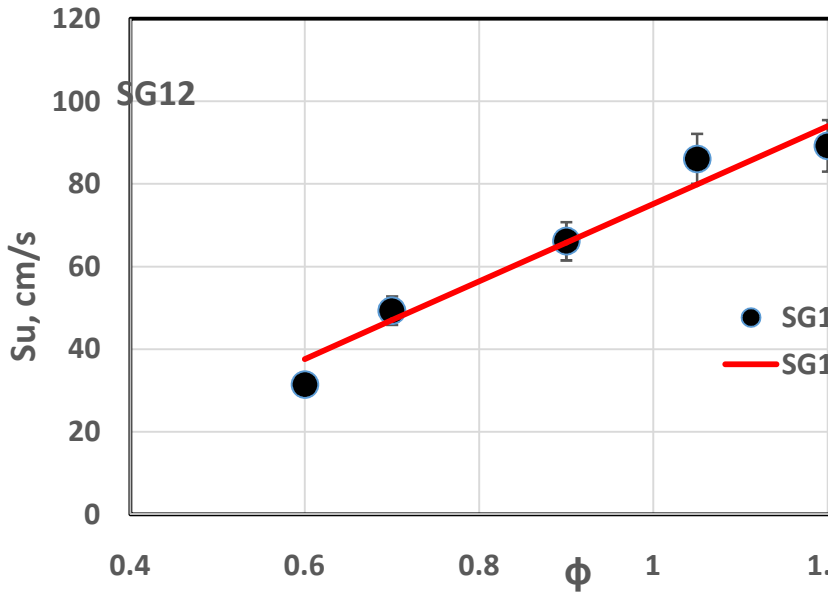


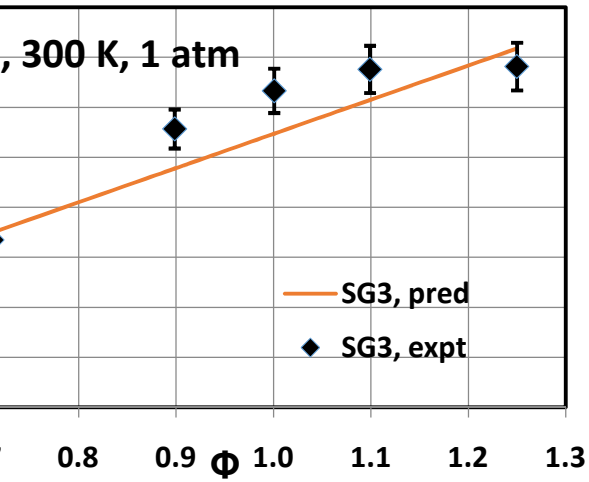


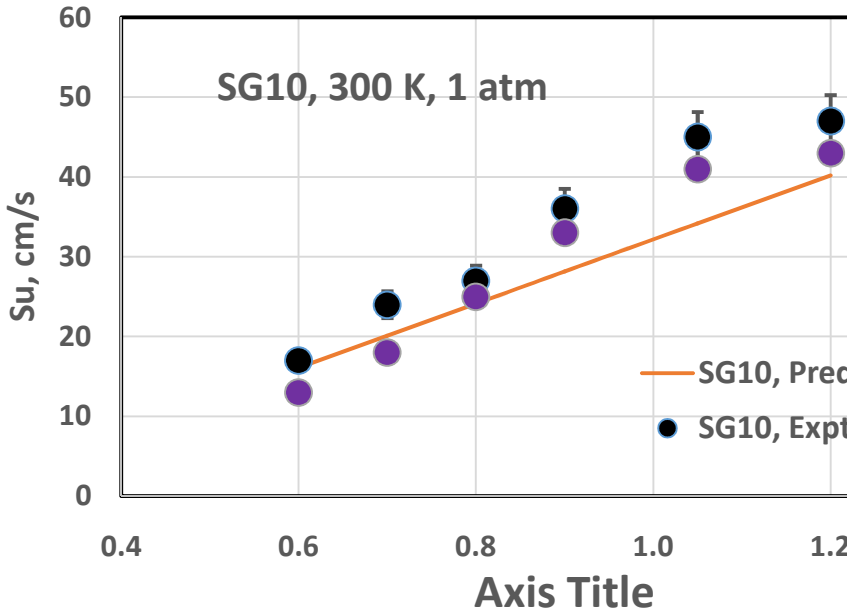
Comparisons are reasonable except for SG10.

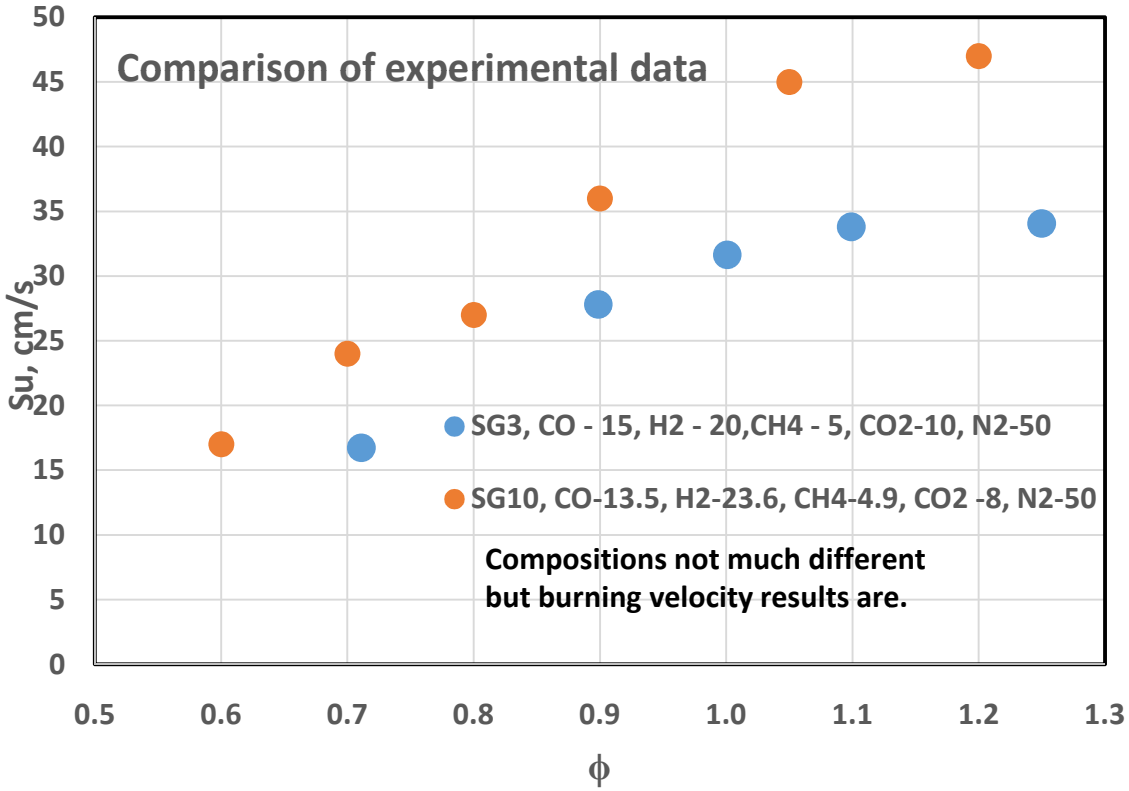
It appears that computational results favor the simpler expectation!





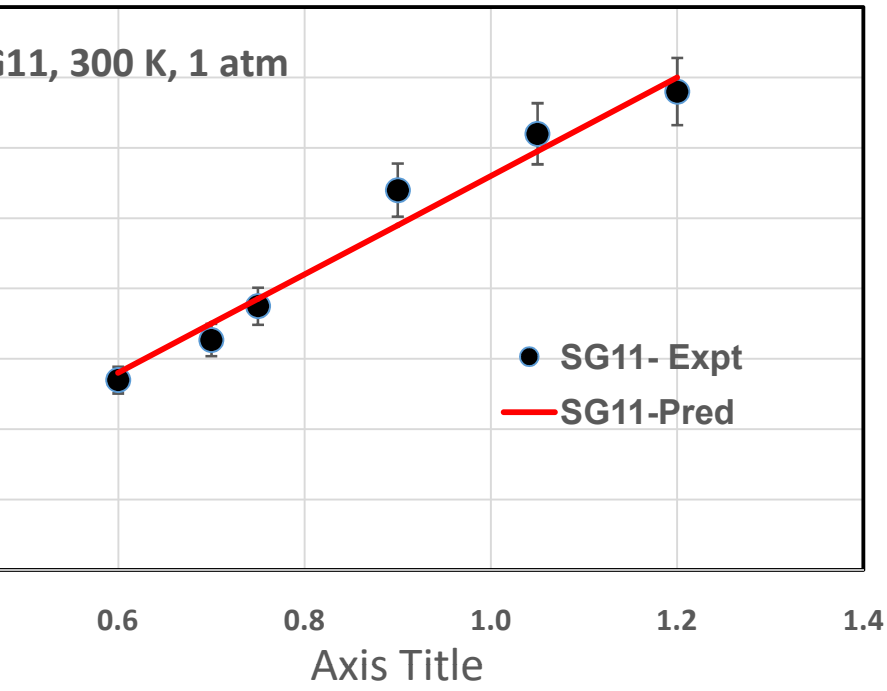




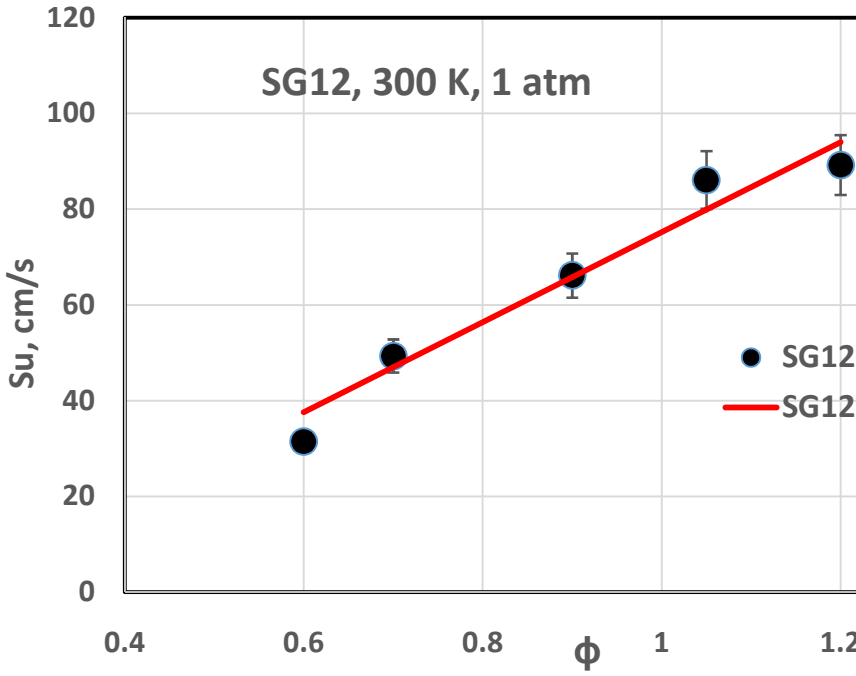


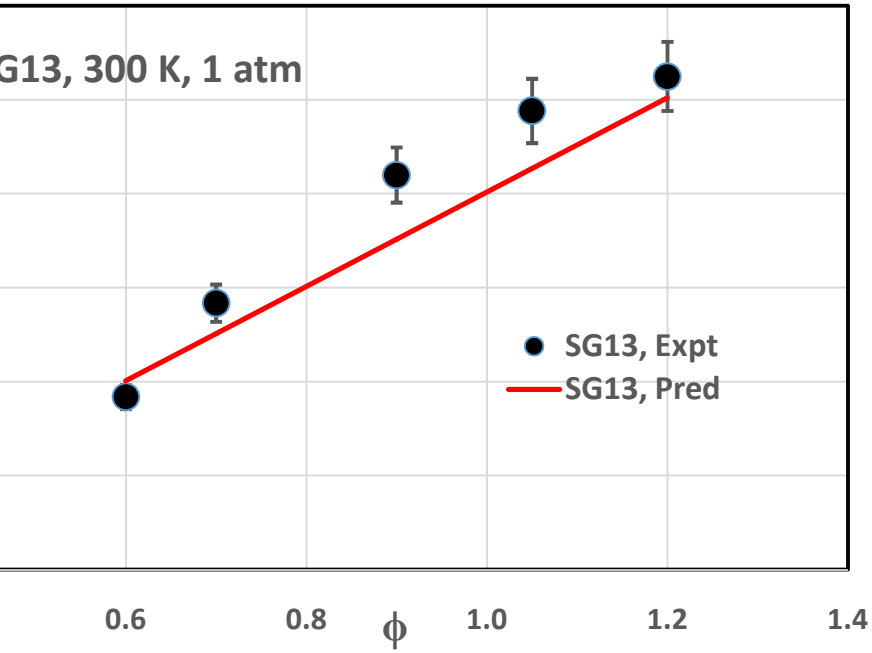
Observation:

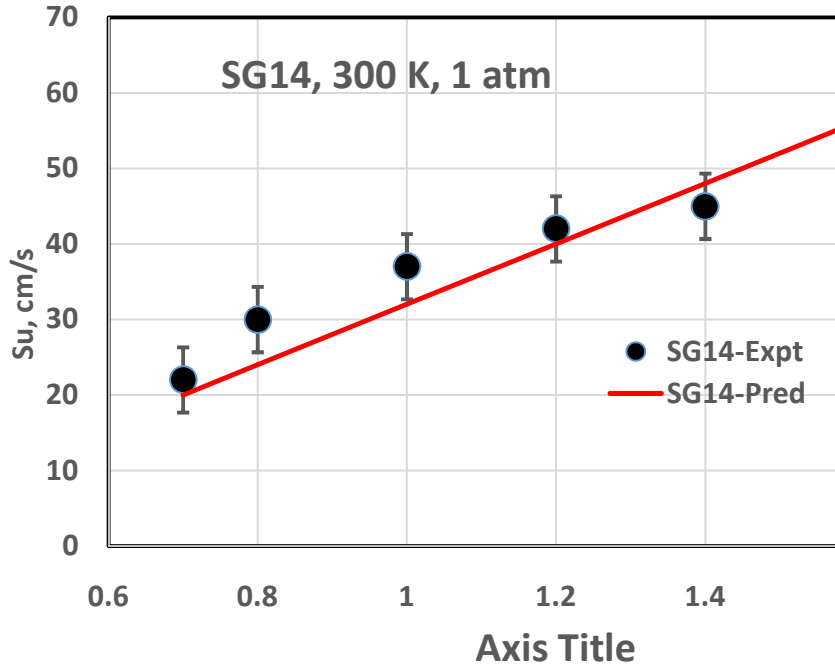
The correlation seems to be able distinguish between close but differently performing compositi

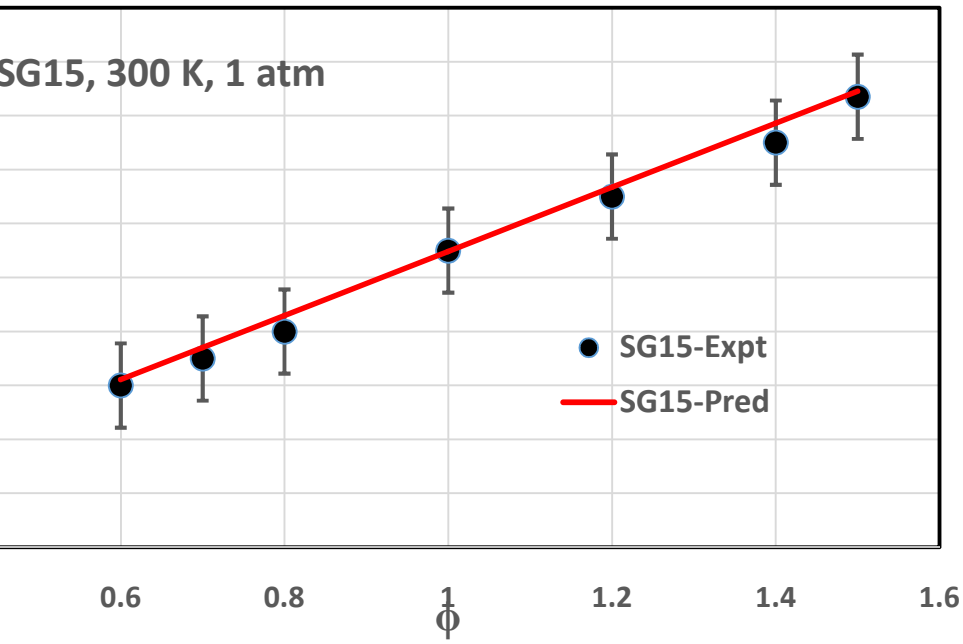


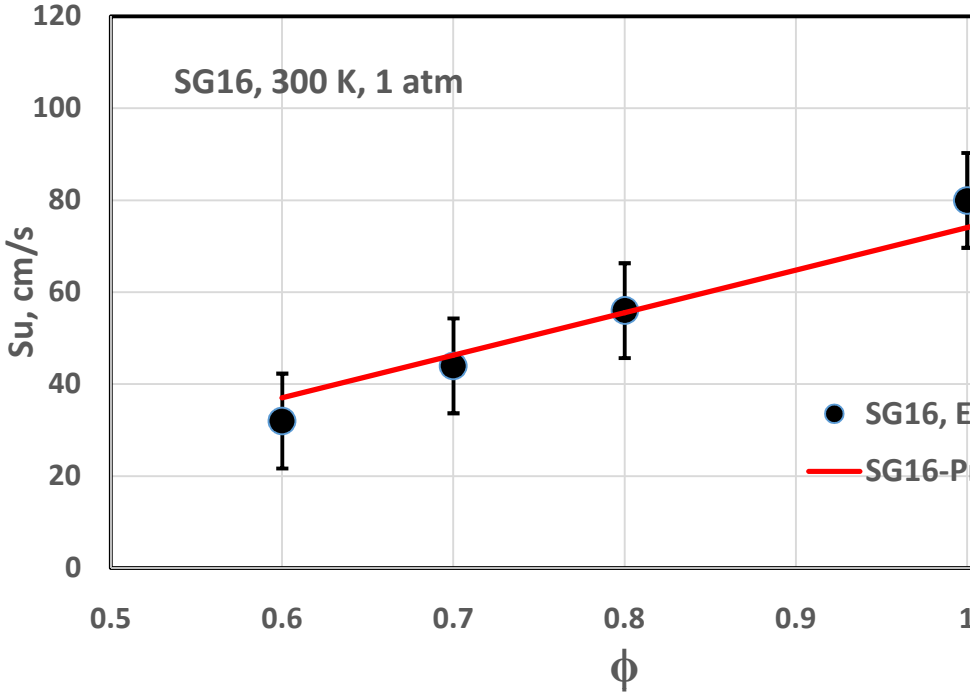
Comparison reasonable





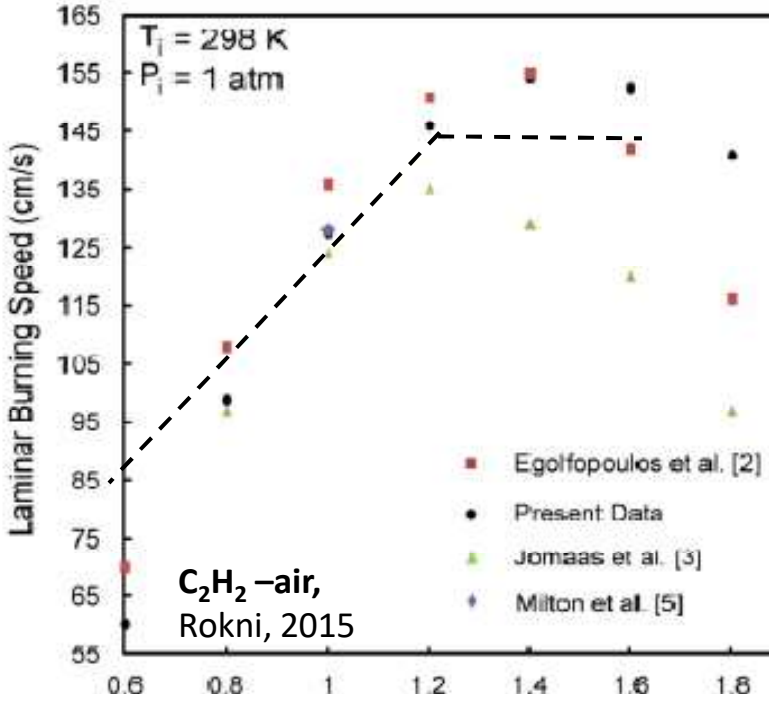




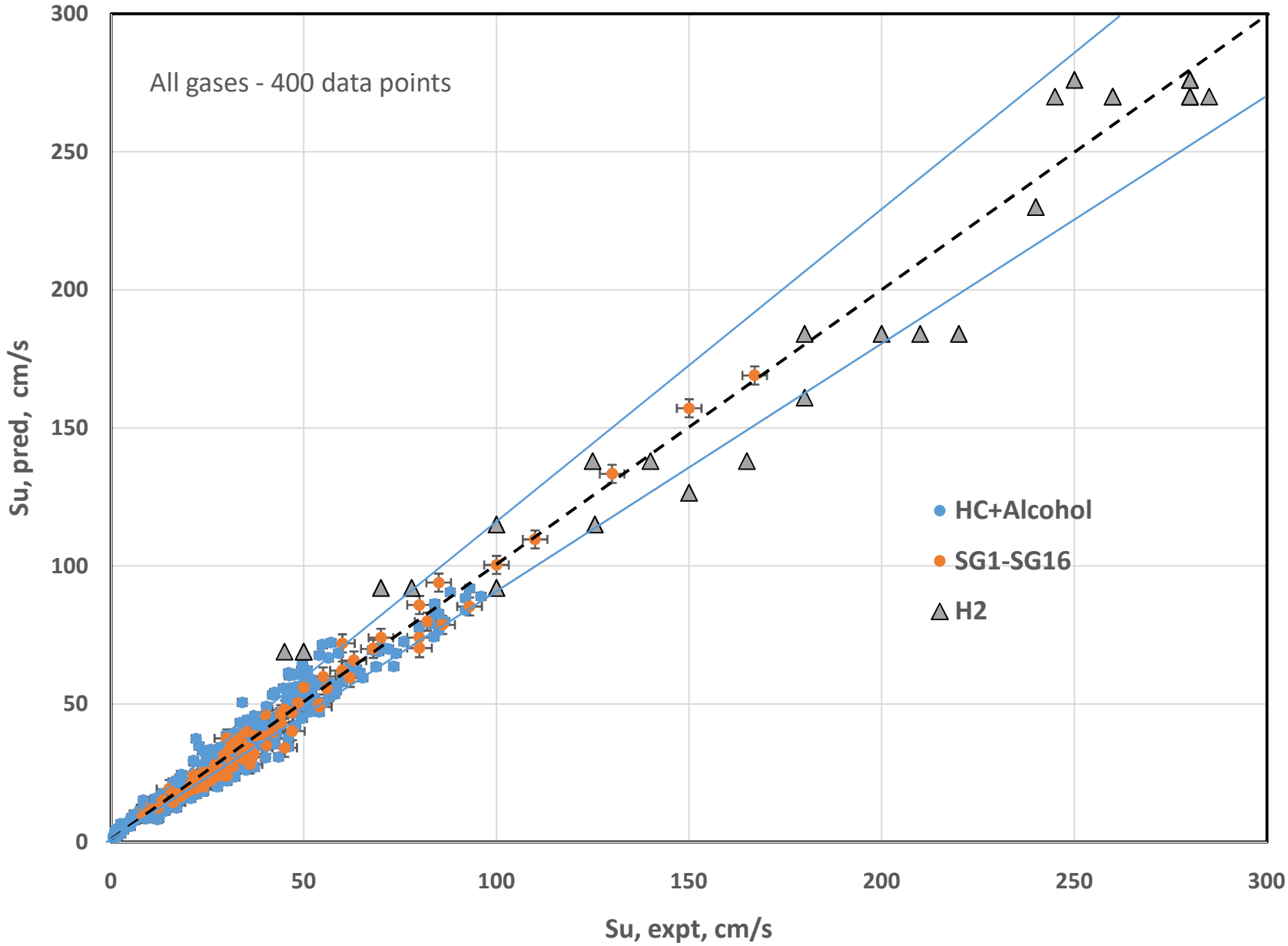


Su (C_2H_2) = 100 ϕ + 25 cm/s, $\phi < 1.2$
= 145 cm/s, $1.8 > \phi > 1.2$

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

emixed flame burning behavior of 45+ compositions of hydrocarbons + alcohols + hydrogen and syngo
ve been considered for study

mplified correlations the burning velocity of hydrocarbons + alcohols and hydrogen and syngas as thr
ts have been attempted.

r hydrocarbons and alcohols for various initial temperatures and pressures (CH_3OH needs more stud

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

r Hydrogen: $Su\ (H_2, cm/s) = 230\ (\phi - 0.2)\ (1-1.9f_{N2})\ (T_{ini}-150)/150$ cm/s for $0.2 < \phi < 1.4$, $= 276\ (1- 1.9f_{N2})\ (Tini-150)/150$ cm/s for 2.

r 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 ϕ =

$Su,min\ (\phi = 0.6) = 1.1\ (P1-11)$

$(Su – Su,min)/(Su,max – Su,min) = (\phi – 0.6)/(1.05 – 0.6)$; 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 com

veral alternate, somewhat more involved correlations did not do as well as the above.

experiments are beset with inaccuracies of measurement, calculations are beset with issues of kine
hemes and other thermochemical details. The final outcome from these efforts do not point to any
em being superior at this stage (accuracies ~ ± 7 to 10 %).

these data are intended for calculating for complex turbulent combusting premixed flows simpler
rrelations may as well do – except close to flammability limits where detailed chemistry matters

References

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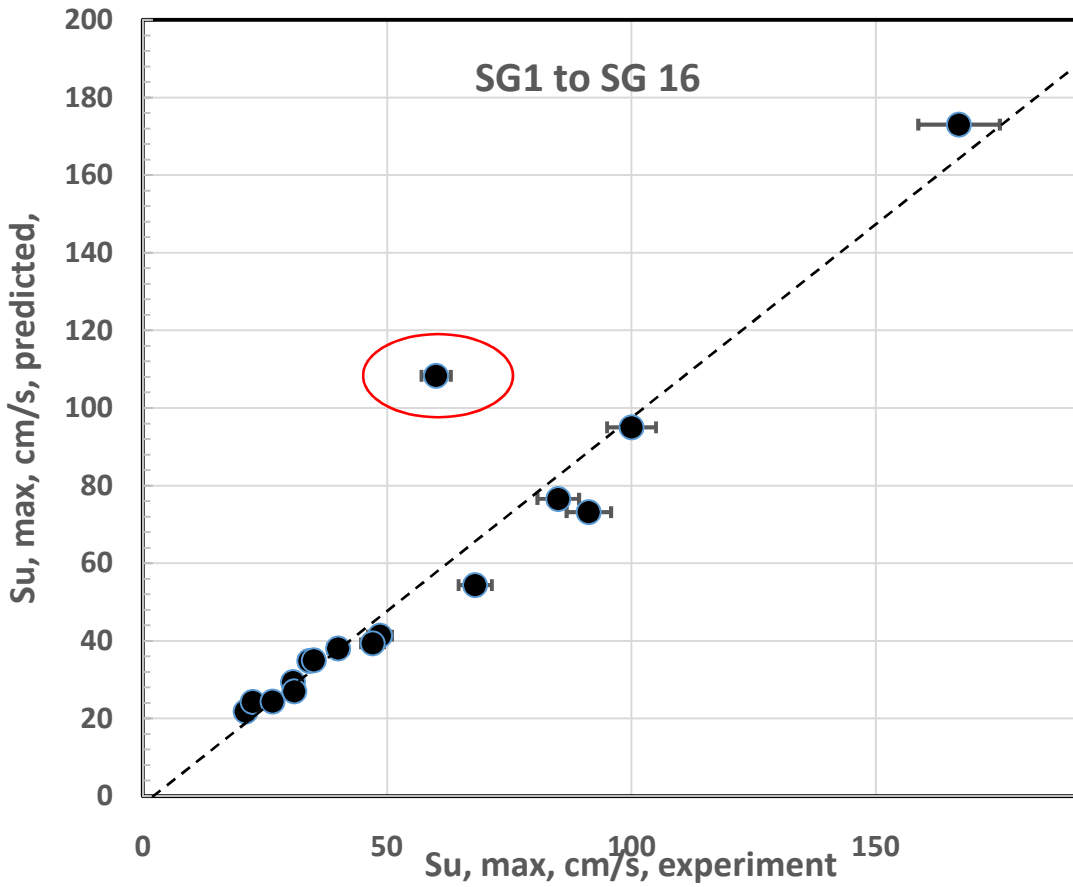
..... Thank yo

Compsn	Expt	Pred
SG1	21.0	21.8
SG2	22.5	24.3
SG3	34.1	34.9
SG4	26.5	24.4
SG5	30.7	29.4
SG6	40.0	38.0
SG7	35.0	35.0
SG8	48.5	41.3
SG9	31.0	27.1
SG10	47.0	39.4
SG11	68.0	54.4
SG12	85.0	76.6
SG13	100.0	95.0
SG14	60.0	115.3
SG15	167.0	181.3
SG16	91.3	73.2



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.

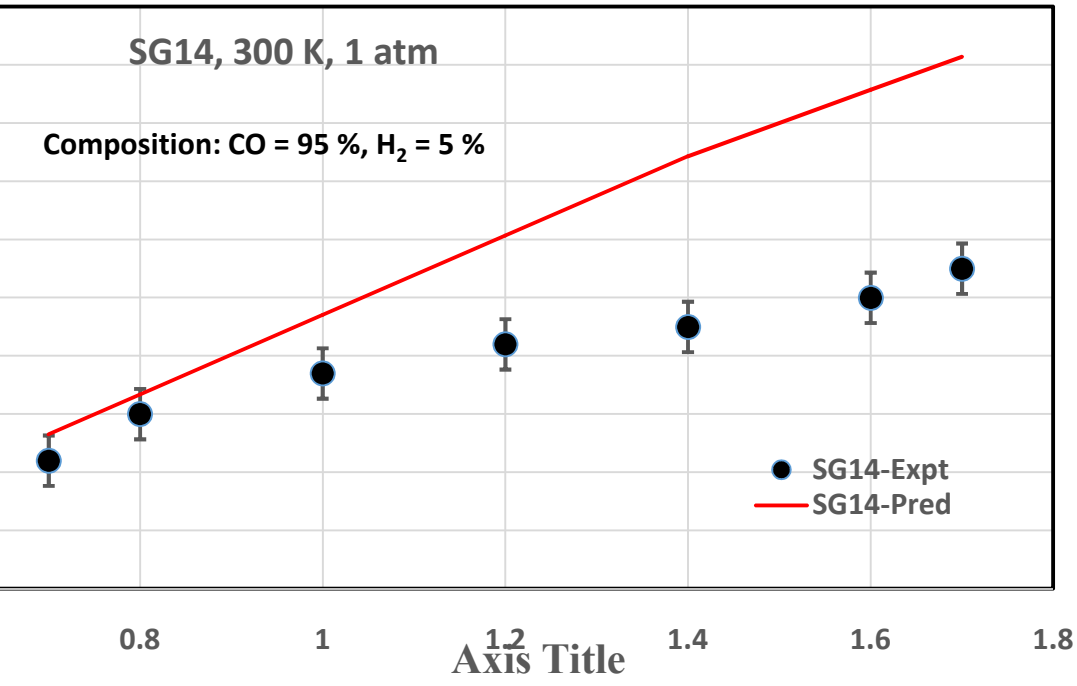
Su (H_2) = 225 (ϕ - 0.2) (T_{ini}-150)/150, for ϕ < 1.4, 270 (T_{ini}-150)/150 f_{H2} for all ϕ > 1.4

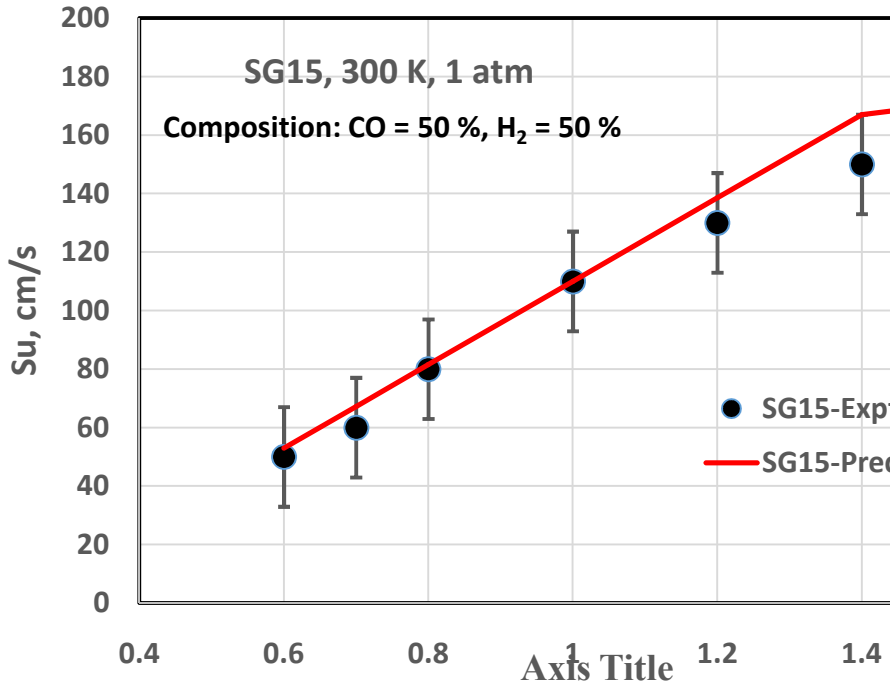
Su(CH_4) = 36.5*(1.71ϕ-0.71) (Tini-150)/150 for ϕ < 1.0

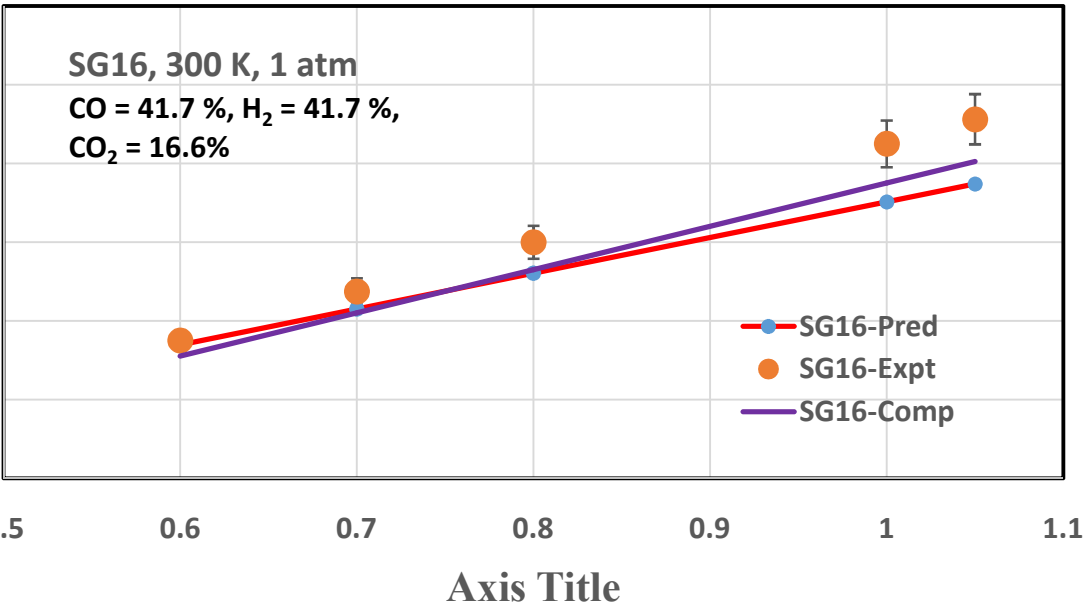
Su(CO) = 60 (ϕ –0.33) (Tini-150)/150 f_{CO} for ϕ < 1.0

Su = [Su (H_2) f_{H2} + Su(CH_4) f_{CH4} + Su(CO) f_{CO}] (1-1.3 f_{CO2}-0.45 f_{N2}) for ϕ < 1

where f_i's are mole fractions of individual species







The poor comparison of composition SG14 cann
understood because any simple modification is
inconsistent with some good comparisons like o

For SG16, it appears that computational result
compare better with simple predictions compar
experiments. CO has been known to burn very
without H_2O (moisture); $CO + OH \longrightarrow CO_2 +$ H
supposedly the most dominant reaction.

CO problem remains to be resolved.