Flame speed: What do we need to measure for practical applications?

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Invited lecture to Workshop on Laminar Burning Velocities:
"New perspectives, Methods, and Applications"
Lisbon April 14, 2019)

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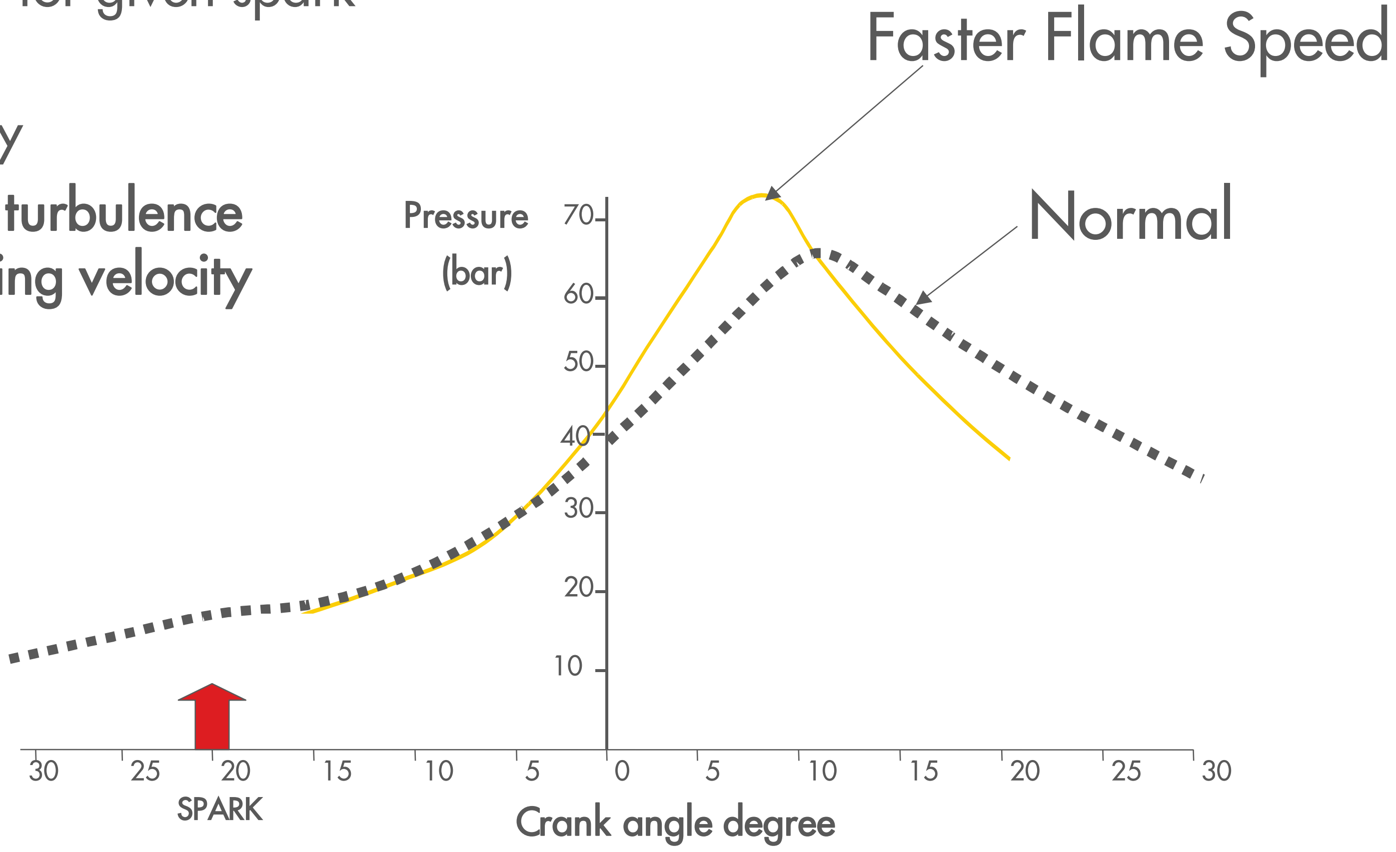
This presentation contains data and analysis from Shell's new Sky Scenario. Unlike Shell's previously published Mountains and Oceans exploratory scenarios, the Sky Scenario is targeted through the assumption that society reaches the Paris Agreement's goal of holding global average temperatures to well below 2°C. Unlike Shell's Mountains and Oceans scenarios which unfolded in an open-ended way based upon plausible assumptions and quantifications, the Sky Scenario was specifically designed to reach the Paris Agreement's goal in a technically possible manner. These scenarios are a part of an ongoing process used in Shell for over 40 years to challenge executives' perspectives on the future business environment. They are designed to stretch management to consider even events that may only be remotely possible. Scenarios, therefore, are not intended to be predictions of likely future events or outcomes and investors should not rely on them when making an investment decision with regard to Royal Dutch Shell plc securities.

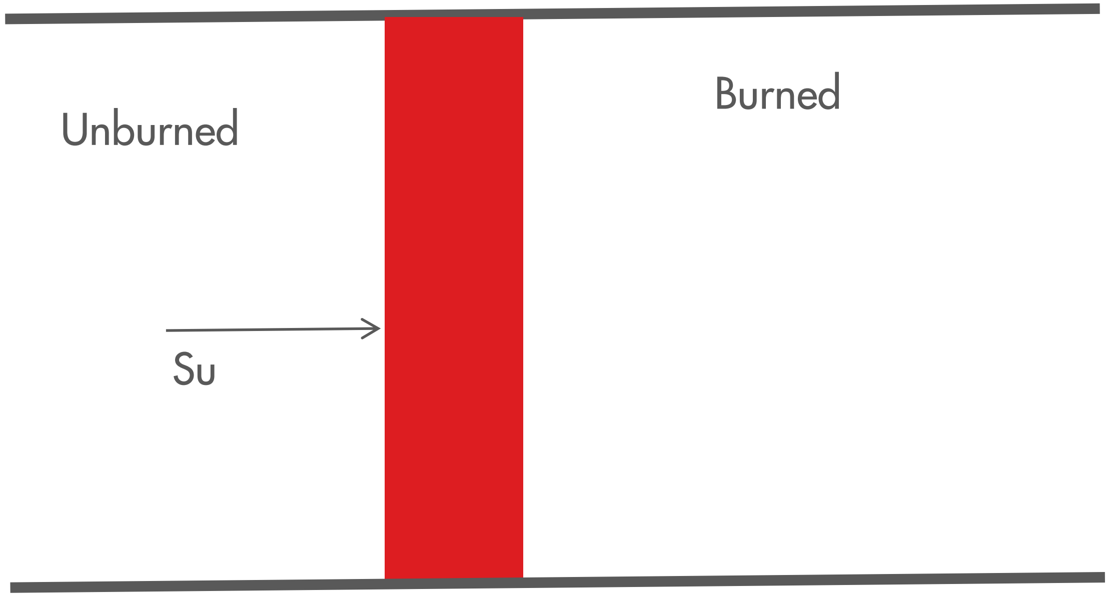
Additionally, it is important to note that Shell's existing portfolio has been decades in development. While we believe our portfolio is resilient under a wide range of outlooks, including the IEA's 450 scenario (World Energy Outlook 2016), it includes assets across a spectrum of energy intensities including some with above-average intensity. While we seek to enhance our operations' average energy intensity through both the development of new projects and divestments, we have no immediate plans to move to a net-zero emissions portfolio over our investment horizon of 10-20 years. Although, we have no immediate plans to move to a net-zero emissions portfolio, in November of 2017, we announced our ambition to reduce our net carbon footprint in accordance with society's implementation of the Paris Agreement's goal of holding global average temperature to well below 2°C above pre industrial levels. Accordingly, assuming society aligns itself with the Paris Agreement's goals, we aim to reduce our net carbon footprint, which includes not only our direct and indirect carbon emissions, associated with producing the energy products which we sell, but also our customers' emissions from their use of the energy products that we sell, by 20% in 2035 and by 50% in 2050.

FASTER FLAME SPEED IN A SI ENGINE

- Decreases burn duration
- Increases P_{max}
- Earlier pressure rise and CA50 for given spark timing.
- Can lead to improved efficiency
- **Strongly influenced by engine turbulence levels as well as laminar burning velocity**



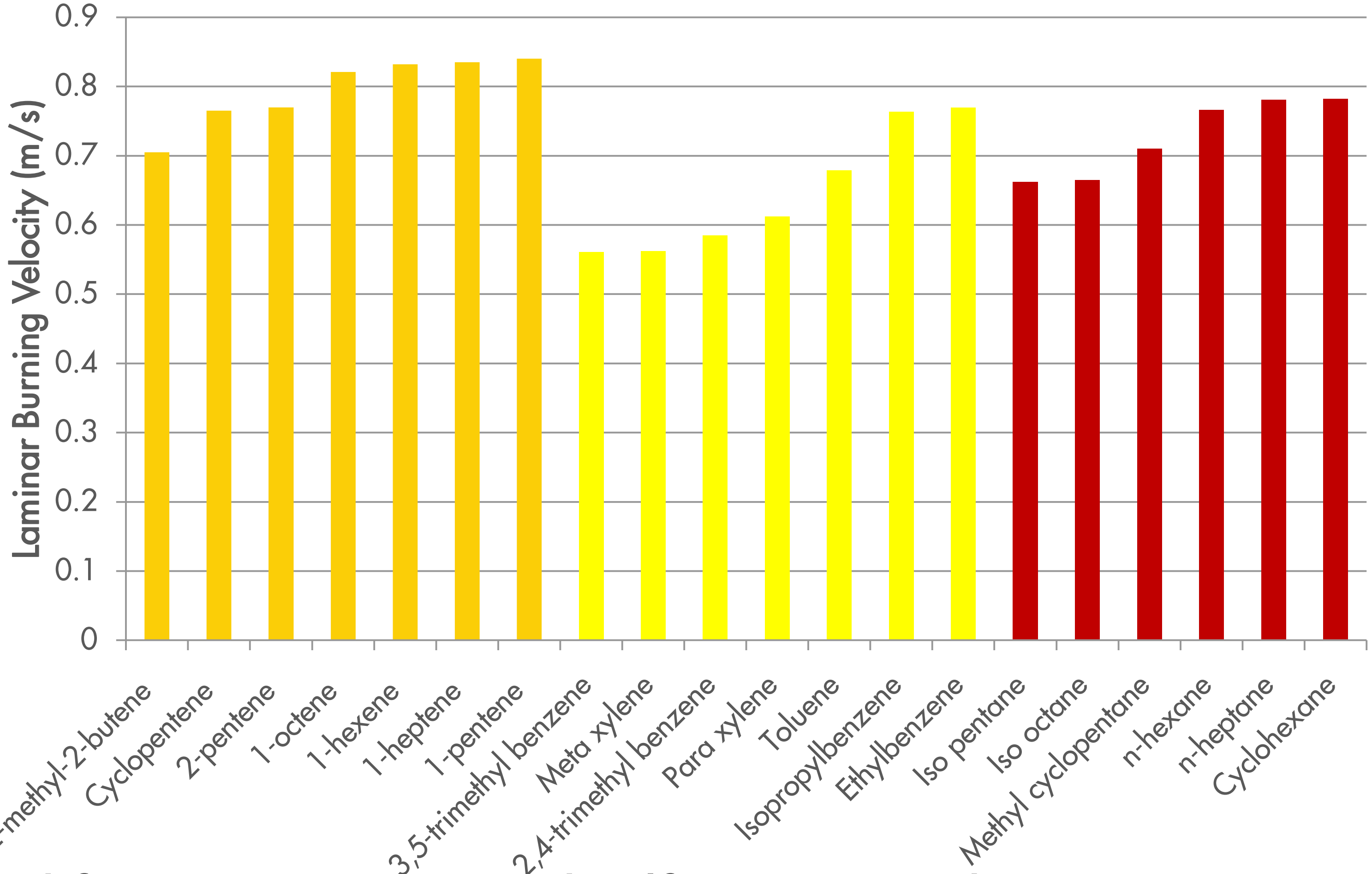
LAMINAR BURNING VELOCITY – A THEORETICAL CONCEPT



(Unstretched) Laminar Burning Velocity is the velocity, relative and normal to the surface of the flame front with which the reactants move into this front and are converted in to products.

- Laminar Burning Velocity typically increases with T and decreases with p
- Typically $S_u \propto T^{1.9} \; p^{-0.2}$ (Marshall et al: Comb. Flame 158 (2011) 1920)
- Desire for a correlation in range 20 -130bar and between 50 -1050K.

GASOLINE COMPONENTS DIFFER IN BURNING VELOCITY



- Need for an extensive and self-consistent data set

- Component S_u from Farrell et al., 2004 (SAE 2004-01-2936 (Combustion bomb - 450 K, 304 kPa))

SINGLE CYLINDER ENGINE TESTS

- Ricardo Hydra engine
- Fixed spark timing - 10° retarded from MBT
- No knock sensor
- Calibrated using base fuel (95 RON EU)
- Run against dynamometer inertia
- Performance : 40 accelerations – last 20 chosen
- Power : steady state at 1500 rpm, 7 bar IMEP
- RUN in sequence A-B-A-B-A-B-A……….

Fuel A= ULG 95 gasoline

Fuel B = 80% Vol. Fuel A + 20% Vol. Single Component (known S_u)

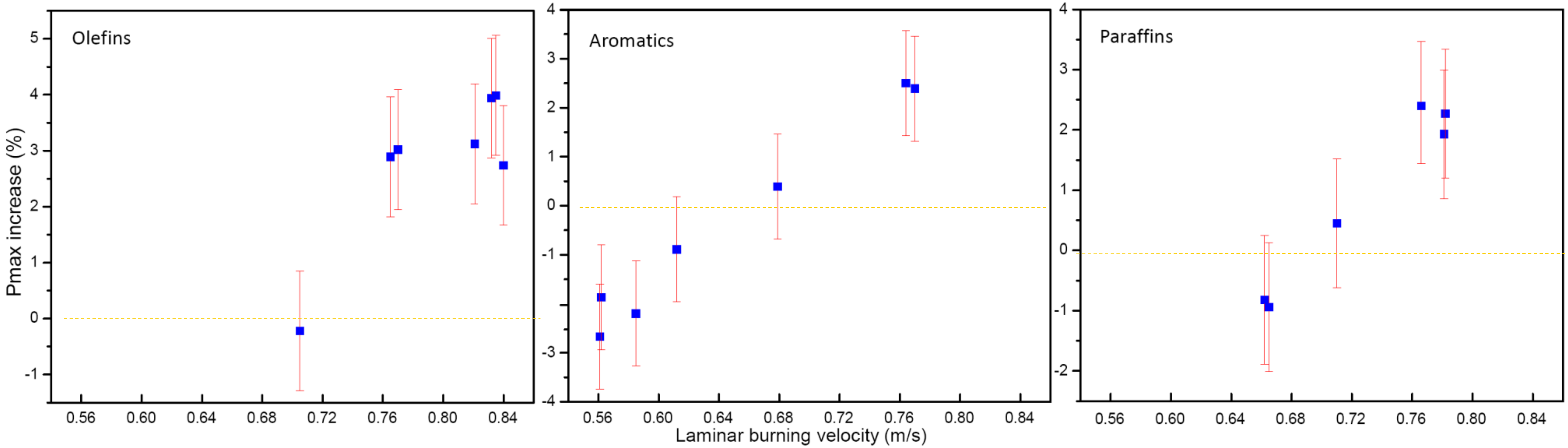
FUEL BLENDS

- Fuel A= ULG 95 gasoline
- Fuel B = 80% vol. Fuel A + 20% vol. Single Component (known S_u)

Component Added	RON	MON	Density (g/cm^3)	Component S_u (450K, 304kPa) (m/s)
Olefins				
2-methyl-2-butene	98.6	86.2	0.7160	0.705
Cyclopentene	96.5	81.2	0.7378	0.765
2-pentene	96.8	85.7	0.7142	0.770
1-octene	84.9	76.1	0.7260	0.821
1-hexene	92.3	82.8	0.7185	0.832
1-heptene	89	80.6	0.7246	0.835
1-pentene	95	84.7	0.7133	0.840
Aromatics				
1,3,5-trimethyl benzene	99.5	89.5	0.7562	0.561
Meta xylene	99.6	88.8	0.7564	0.562
1,2,4-trimethyl benzene	96.2	86.3	0.7585	0.585
Para xylene	99.4	89.4	0.7556	0.612
Toluene	99.5	88.4	0.7564	0.679
Isopropylbenzene	99.1	89.4	0.7558	0.764
Ethylbenzene	99.4	89.3	0.7566	0.770
Paraffins				
Iso pentane	94.7	87.3	0.7079	0.662
Iso octane	96.2	88.4	0.7214	0.665
Methyl cyclopentane	94.3	85.4	0.7322	0.710
n-hexane	84.2	78.8	0.7163	0.766
n-heptane	79.9	76.1	0.7200	0.781
Cyclohexane	92.5	84.1	0.7379	0.782

Component S_u from Farrell et al., 2004 (SAE 2004-01-2936)
Measured in a Combustion bomb - 450 K, 304 kPa

RELATIONSHIP of S_u ON P_{max}

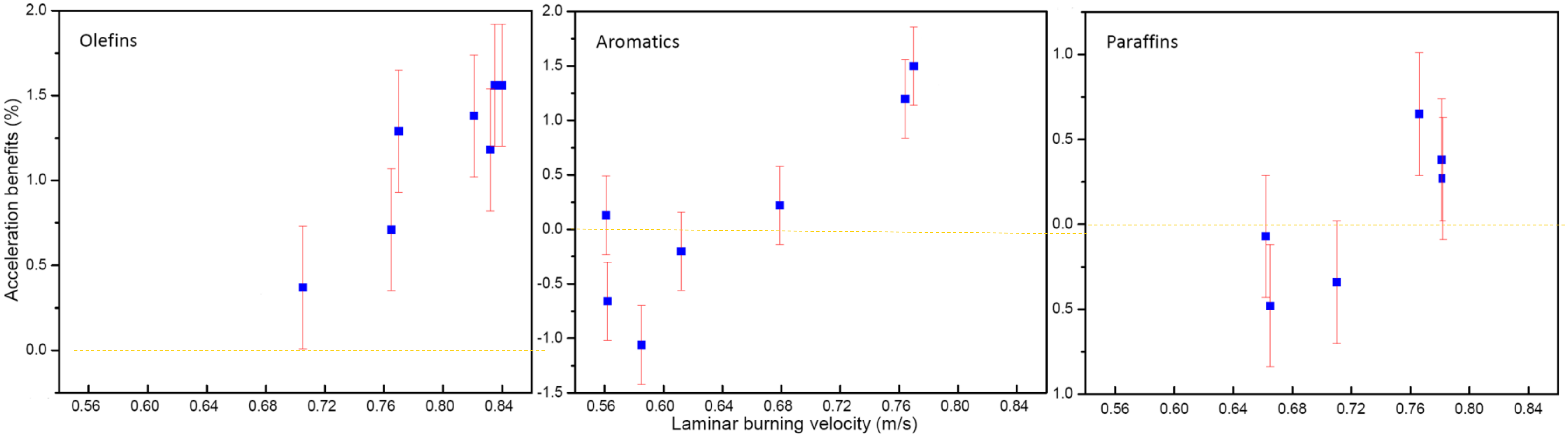


- Laminar Burning Velocity of component (added at 20%) DOES affect Pmax.
- BUT what happens to performance?

Component S_u from Farrell et al., 2004 (SAE 2004-01-2936) Measured in a Combustion bomb - 450 K, 304 kPa

SAE 2012-01-1742

RELATIONSHIP BETWEEN ACCELERATION TIME AND S_U

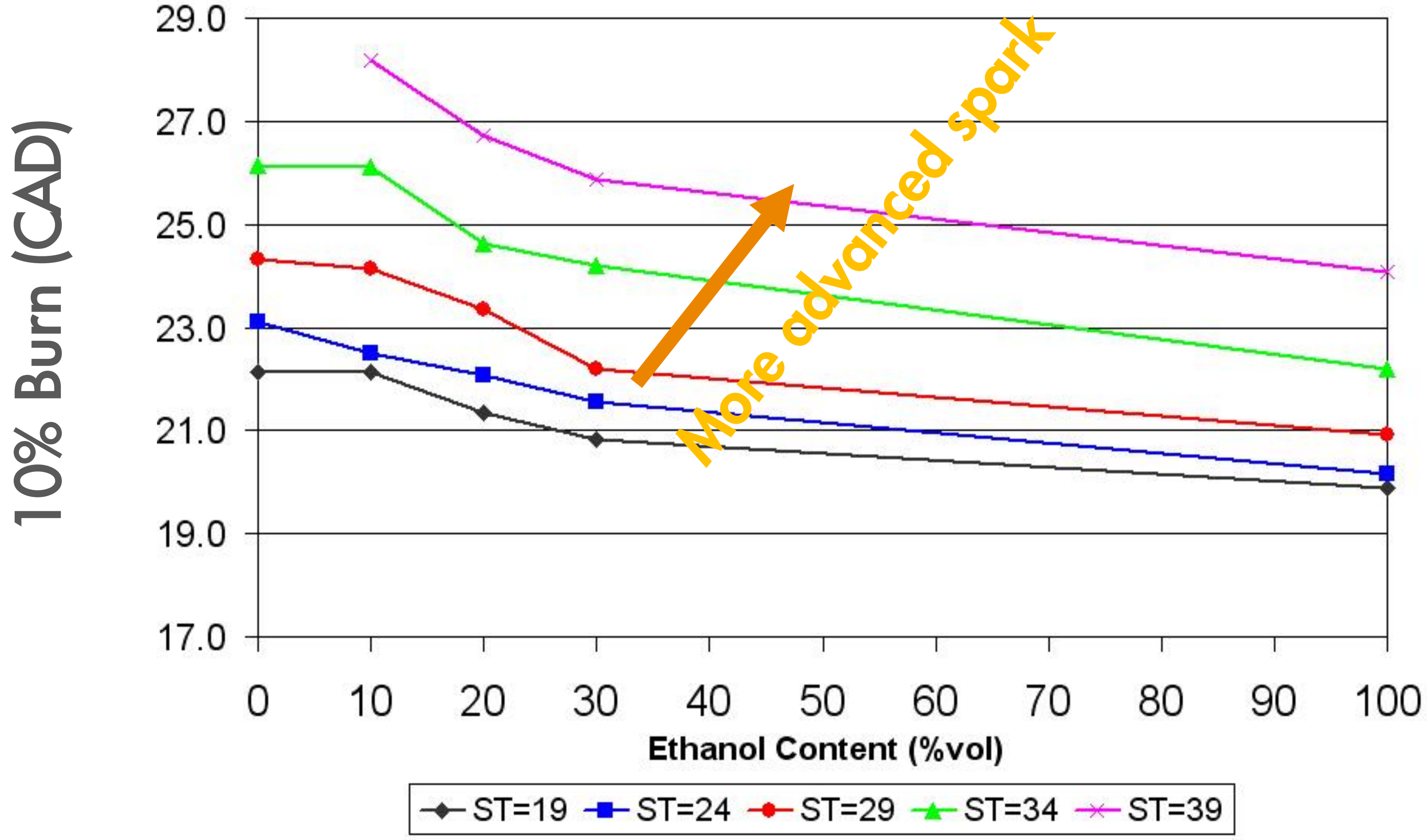


- Laminar Burning Velocity of component (added at 20%) correlates with acceleration.

Component S_u from Farrell et al., 2004 (SAE 2004-01-2936 (Combustion bomb - 450 K, 304 kPa))

SAE 2012-01-1742

ETHANOL BLENDS- FLAME SPEED IN DISI ENGINES



- 3.4 bar IMEP
- Single injection:280° BTDC

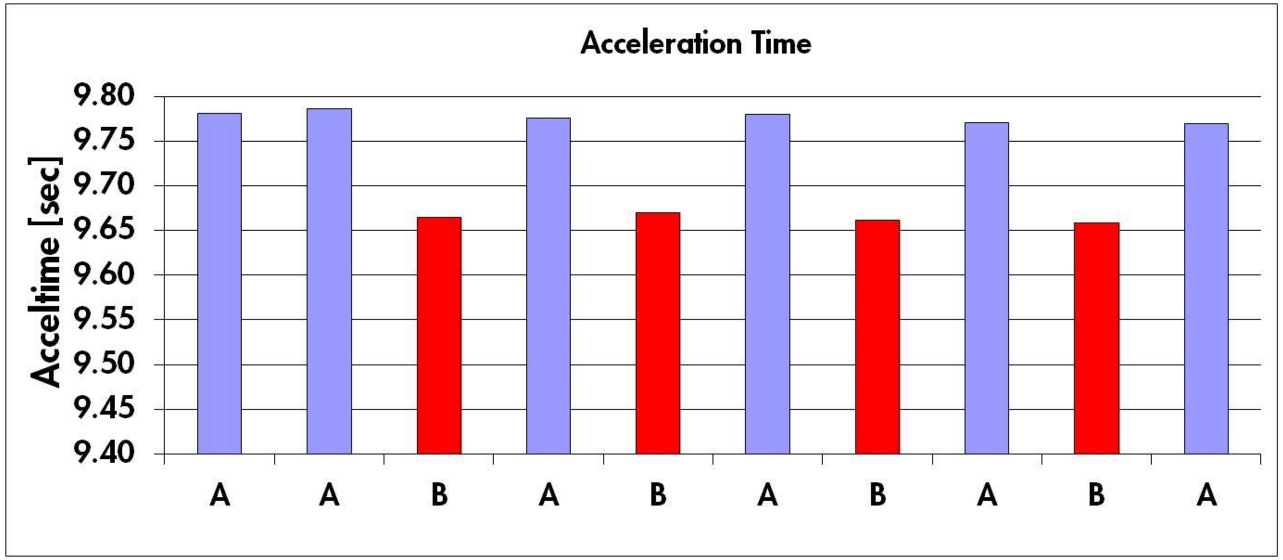
- Higher ethanol content leads to faster combustion

Turner et al: Fuel 90 (2011) 1999

VEHICLE TESTS (1)

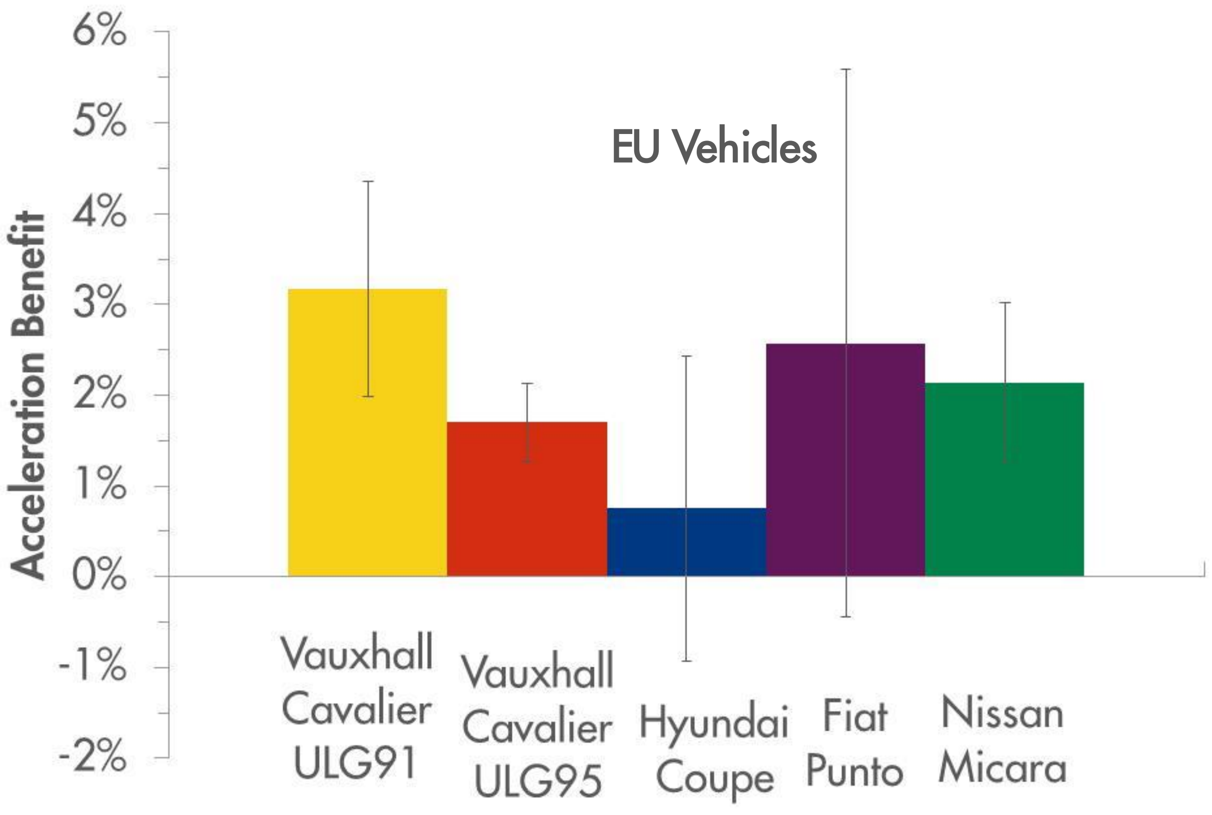
- Five US vehicles and 4 European vehicles
- Test fuel blend (35% aromatics, 18% olefins - selected for higher S_u), same reference fuel
- 70-120 km/h accelerations on Chassis Dynamometer
- A-A-B-A-B-A-B-A-B-A sequence
- Desire to separate potential flame speed benefits from octane effects
  - Vehicles selected to be insensitive to octane in range tested
  - Confirmed by looking at spark timings

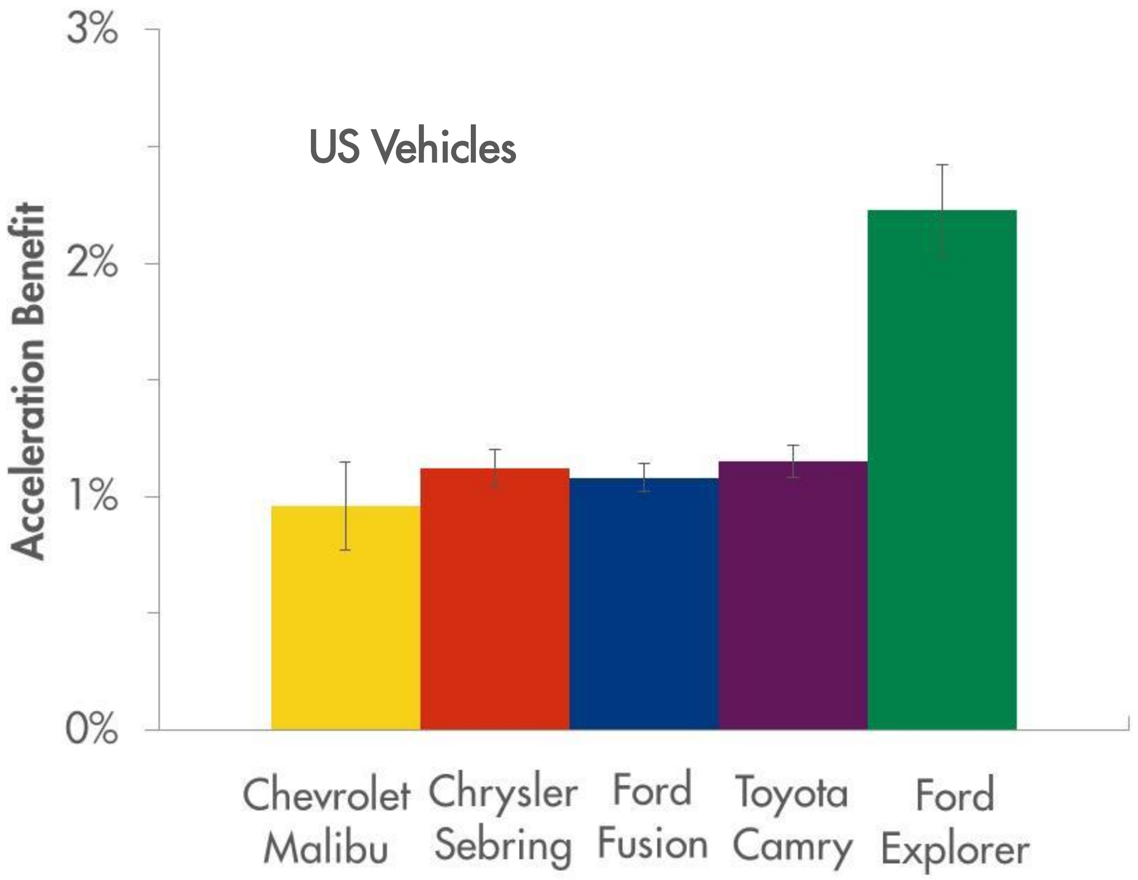
Toyota Camry Results



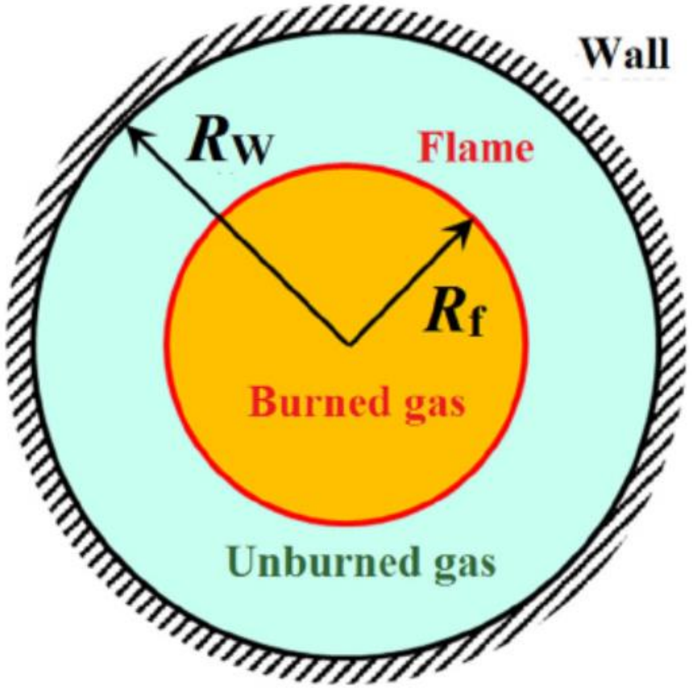
SAE 2012-01-1742

VEHICLE TESTS (2)





BOMB (SEF) METHODS TO DETERMINE FLAME SPEED

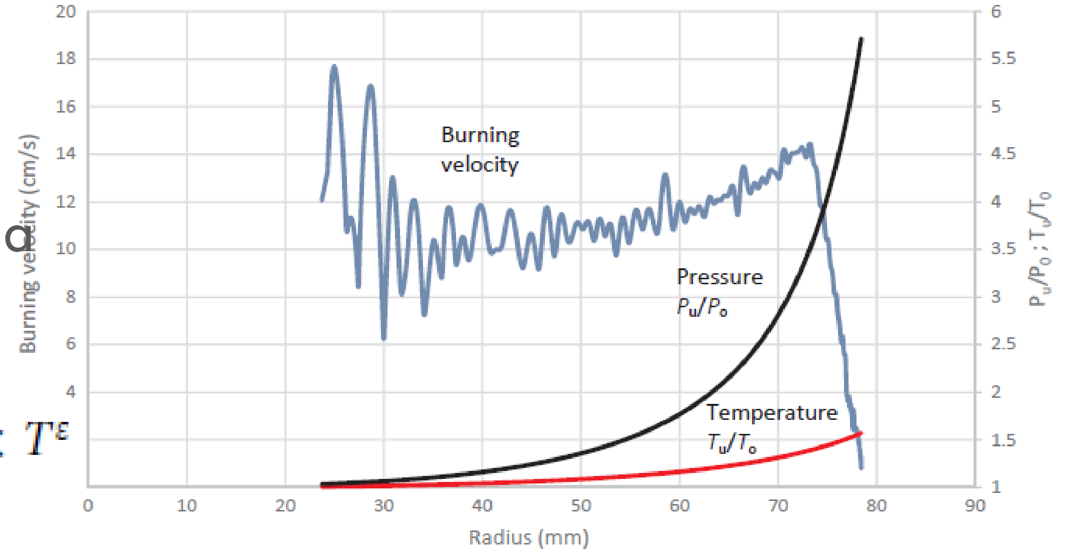


- Use data at small flame radius before significant pressure rise
  - Use Schlieren images. (Need to correct for flame stretch)
  - Use early pressure rise data and assume *Su* is relatively independent of T and P. Use thermodynamic model to calculate R

$$S_u = \frac{dR_f}{dt} - \frac{(R_w^3 - R_f^3)}{3R_f^2\gamma_u P}\frac{dP}{dt}$$

(Need to correct for flame stretch)

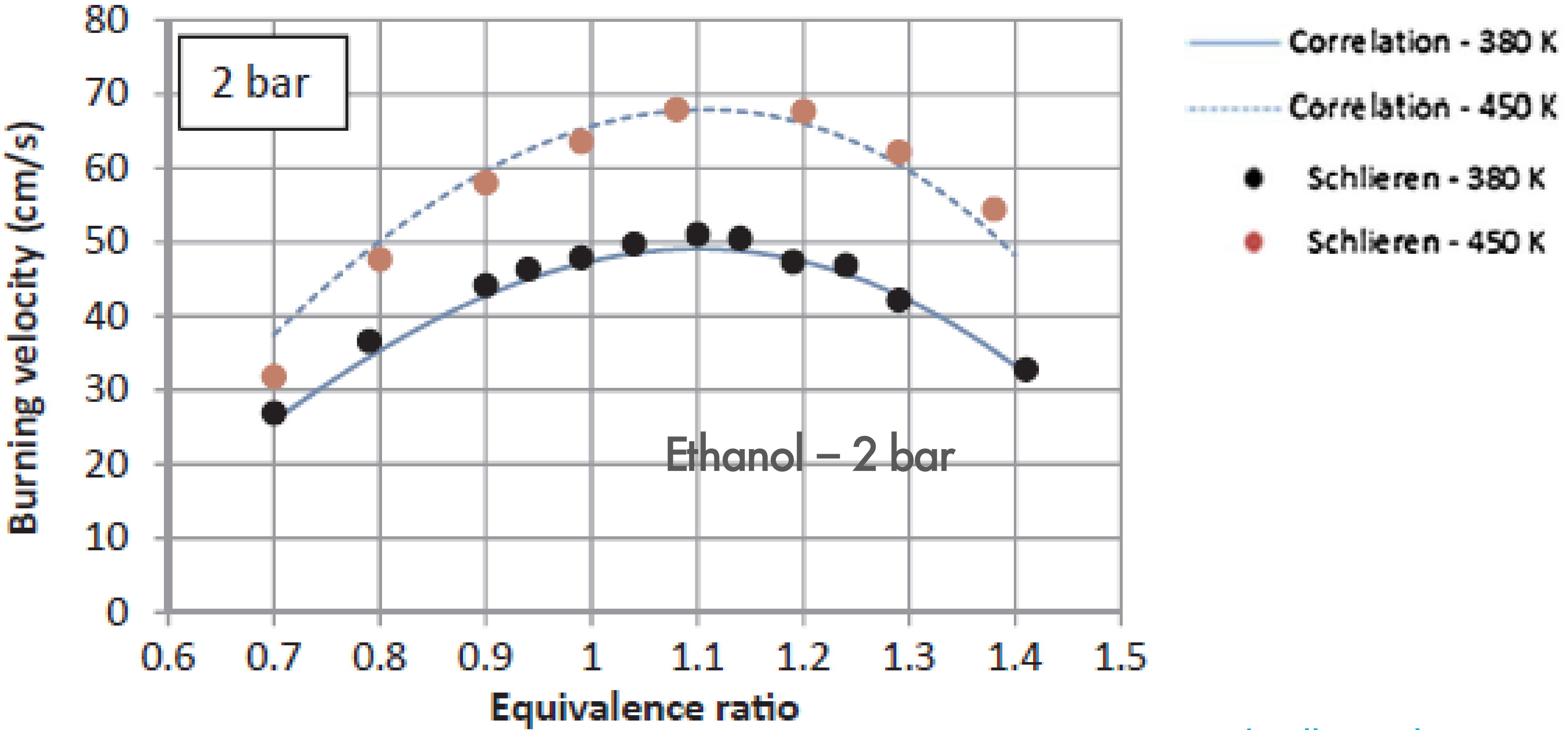
- Use full pressure rise data and acknowledge that Su is a function of T, P and φ. Use thermodynamic model Fit to a function – e.g.



$$S_u = [S_{u,0} + S_{u,1}(\phi-1) + S_{u,2}(\phi-1)^2 + S_{u,3}(\phi-1)^3 + S_{u,4}(\phi-1)^4] \times T^{\varepsilon}$$
$$\times P^{\beta} \times (1-\mu_1 x_r^{(\mu_2+(\phi-1)\mu_3)})$$

AGREEMENT BETWEEN BOMB METHODS

- Pre-pressure: Radius development early flame determined via Schlieren. Extrapolation to zero stretch
- Pressure: Fit to function and get correlation depending on P, T and φ

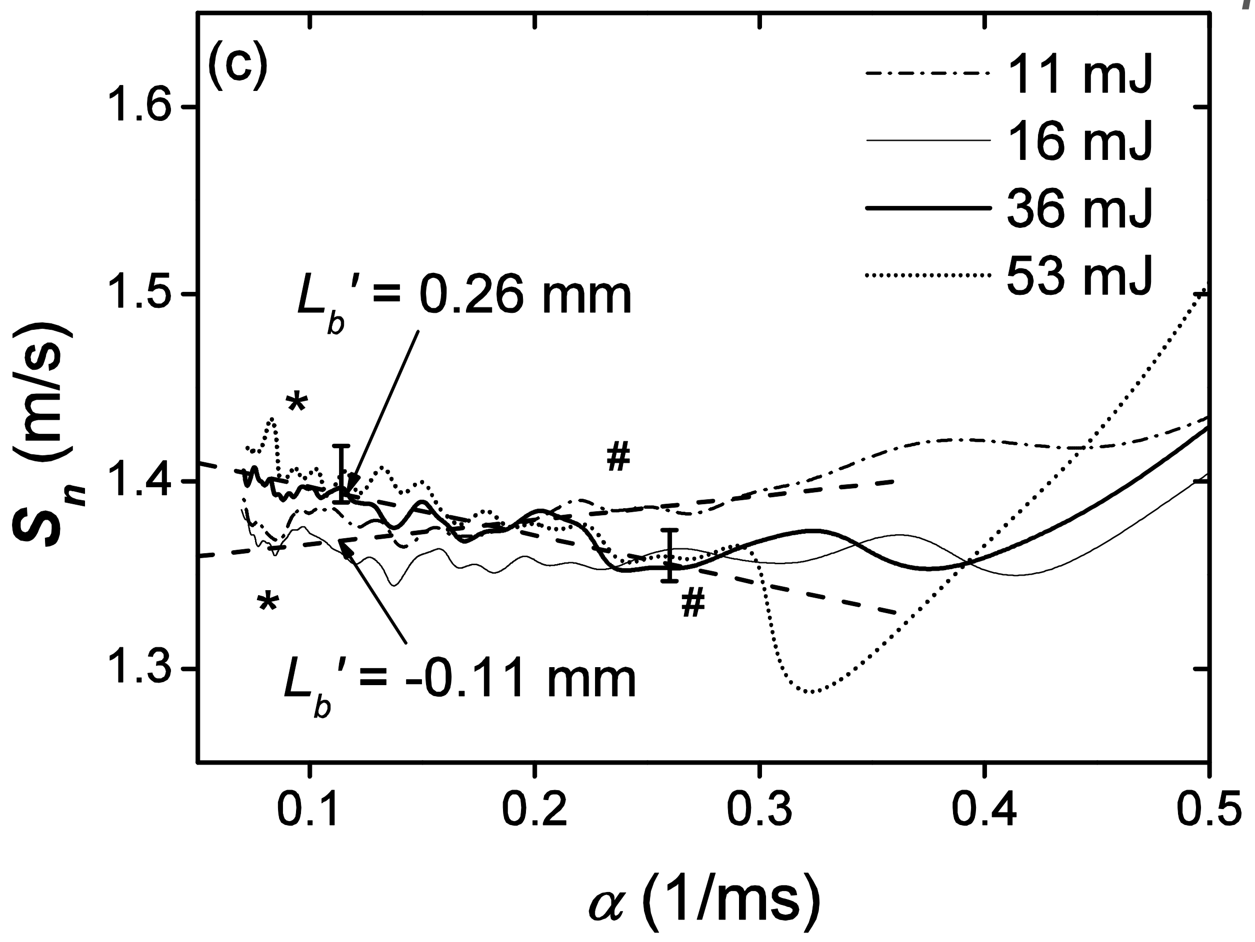


N. Hinton, C.R. Stone, R.F. Cracknell: Fuel 211 (2018) 446–457

ISSUES WITH BOMB EXPERIMENTS (1)

- Xiouris et al (CNF 163 (2016) 270) claim that neglecting radiation can lead to an error of up to 15%.
  - Built a radiation model into thermodynamics calculations
- Linear versus non-linear extrapolation to zero stretch (Kelley and Law; CNF 156, (2009), 1844)
- Cellularity and Effect of spark

ISSUES WITH BOMB EXPERIMENTS (2)



Methane-air mixture (ϕ=0.8, T=358 K, P=0.3 MPa).

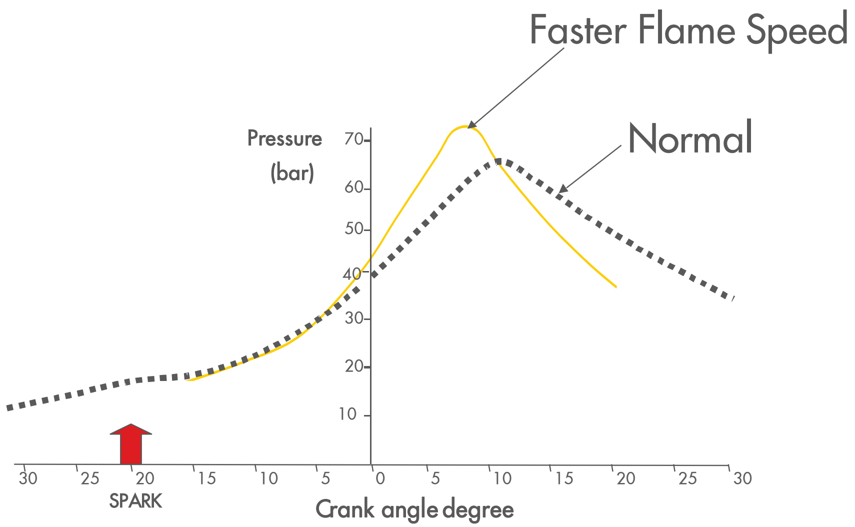
- For low/negative Markstein lengths, it can be difficult to find a region to extrapolate to zero stretch, which is independent of spark strength AND without a cellular flame.

  - Apparent Markstein length can depend on spark energy

Lawes, M, Sharpe, GJ, Tripathi, N and Cracknell R.F.: Fuel, 186. (2017) pp. 579-586.

DISCUSSION – IS LAMINAR BURNING VELOCITY THE RIGHT TARGET TO BE MEASURED?

- Faster combustion in engines can lead to improved efficiency, but is strongly influenced by engine turbulence levels as well as laminar burning velocity



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- Laminar Flame Speed is a theoretical concept:
  - For some systems (e.g. with low or –ve Markstein length) an unstretched laminar flame speed may not be definable at all
  - Attempts to correct for stretch lead to error

- Need an extensive and self-consistent data set. Results in an engine <u>do</u> correlate with measured LBV

- Key question in engines is "How fast does the pressure rise"
  - Can we just compare pressure rise rates and compare to standard components (e.g. iso-octane and n-heptane)

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Questions and Answers

Q&A