3D Engine knock prediction and evaluation based on detonation theory

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Outline

I. Objective

II. Combustion model

III. Detonation theory

IV. SI Engine Application

V. Summary and Conclusions

Objective

- SI engine development tends towards downsizing and increase in compression ratio to improve efficiency
  - Increased knock tendency

- Demand on SI engine simulations
  - Predict auto-ignition events
  - Reproduce physical sensitivities
  - Predict auto-ignition as function of fuel octane ratings
  - Evaluate the transition of harmless deflagration to undesirable knocking combustion
  - Classify the severity of the auto-ignition event

Our approach:
Detailed chemistry, laminar flame speed tabulation, evaluation with the detonation diagram by Bradley

LUND COMBUSTION ENGINEERING

COMBUSTION MODELING

Combustion Model Approach

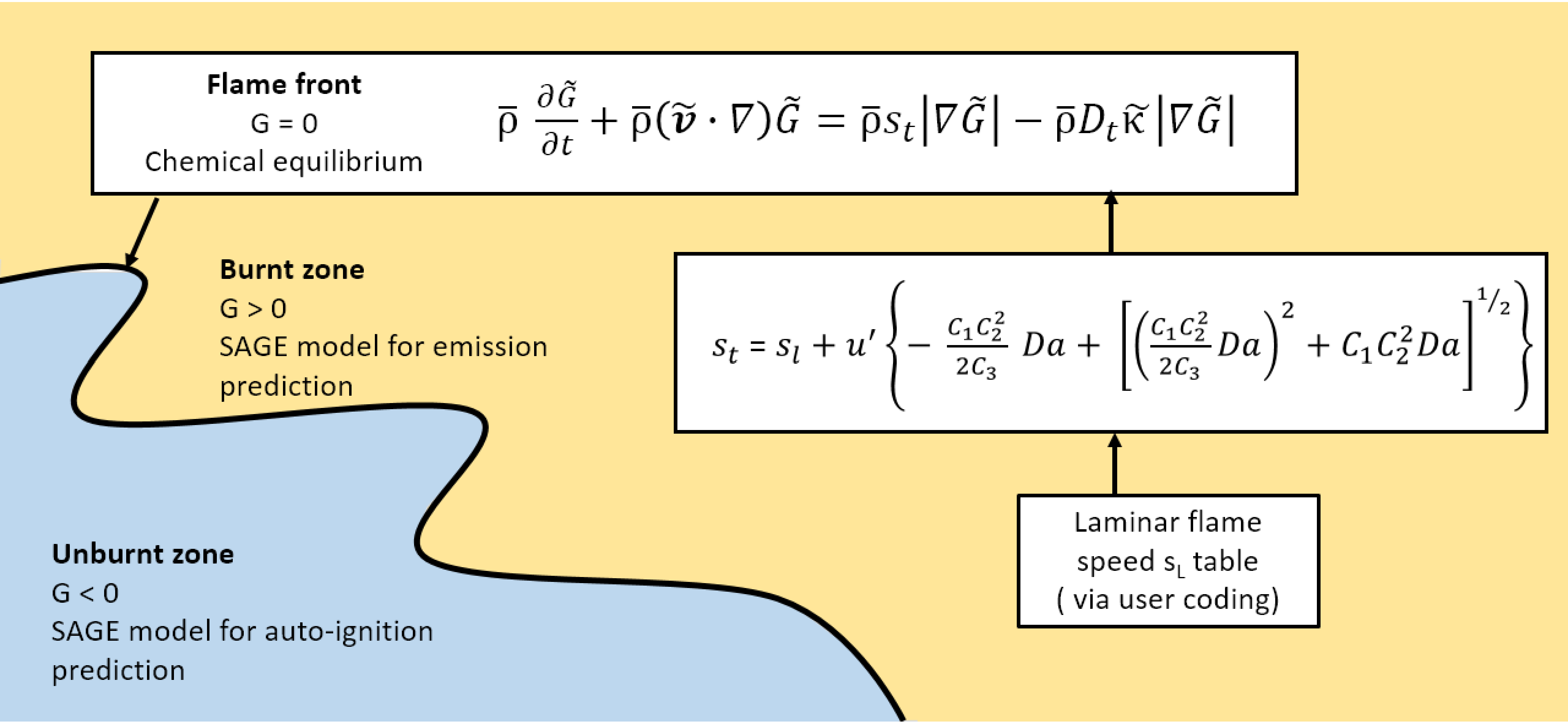
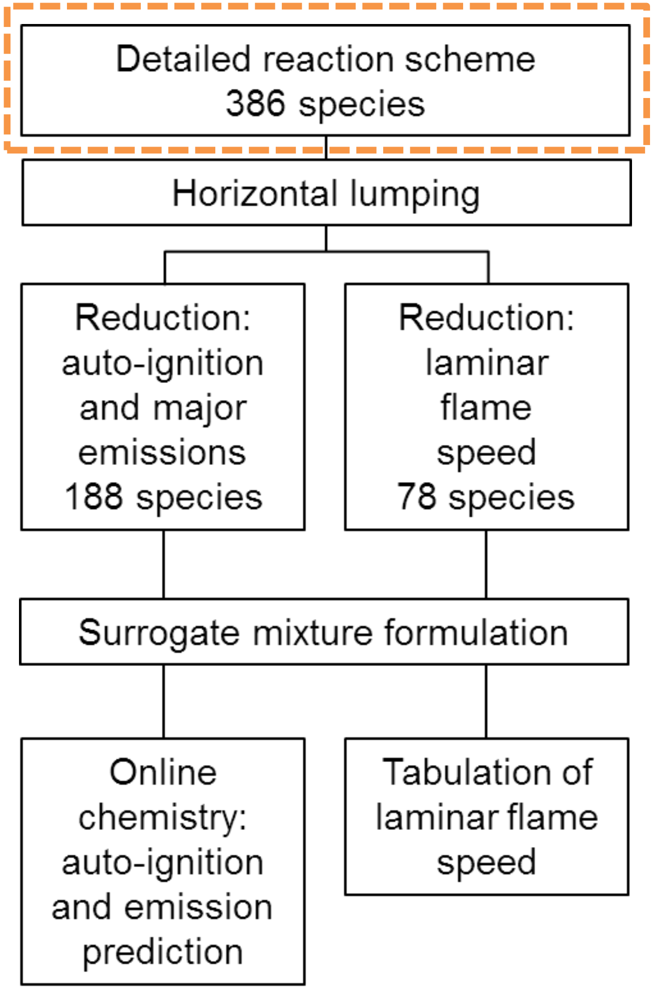


Figure 1: Schematic illustration of the combustion modelling approach

Gasoline Surrogate Chemistry

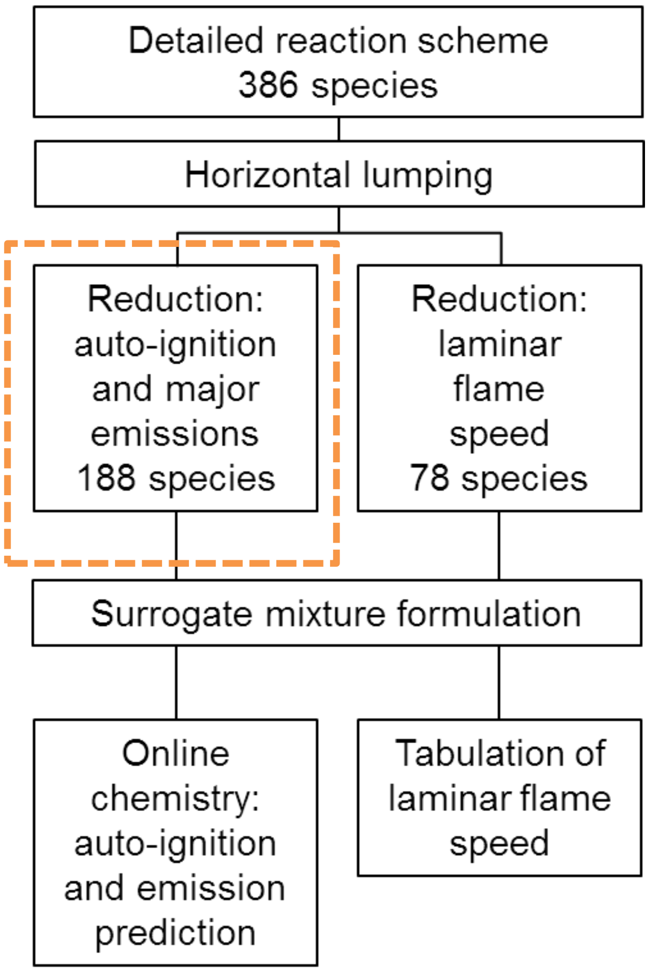
- Detailed reaction mechanism



- Latest LOGE GASOLINE
  - Fuel species (ETRF):
    - Ethanol C_2H_5OH
    - Toluene A_1CH_3
    - Iso-octane $i\text{-}C_8H_{18}$
    - N-heptane $n\text{-}C_7H_{16}$
  - Oxidation chemistry for C_1-C_5 species
  - Major exhaust-out emissions
  - Thermal NO_x
  - Growth pathways for poly-aromatic hydrocarbons
  - 386 species and 4511 reactions

Gasoline Surrogate Chemistry

- Skeletal scheme for auto-ignition and emissions



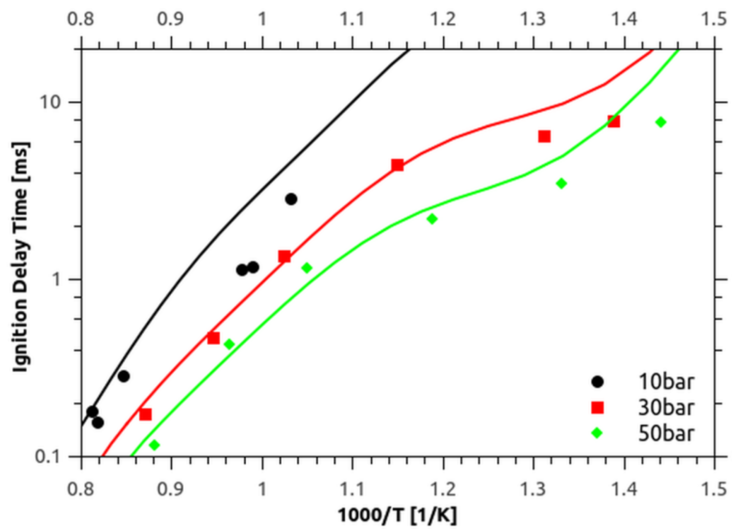


Figure 2: Ignition delay time for a mixture of 0.72 toluene and 0.28 n-heptane (mole fraction) at φ = 0.3, p = 10, 30, 50 bar. Experimental data from Herzler et al. [5]

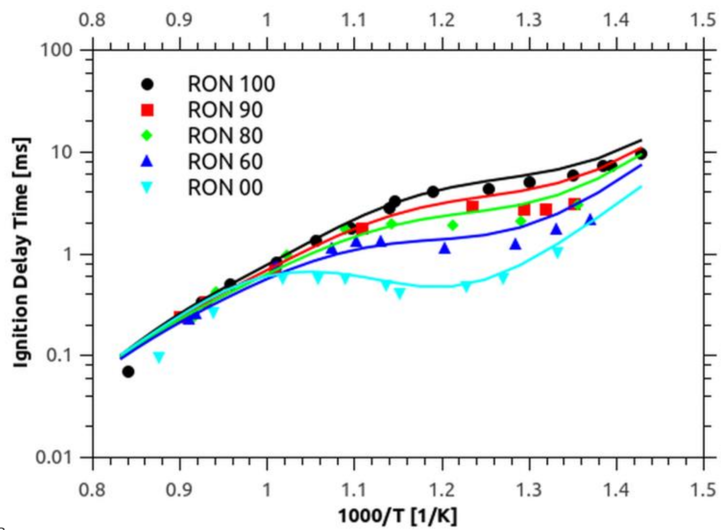
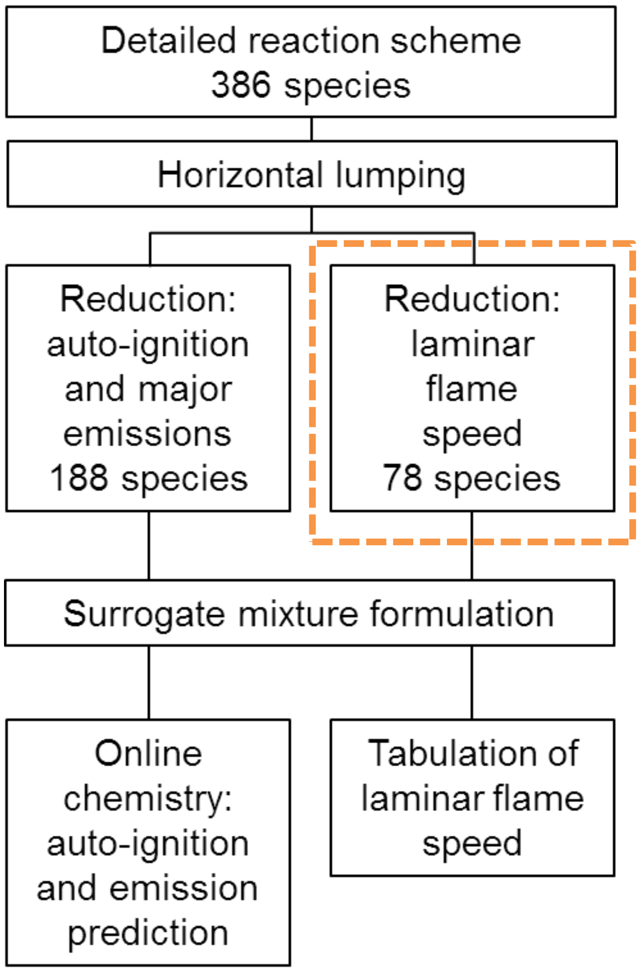


Figure 3: Ignition delay time of iso-octane/n-heptane mixtures at 40 bar, φ = 1. Experimental data from Fieweger et al. [6]

Gasoline Surrogate Chemistry

- Skeletal scheme for laminar flame speed only



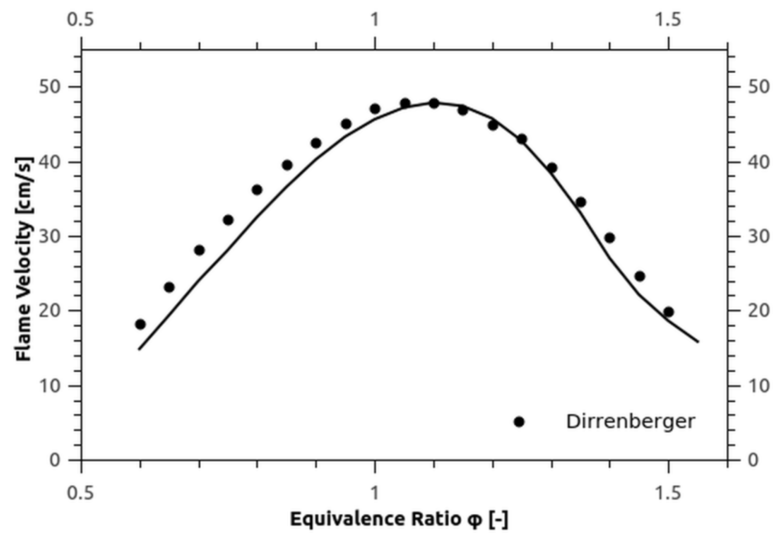


Figure 4: Laminar flame speeds at 1 atm and 358 K with air as oxidizer for a mixture of 11.65% n-heptane, 36.47% iso-octane, 36.89% toluene and 15.0% ethanol (liquid volume fraction) Experimental data from Dirrenberger et al. [7]

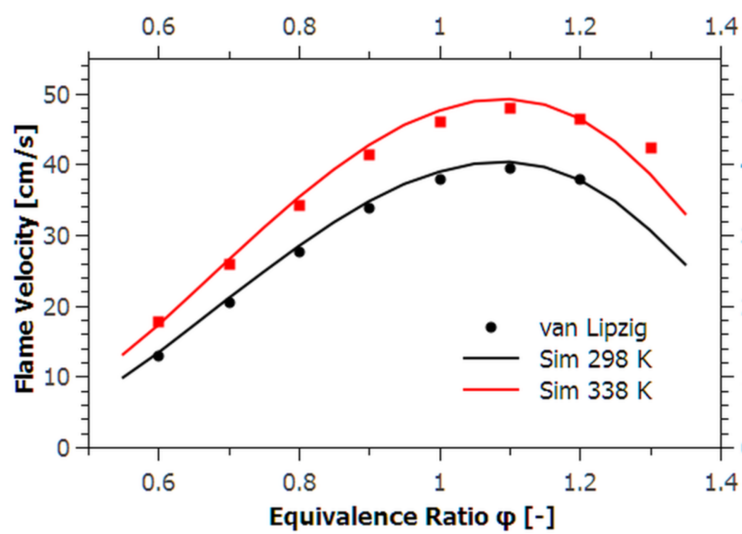
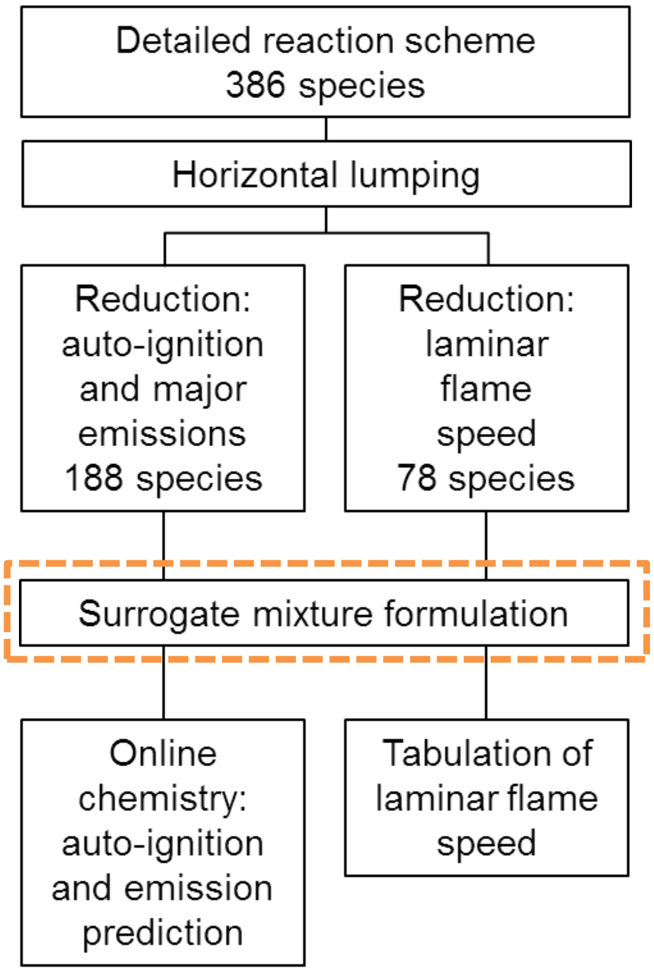


Figure 5: Laminar flame speeds at 1 atm and 358 K with air as oxidizer for a mixture of 33.3% n-heptane, 33.33% iso-octane, and 33.3% ethanol (liquid volume fraction) Experimental data from van Lipzig et al. [8]

Gasoline Surrogate Chemistry

- Surrogate mixture formulation



- Based on published correlations (Anderson et al. [3] and Morgan et al. [4])
- Input parameters from fuel data sheet:
  - RON
  - Aromatic content (Toluene)
  - Ethanol content
- Output: Surrogate mixture formulation

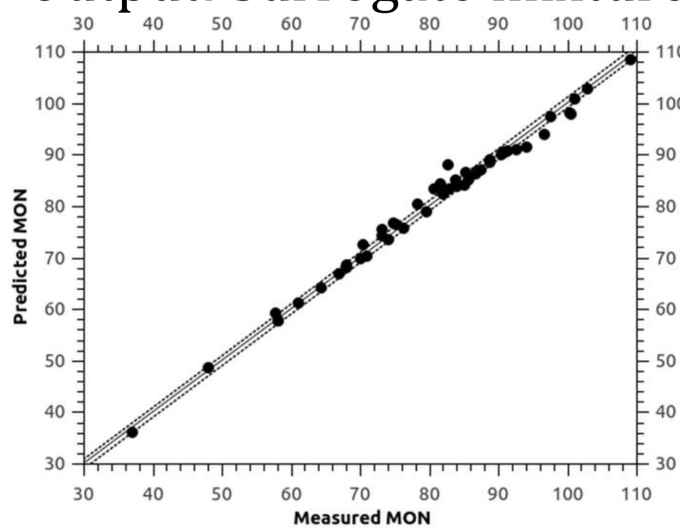
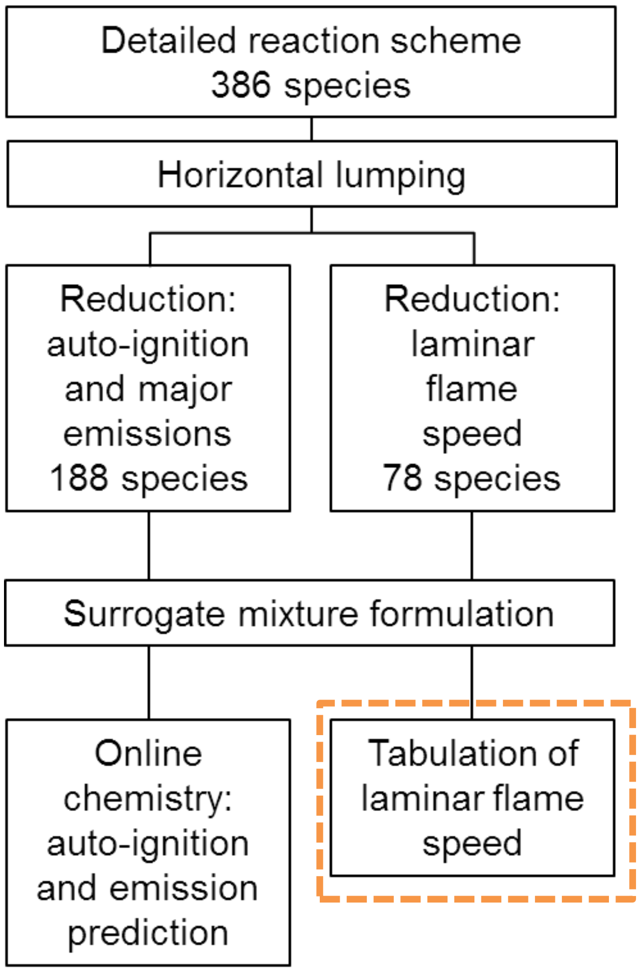


Figure 6: Predicted MON vs. measured MON.. Dashed line shows an uncertainty of 1 octane point

Gasoline Surrogate Chemistry

- Tabulation of laminar flame speed



  - Table generated with LOGEsoft based on reaction scheme or correlations (faster)
  - Fast tabulation due to reduced reaction scheme
  - Tabulated in wide engine relevant range

Table 1: Ranges for tabulation of the laminar flame speed

Property	Range	Step size
Pressure	1bar to 150 bar	Up to 10 bar: 1 bar 10 to 150 bar: 10 bar
Unburnt zone temperature	350 K to 1600 K	50 K
Fuel-air equivalence ratio	0.5 to 1.5	0.05
EGR level	0 % to 30 %	10 %

DETONATION THEORY

Engine Knock Evaluation

- Detonation diagram by Bradley et al.

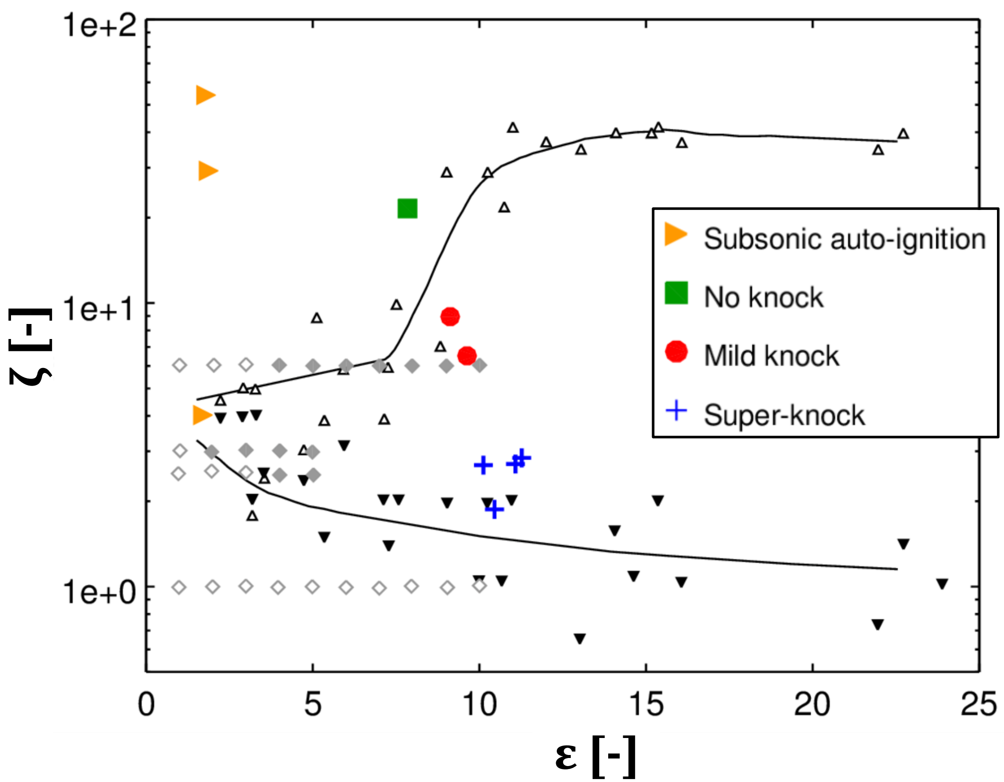


Figure 7: Detonation diagram; Black symbols and lines: experiments Bradley et al. [1]; Grey symbols 1D simulations – open symbols: no detonation, filled symbols: developing detonation Peters et al. [9]; Colored symbols LES engine simulations: green stars: subsonic auto-ignition, blue squares: no knock, red circle: mild knock, oranges crosses: super-knock Bates et al. [10]

– Severity of auto-ignition event based on two dimensionless parameters:

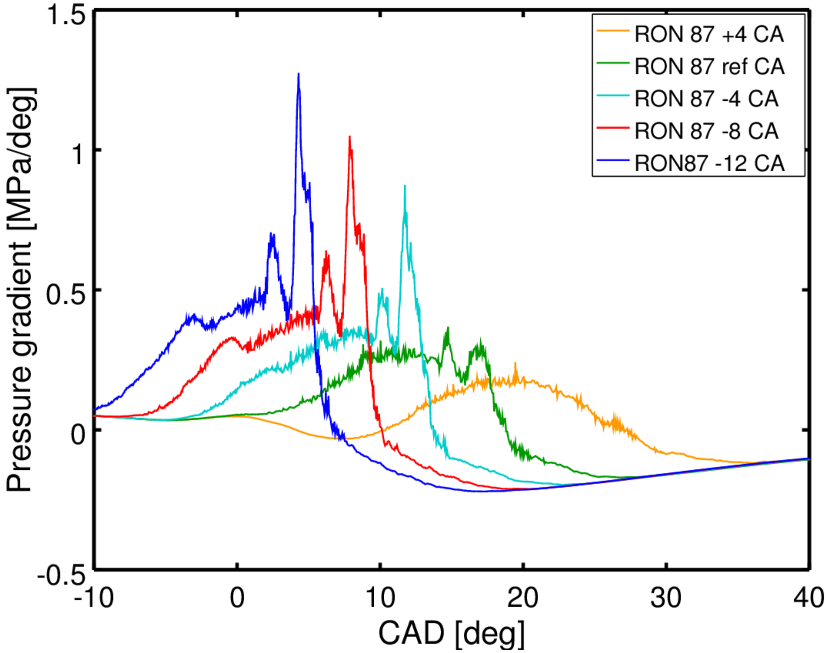
$$\boldsymbol{\zeta = \frac{a}{u} = a \cdot \frac{\partial T}{\partial x} \cdot \frac{\partial \tau}{\partial T}}$$

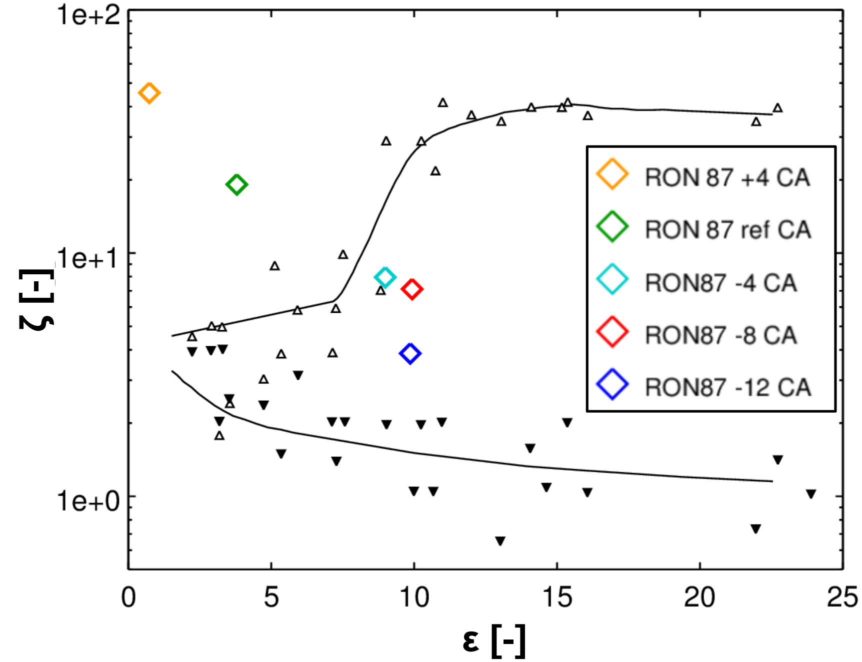
$$\boldsymbol{\varepsilon = \frac{l}{a \cdot \tau_e}}$$

- speed of sound **a**
- reaction front velocity **u**
- Ignition delay time **τ**
- kernel size **l** in which the temperature gradient is
- Excitation time $\boldsymbol{\tau_e}$ (time from 5% to maximum heat release)

SI ENGINE APPLICATION

Sensitivity Spark Advancing



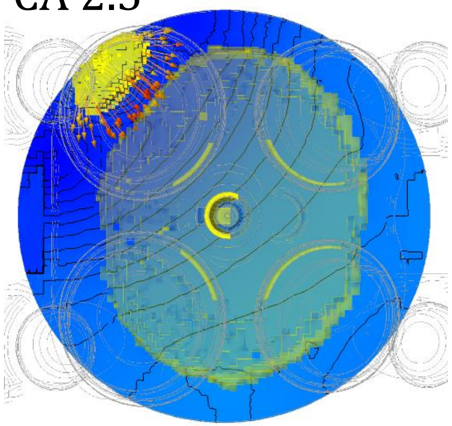


- Only the most severe auto-ignition event per calculation is shown
- Transition from acceptable subsonic auto-ignition over light knock to heavy knock go well together with the predicted pressure gradients

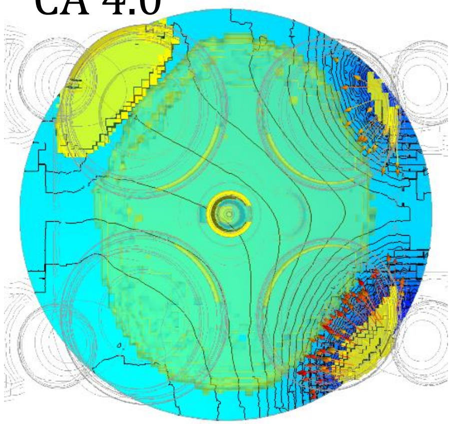
Detailed Investigations

- Investigation: severity of different ignition kernels

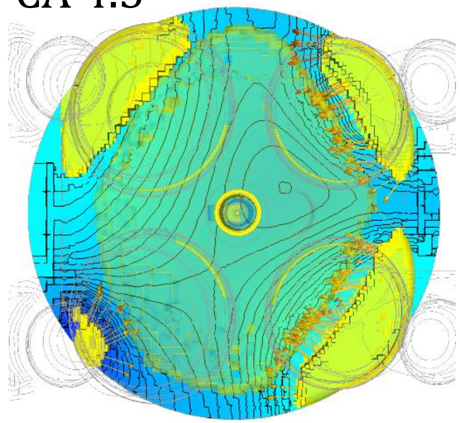
CA 2.5



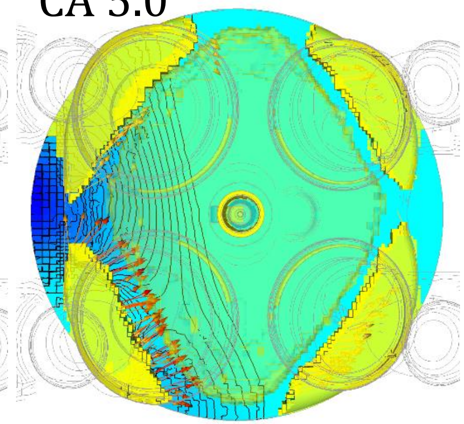
CA 4.0

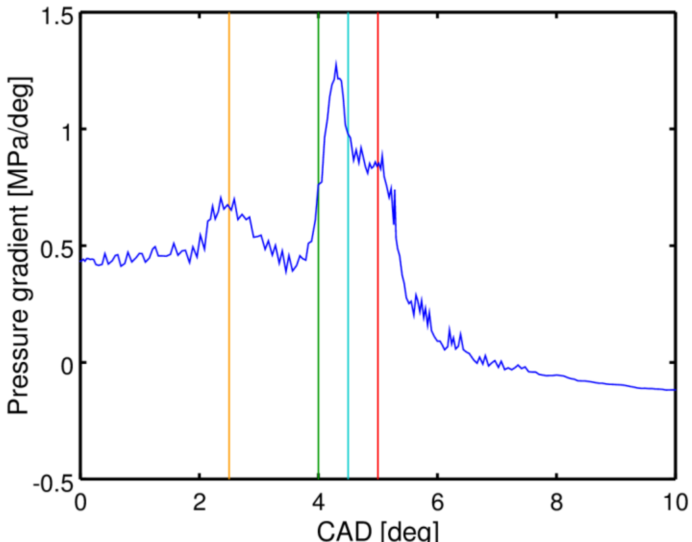


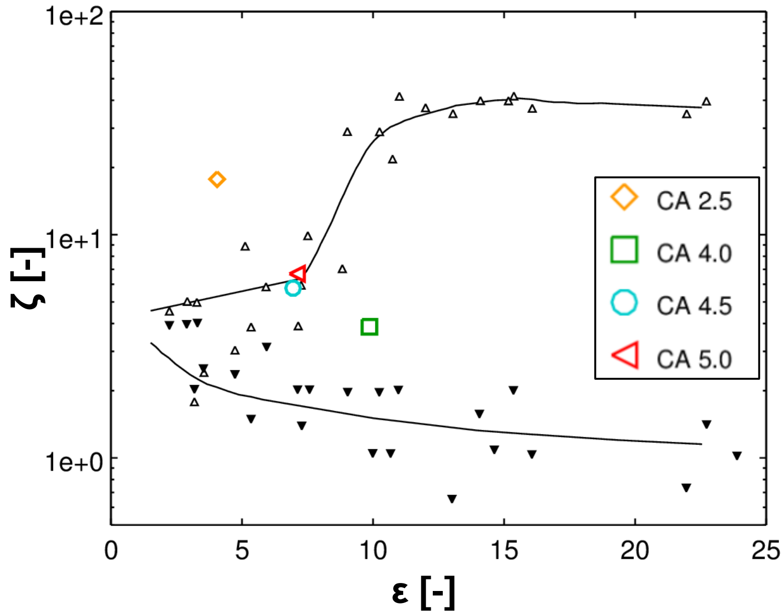
CA 4.5



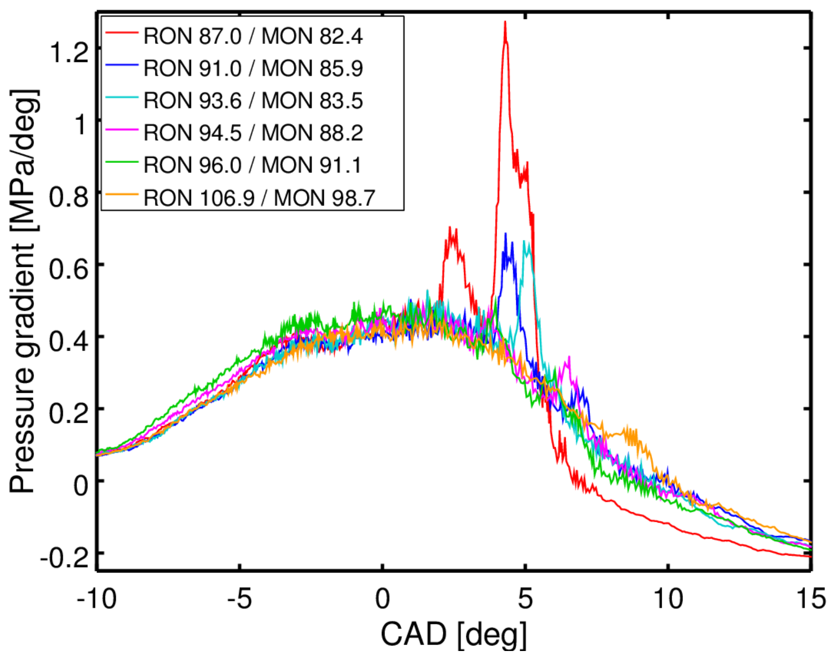
CA 5.0

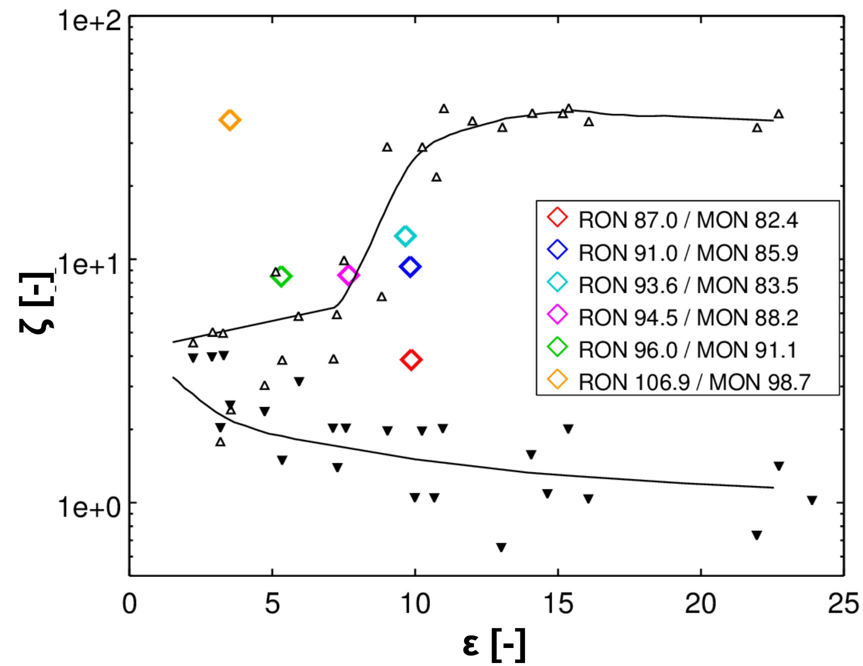






Sensitivity Fuel Octane Rating





- Study: same operating point with different fuel octane ratings and corresponding laminar flame speed tables
- The severity of the auto-ignition event decreases with increased fuel RON

Sensitivity Fuel Octane Rating

- Investigation: first appeared ignition kernel

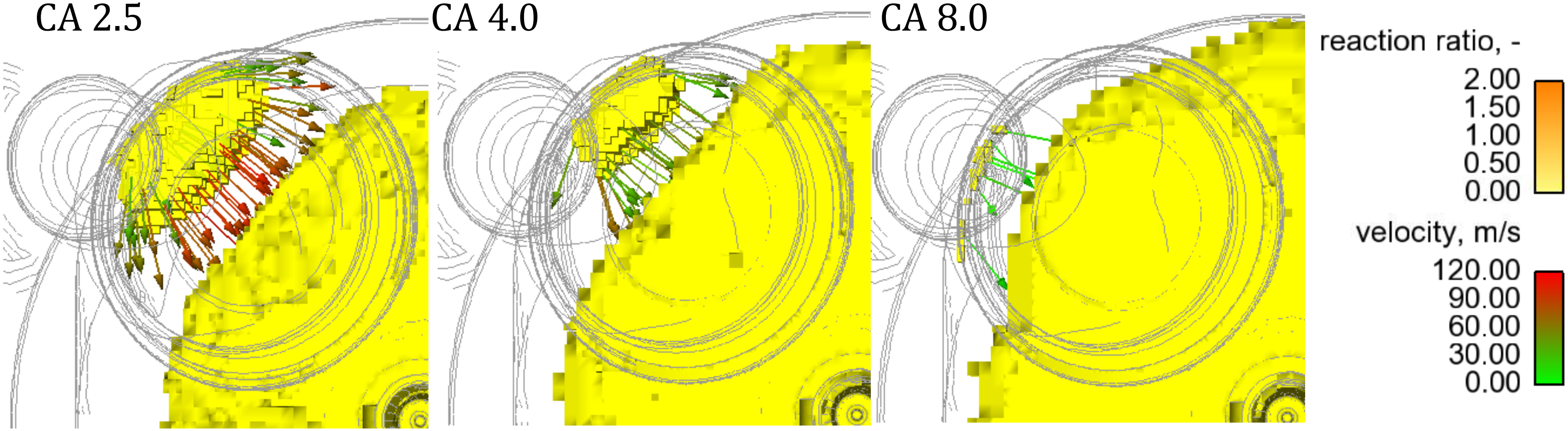
RON

Auto-ignition appearance CA

RON 87.0 /MON 82.4
CA 2.5

RON 96.0 /MON 88.2
CA 4.0

RON 106.9 /MON 98.7
CA 8.0



Auto-ignition severity

Ignition kernel size

Conclusions

- **Engine knock prediction based on**
  - detailed chemistry
  - tabulated laminar flame speeds
  - SAGE for auto-ignition prediction

- **Physical sensitivity to**
  - spark advancing
  - fuel quality

- **The knock severities based on the detonation diagram go well together with the predicted pressure traces.**

- **Suggested tool chain can be used efficiently to predict knock severity of different operating conditions and fuel octane ratings.**

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Acknowledgements

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