Impact of Gasoline Surrogates with Different Fuel Sensitivity (RON-MON) on Knock Prediction

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Introduction

The trade-off between maximizing the fuel efficiency and avoiding harmful engine knock is dominating the development of Spark Ignition (SI) engines. The knock tendency of a fuel is characterized by the octane rating: Research Octane Number (RON) and Motored Octane number (MON). Frequently, Primary Reference Fuels (PRF) are applied to predict engine knock, regardless that their composition of iso-octane (RON=MON=100) and n-heptane (RON = MON = 0) can represent the RON of a commercial gasoline fuel, but never at the same time the correct MON or octane sensitivity S=RON-MON. The use of more complex surrogates such as ethanol containing Toluene Reference Fuels (ETRF) overcomes this drawback.

In this work, we analyze the effect of different surrogates on the engine knock prediction using 3D CFD (Converge 2.4). Surrogates composed of different species (PRF, TRF, ETRF), that have the same RON, but differ in MON are compared to each other regarding their prediction of strength and onset of engine knock.

Surrogate Formulation

Different surrogates with same RON, but different number of surrogate fuel species and different MON are composed using the methodology developed in [1], where correlations from Morgan et al. [2] and Anderson et al. [3] are applied.

Table 1: Properties of the commercial gasoline (fuel analysis) and the surrogates (calculated). *Input properties: RON, content of aromatics and ethanol

		Gasoline	PRF	TRF	ETRF 1	ETRF 2	ETRF 3
RON*	-	94.5	94.5	94.5	94.5	94.6	94.4
MON	-	84.1	94.5	88.2	88.1	87.6	84.3
S	-	10.4	0	6.3	6.4	7	10.1
aromatic content*	vol%	32.6	0	32.6	22.5	18.8	44.6
ethanol content*	vol%	0	0	0	5.1	10.9	10.4
ρ	kg/m³	747.5	691.3	747.3	735.3	728.5	769.6
LHV	MJ /kg	42.9	44.4	42.9	42.4	41.7	40.9
M	g/mol	-	113.4	103.1	98.4	93.3	89
C:H:O–ratio	mass%	87:13:0	84:16:0	87:13:0	84:14:2	82:14:4	84:12:4
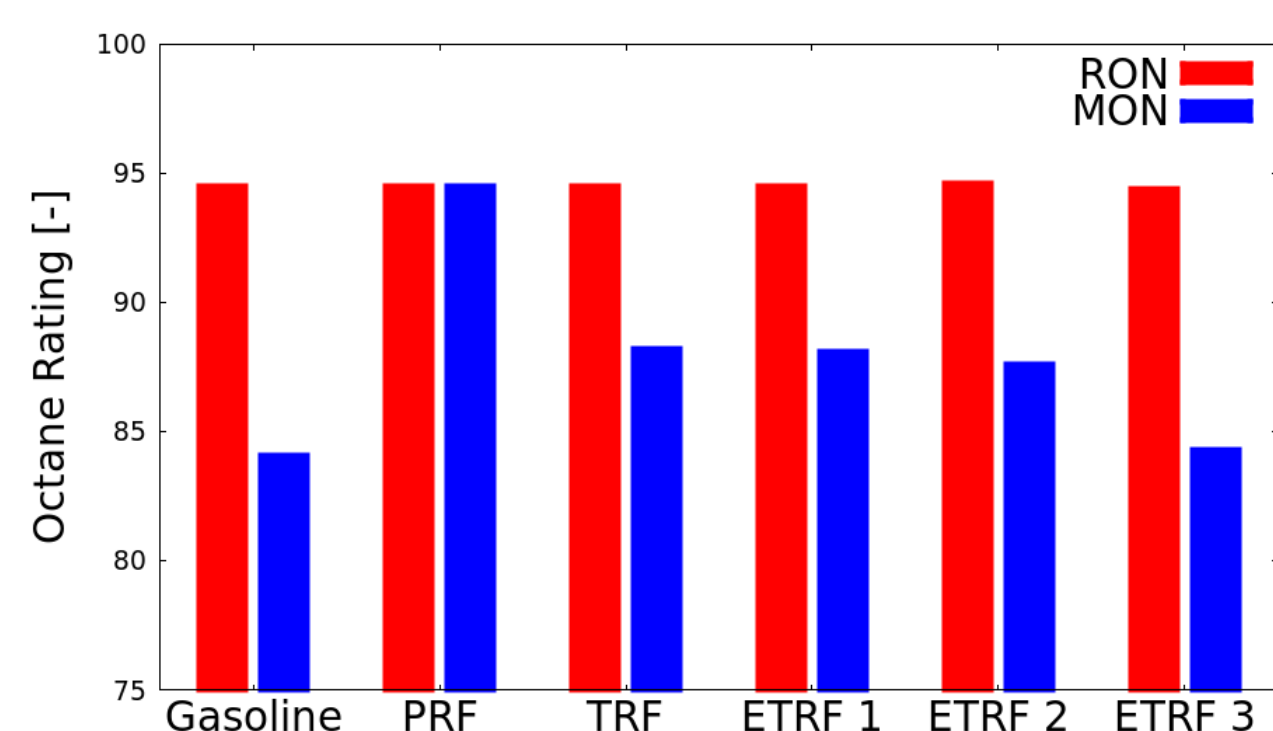
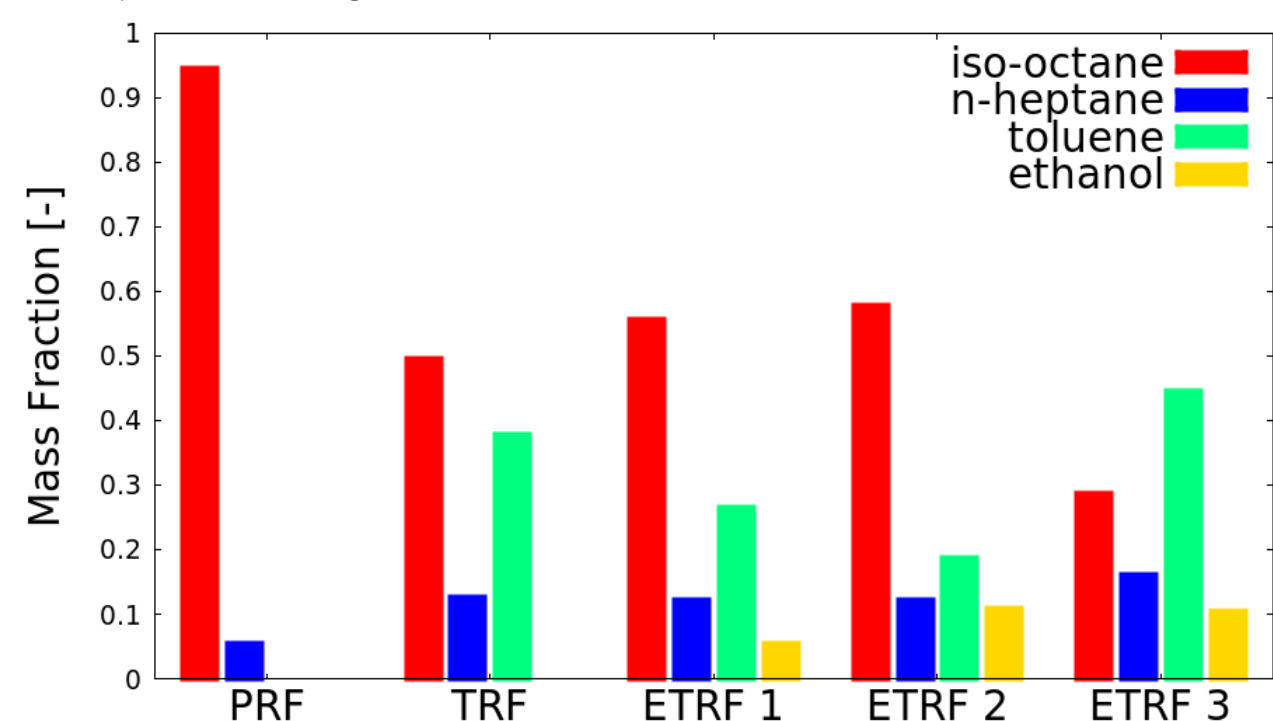Figure 1: RON and MON of the commercial gasoline and the analyzed surrogates.

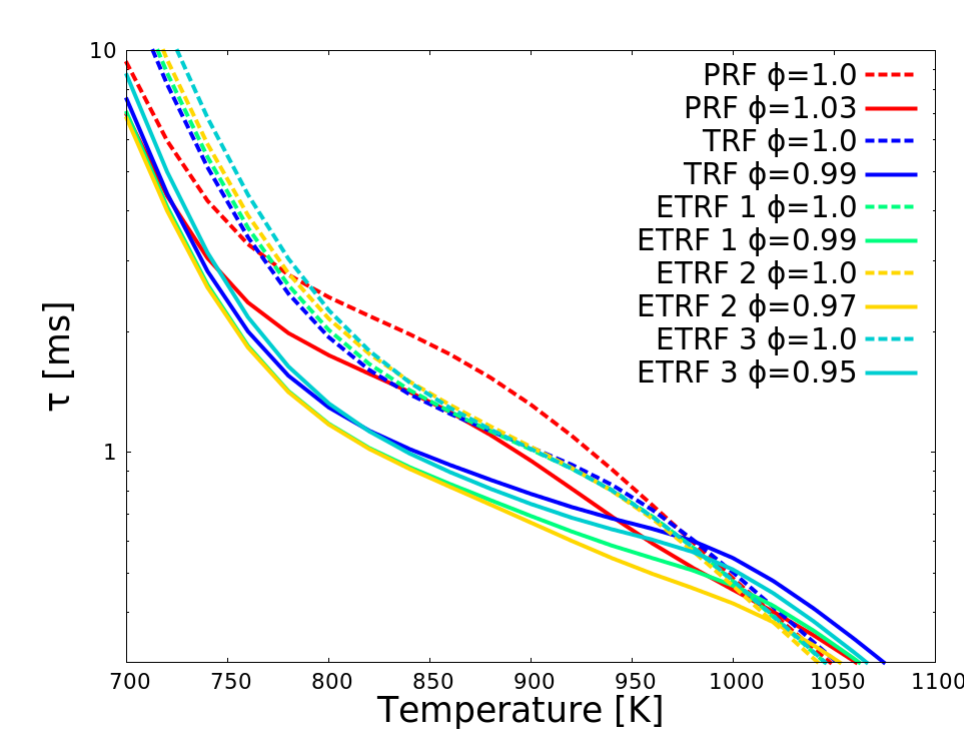Figure 3: Predicted ignition delay time for different mixtures with air as oxidizer at 60 bar using constant volume reactors.

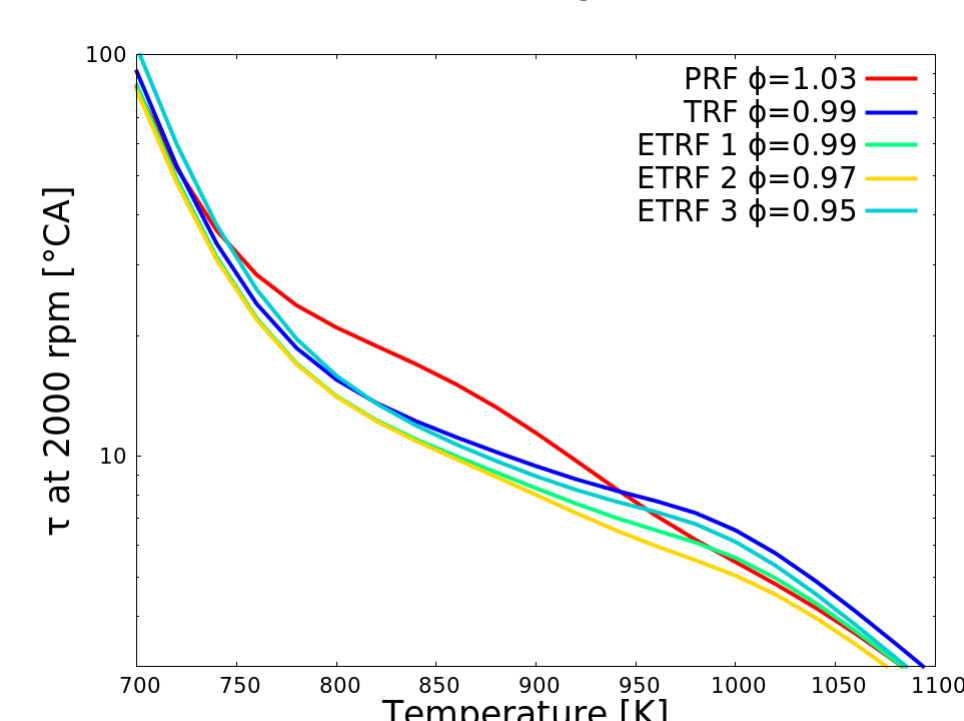Figure 2: Composition of the analyzed surrogates in mass fraction.

Figure 4: Ignition delay time converted from milliseconds to crank angle degree for a speed of 2000 rpm.

Combustion modelling approach

The combustion is predicted using the G-equation [4] and well stirred reactors [5] in the unburned zone to predict auto-ignitions. Auto-ignitions and laminar flame speed are predicted applying the ETRF reaction scheme from Seidel [1].]. The laminar flame speed is predicted and stored in look-up tables using LOGEresearch [6].

Flame front: $G(x_i, t) = G_0$

$$\frac{\partial(\bar{\rho}\tilde{G})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{G})}{\partial x_i} = \bar{\rho}_u s_t \left|\frac{\partial\tilde{G}}{\partial x_i}\right| + D'_t\kappa\left|\frac{\partial\tilde{G}}{\partial x_i}\right|$$

Burnt zone: $G > G_0$

$$s_t = s_l + u'\left\{-\frac{a_4 b_3^2}{2b_1}Da + \left[\left(\frac{a_4 b_3^2}{2b_1}Da\right)^2 + a_4 b_3^2 Da\right]^{1/2}\right\}$$

WSR model for emission prediction based on detailed chemistry [1]

Unburnt zone: $G < G_0$

WSR model for auto-ignition prediction based on detailed chemistry [1]

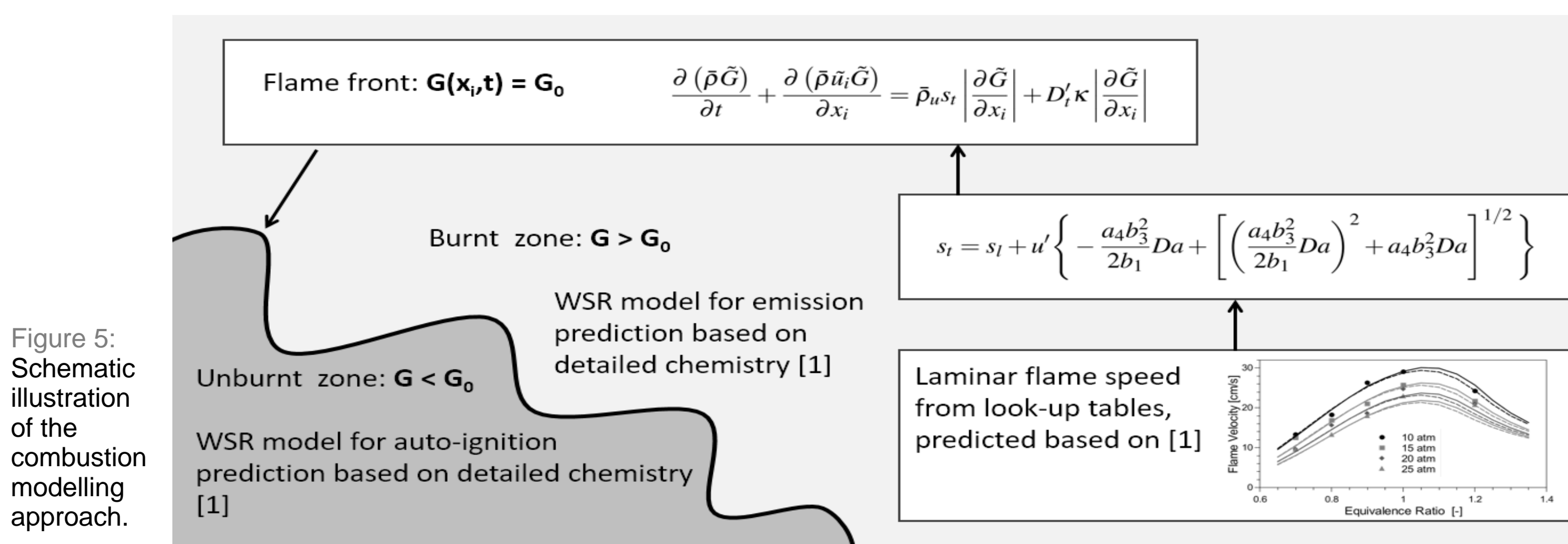Laminar flame speed from look-up tables, predicted based on [1]

Figure 5: Schematic illustration of the combustion modelling approach.

Knock evaluation

To make the study comparable, the same flow field in the CFD simulation was achieved by keeping air mass and fuel mass constant and applying the same laminar flame speed table. This leads to ignition kernel appearance at the same position, but also to a deviation in equivalence ratio of $\phi = 1 \pm 0.05$.
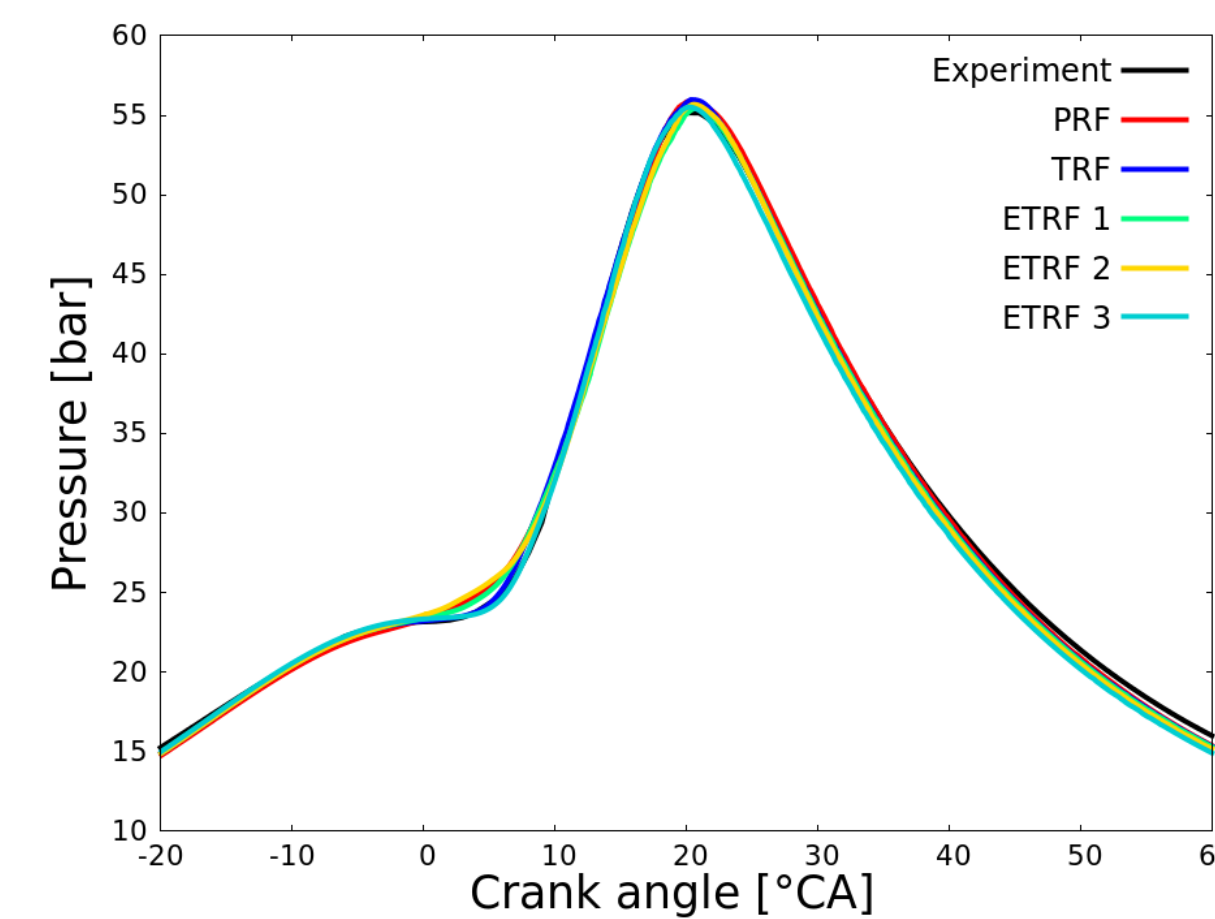

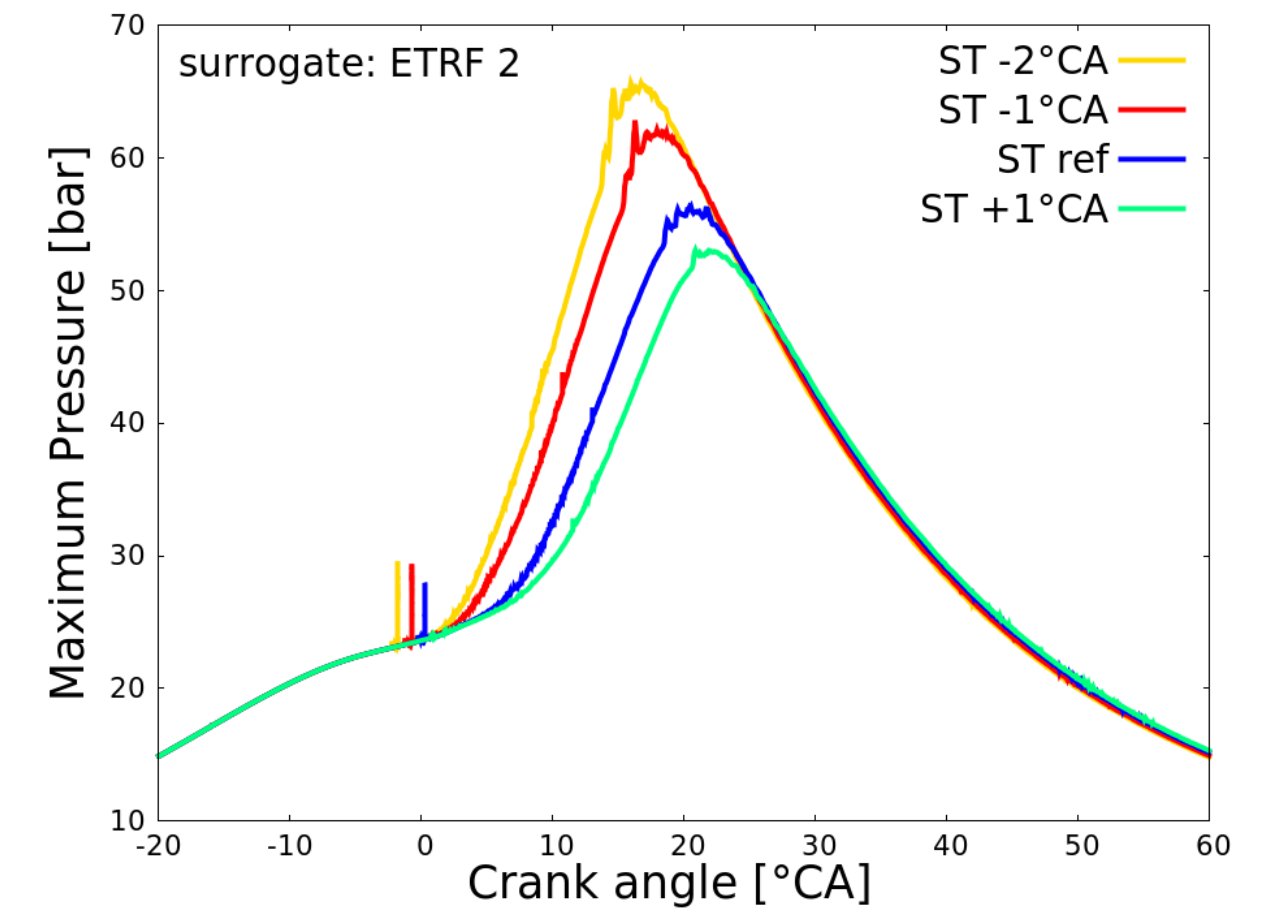Figure 6: Predicted mean pressure for the analysed surrogates.

Figure 7: Maximum predicted pressure for the spark timing sweep using surrogate ETRF 2.
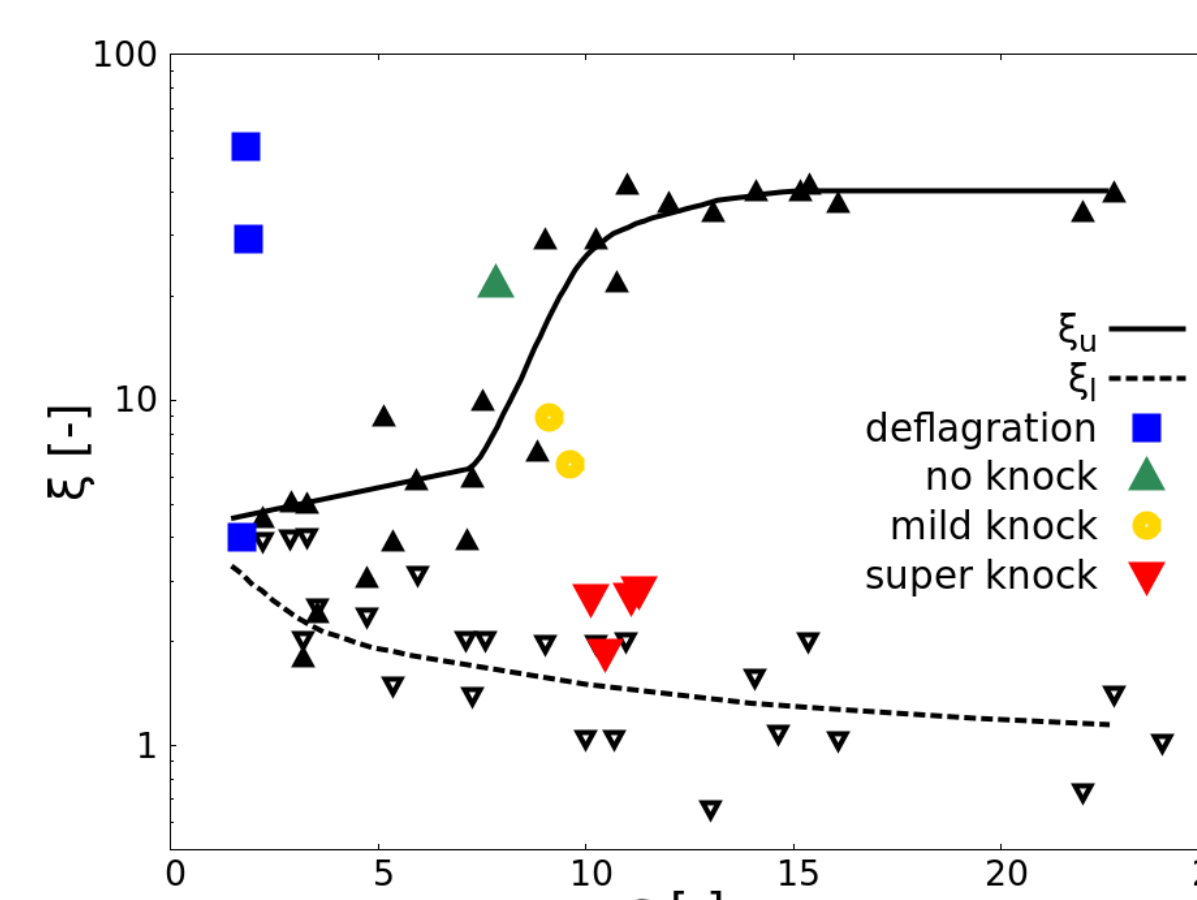

Figure 8: Developing detonation peninsula by Bradley et al. [7] and Gu et al [8]. Engine regime definition are taken from Bates et al. [9].
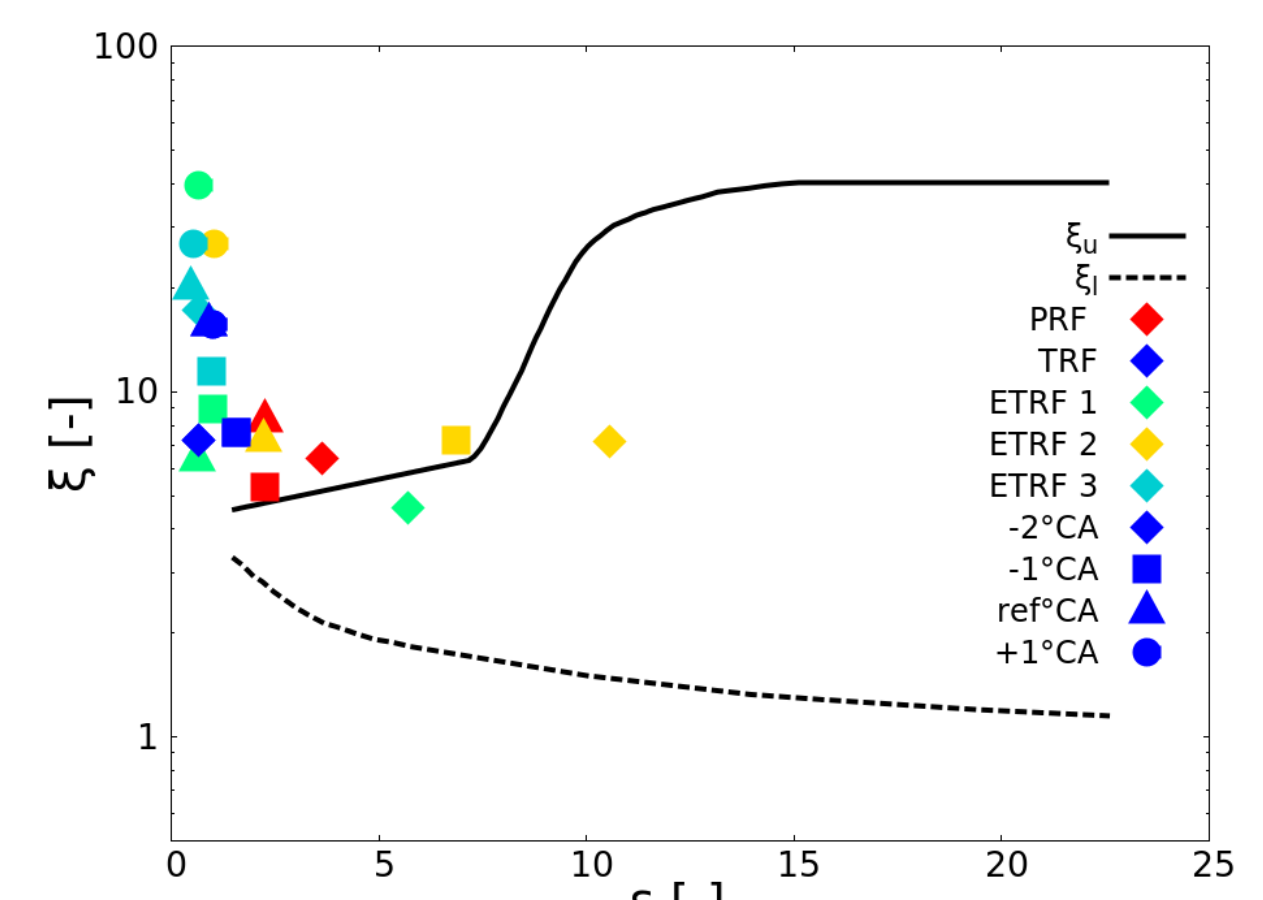

Figure 9: Evaluation of the auto-ignitions for the different surrogates and the spark timing sweep, as introduced in [10]. If more than one auto-ignition is predicted, only the strongest is shown.
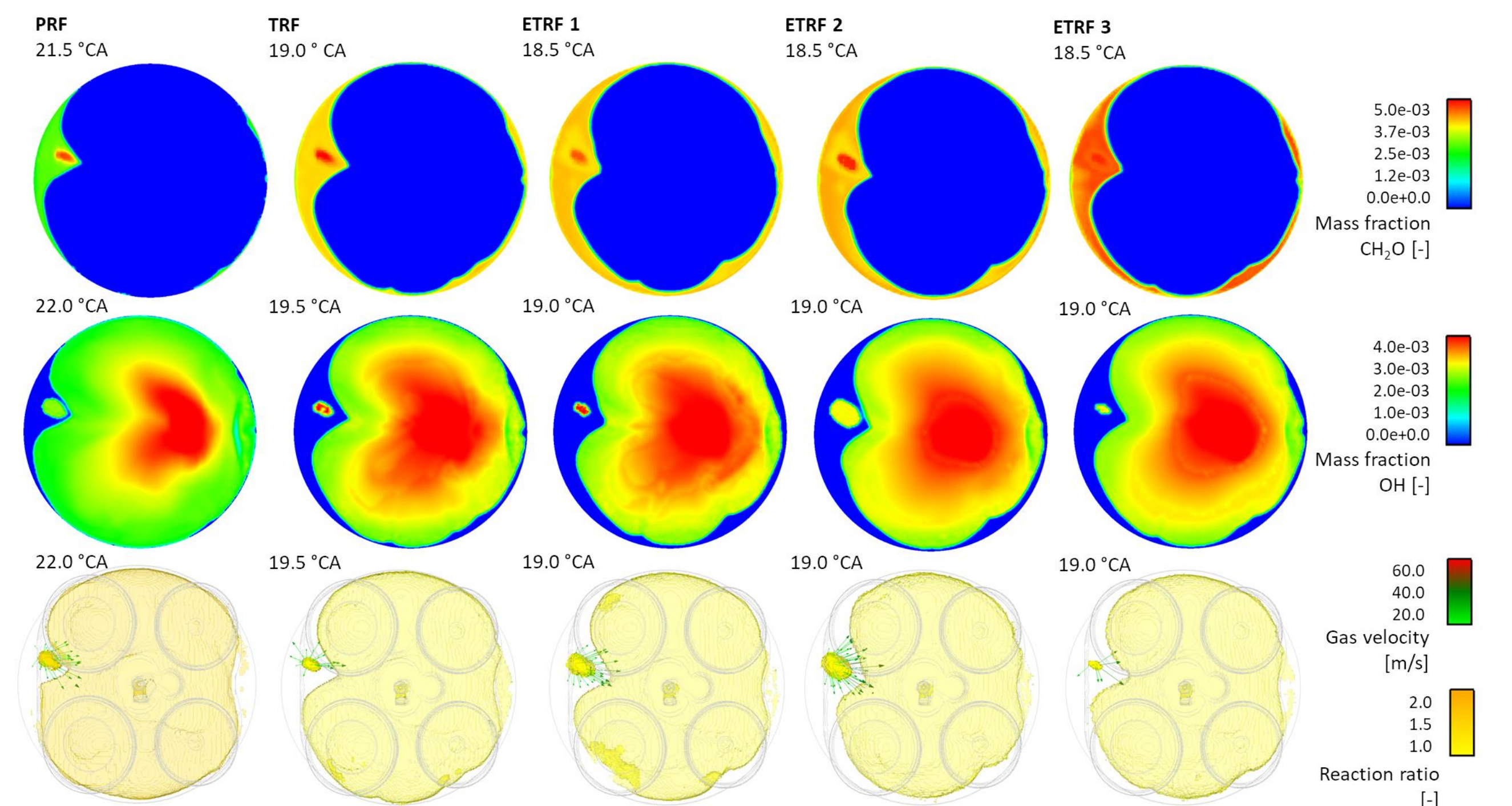

Figure 10: Time step of first auto-ignition event and previous. From left to right: Mass fraction CH₂O, mass fraction OH and flame propagation determined from an iso-volume at reaction ratio ≥ 1.0 and gas velocity. View from top.
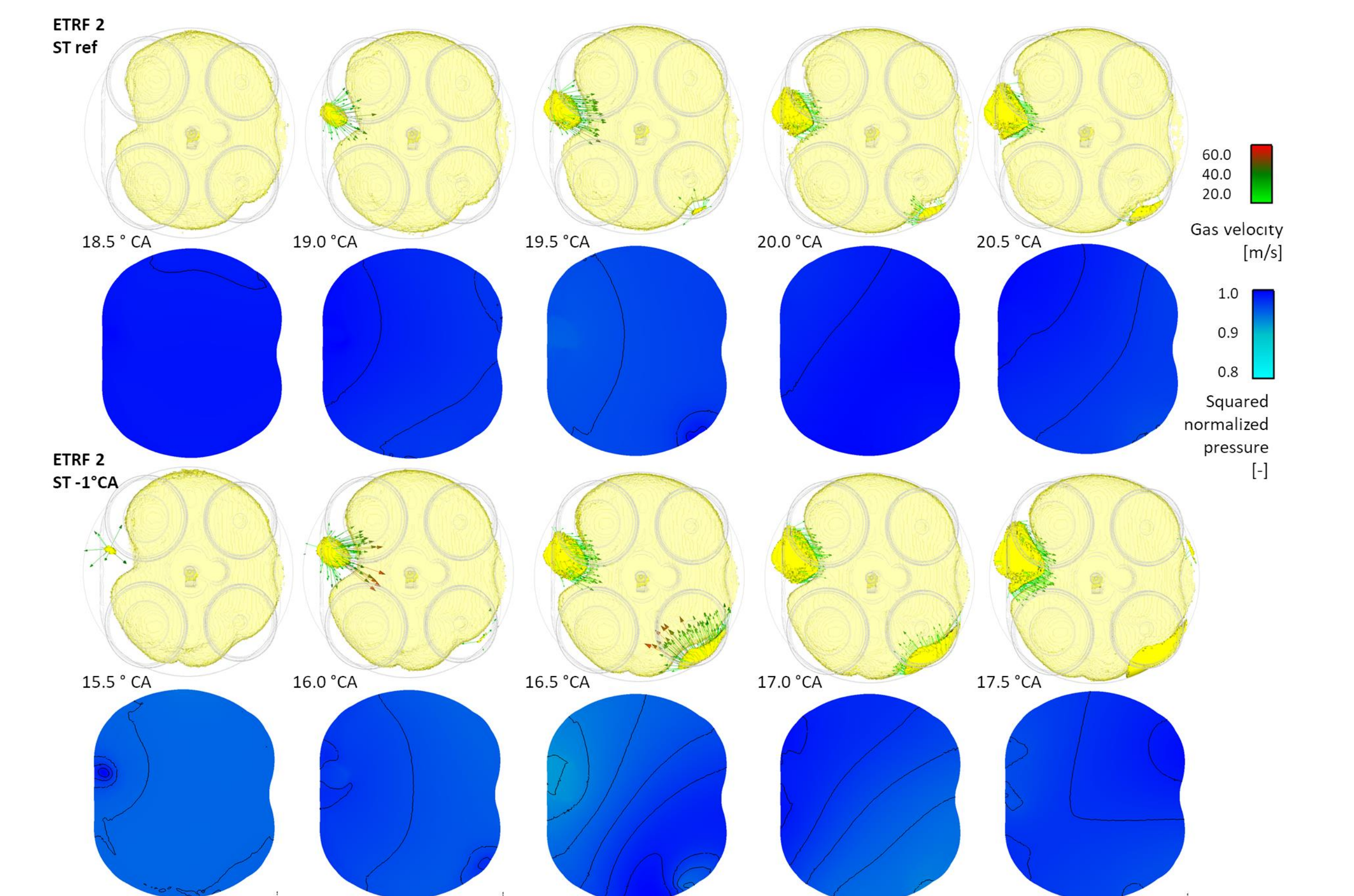

Figure 11: Transition from deflagration to knocking combustion illustrated using the ignition kernels, gas velocities and local pressure gradients. View from top.

Conclusions

Even though the surrogates have the same RON, the tendency to auto-ignite in the engine simulations is very different. The found shift in KLSA is 2°CA and bigger. The predicted sensitivities may also depend on the specific surrogate properties such as density, heat capacity, lower heating value and C:H:O-ratio.

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