CONVERGE User Conference–North America

Surrogate Impact on Flame Propagation and Knock Prediction

C. Netzer, F. Mauss,
Brandenburg University of Technology, Cottbus, Germany

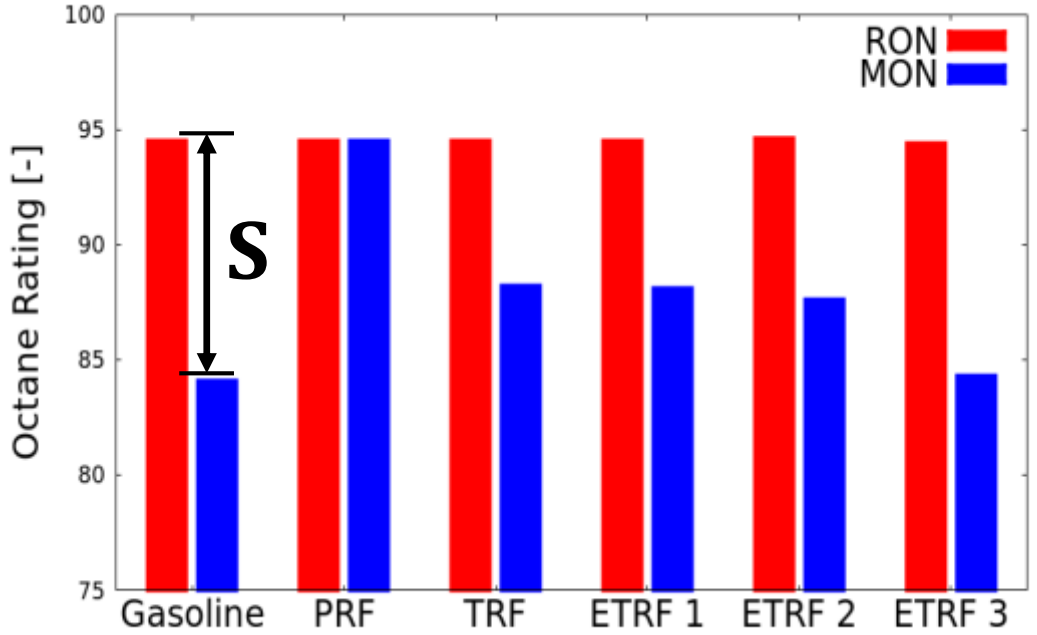
L. Seidel, H. Lehtiniemi
LOGE AB, Lund, Sweden

September 24–28, 2018, Madison, USA

Objective

Fuel octane rating characteristics:

- Research Octane Number *RON*
- Motored Octane Number *MON*
- Octane Sensitivity *S = RON – MON*



Fuel surrogate

- Pure *iso*-Octane
- Primary Reference Fuels (PRF)
  - *iso*-Octane (RON = MON = 100)
  - *n*-Heptane (RON = MON = 0)
- Toluene Reference Fuels (TRF) and Ethanol containing Toluene Reference Fuels (ETRF)
  - *iso*-Octane (RON = MON = 100)
  - *n*-Heptane (RON = MON = 0)
  - Toluene (RON = 120 / MON = 109)
  - Ethanol (RON = 109 / MON = 90)

Outline

I. Objective

II. Combustion Modeling Approach

III. Impact of Gasoline Surrogate on Flame Propagation

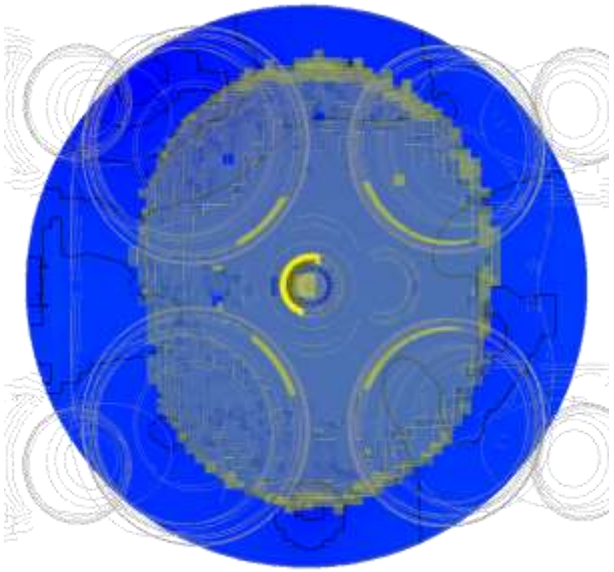
IV. Impact of Gasoline Surrogate on Knock Prediction

V. Summary and Conclusions

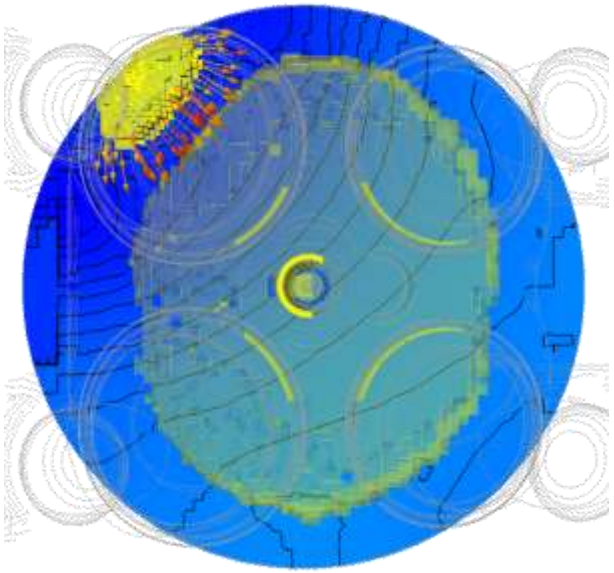
MODEL APPROACH

Knock Prediction

- G-equation and well stirred reactors in the unburned zone
  - both available in Converge 2.4.9
- Laminar flame speed is retrieved from a look-up table composed for a surrogate

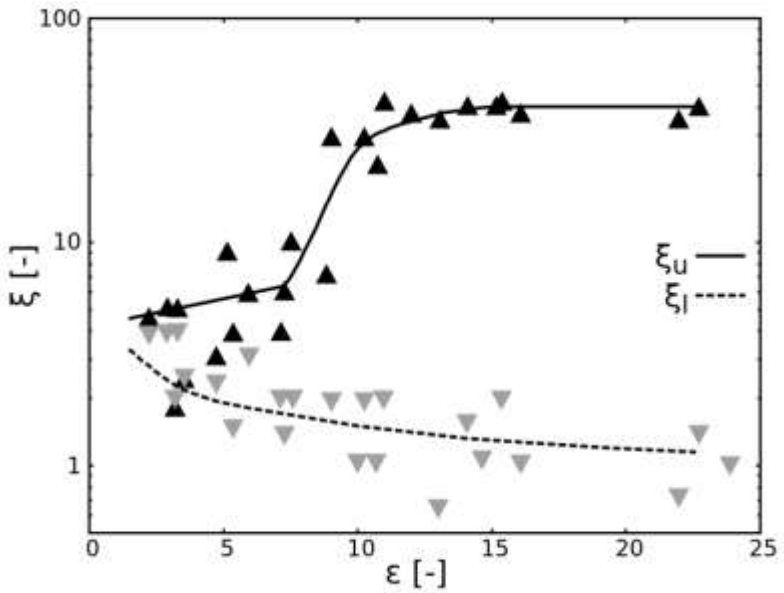


- Auto-ignition in the unburned zone is predicted using the ETRF mechanism by Seidel (2017)
  - ETRF: Ethanol, Toluene, iso-Octane & n-Heptane
  - 188 species and 1049 reactions
  - Major exhaust-out emissions
  - Thermal NOx

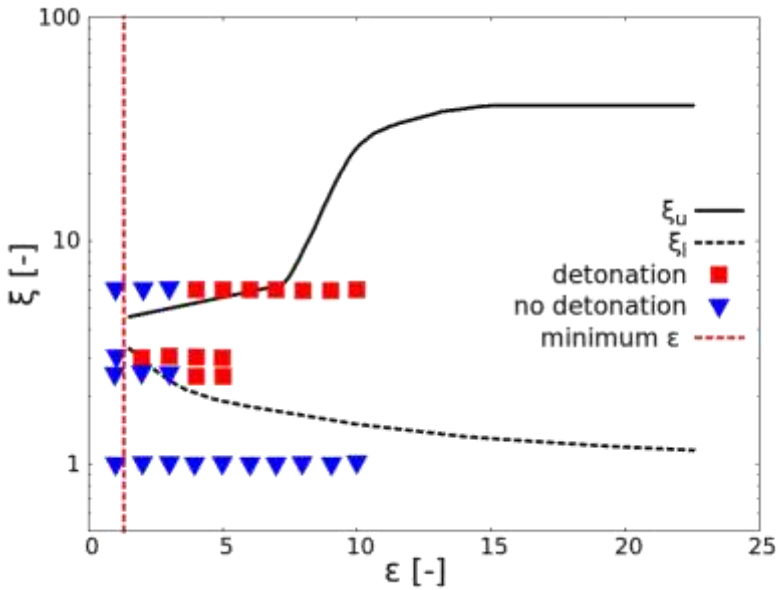


Knock Evaluation

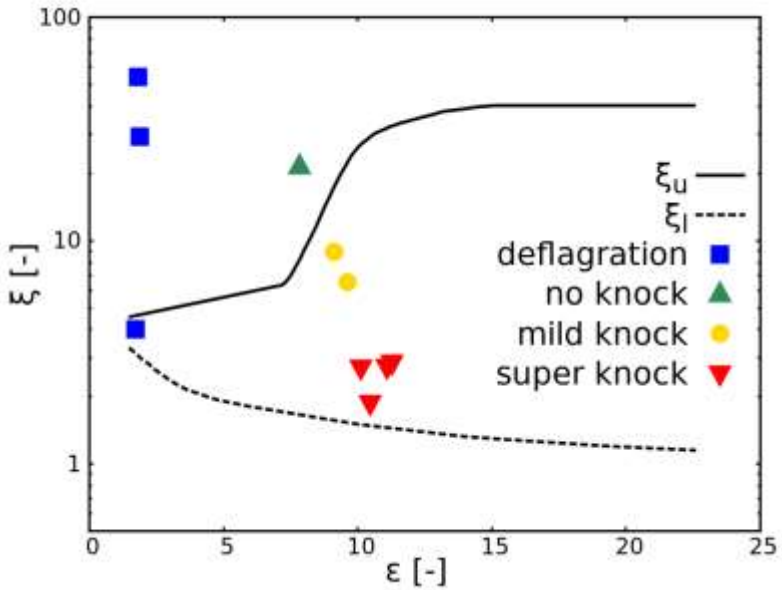
- Detonation diagram by Bradley and co-workers (2002)
  - Resonance parameter: $\xi = \frac{a}{u} = a \frac{\partial T}{\partial x} \frac{\partial \tau}{\partial T}$
  - Reactivity parameter: $\varepsilon = \frac{l}{a \tau_e}$



Bradley et al. 2002



Peters et al. 2013



Bates et al. 2016

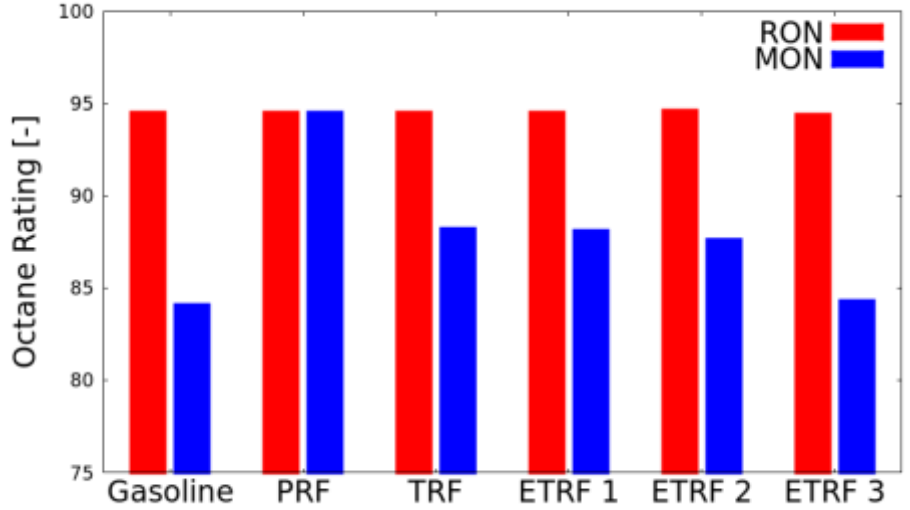
SURROGATE FORMULATION

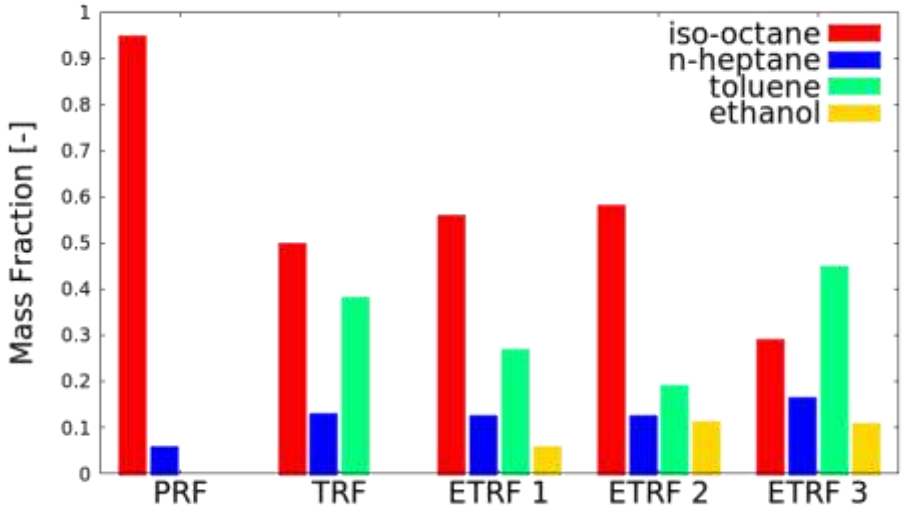
Surrogate Formulation

- Composed using the correlations by Morgan et al. (2010) and Anderson et al. (2010)

		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/m^3	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

*Input properties





FLAME PROPAGATION

Laminar Flame Speed Prediction

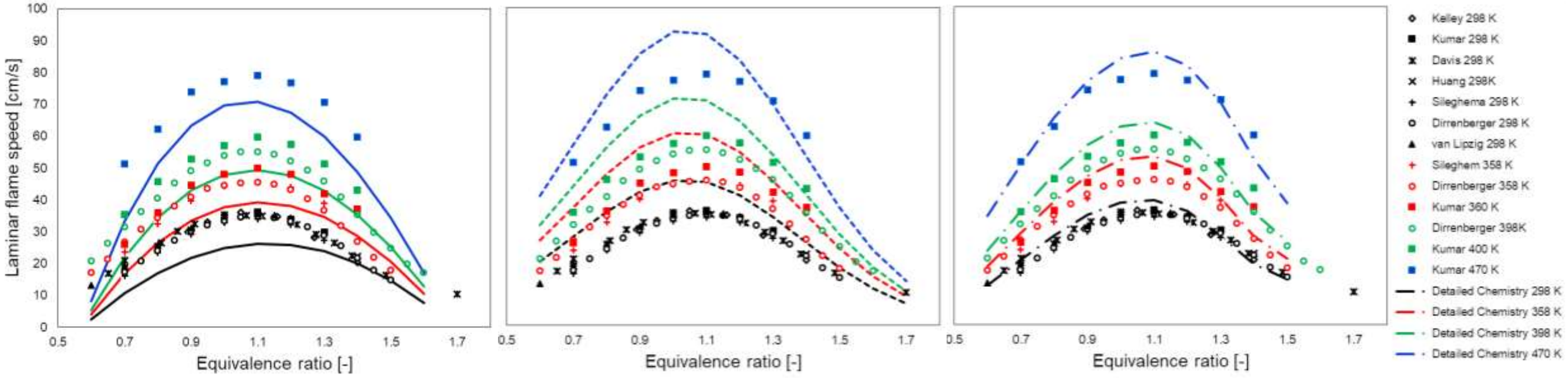
- Fuel: iso-octane
- Correlation by Metghalchi and Keck (1982)
- Correlation by Gülder et al. (1984)
- Prediction using the ETRF LOGEGasoline by Seidel (2017)

- Temperature dependency:

Metghalchi and Keck

Gülder et al.

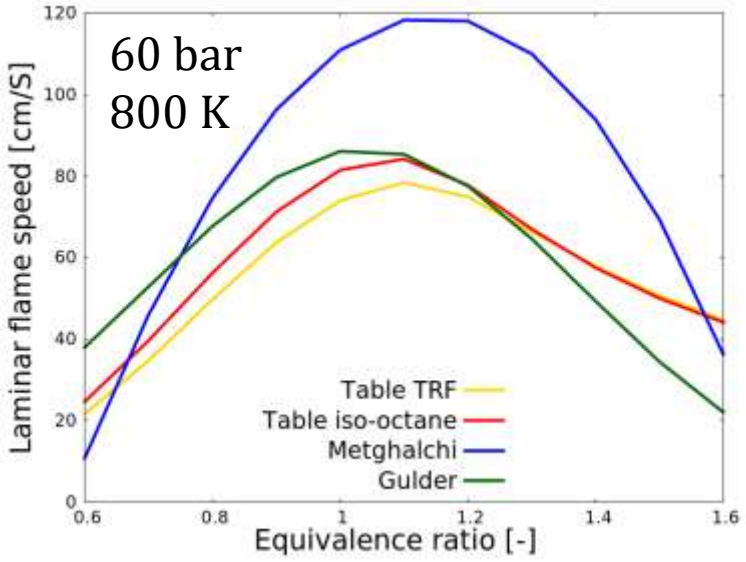
Seidel



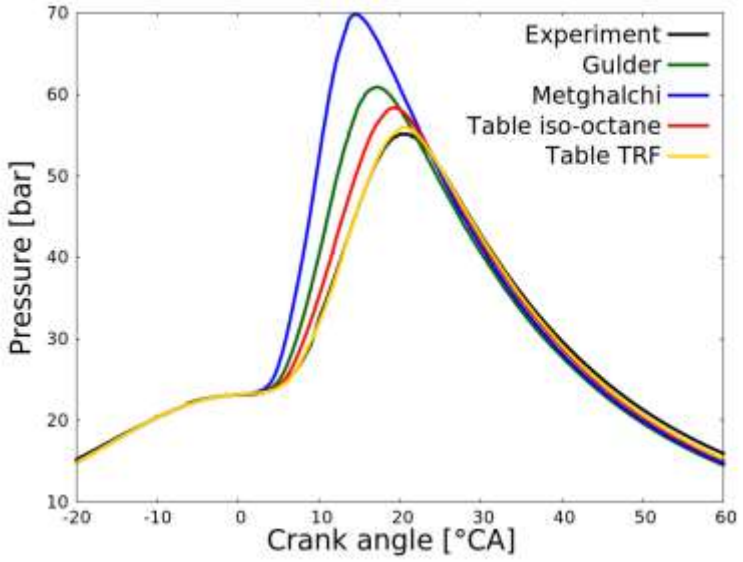
Engine Conditions iso-Octane

- Simulations
  - Correlation by Metghalchi and Keck (1982)
  - Correlation by Gülder et al. (1984)
  - Detailed chemistry flame speed tables using LOGEgasoline by Seidel (2017)
    - Iso-Octane
    - TRF RON 94.5 (used for calibration!)

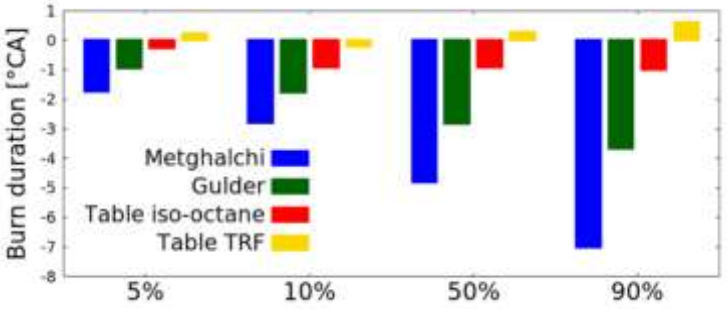
- Laminar Flame Speed



- Combustion Prediction



- Burn duration Sim vs Exp

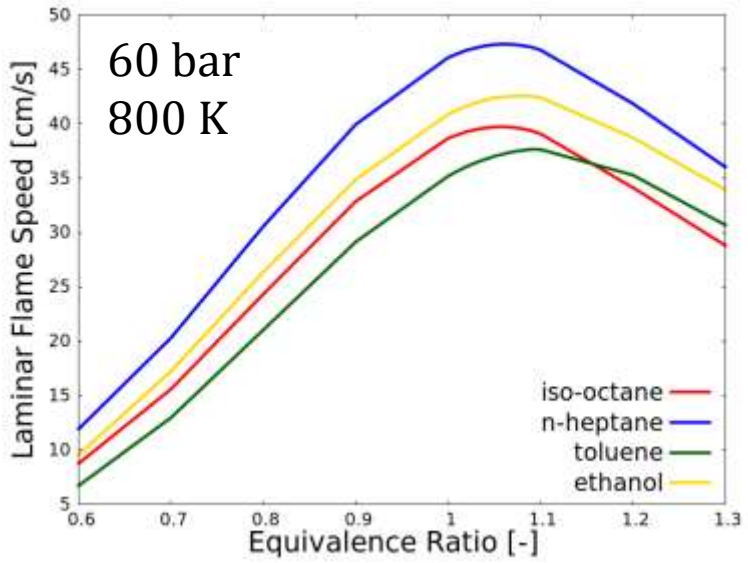


	ΔCA_{50}	Δp_{max}
Iso-octane models	4°CA	12 bar
Detailed chemistry Iso-octane vs TRF	1.5°CA	3 bar

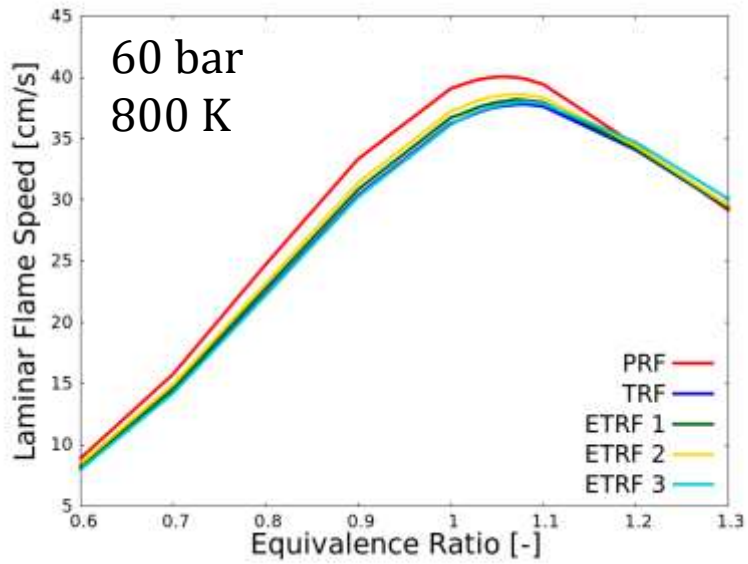
Engine Conditions ETRF Surrogates

- Simulations
  - Detailed chemistry flame speed tables using LOGEgasoline by Seidel (2017) for the 5 surrogates

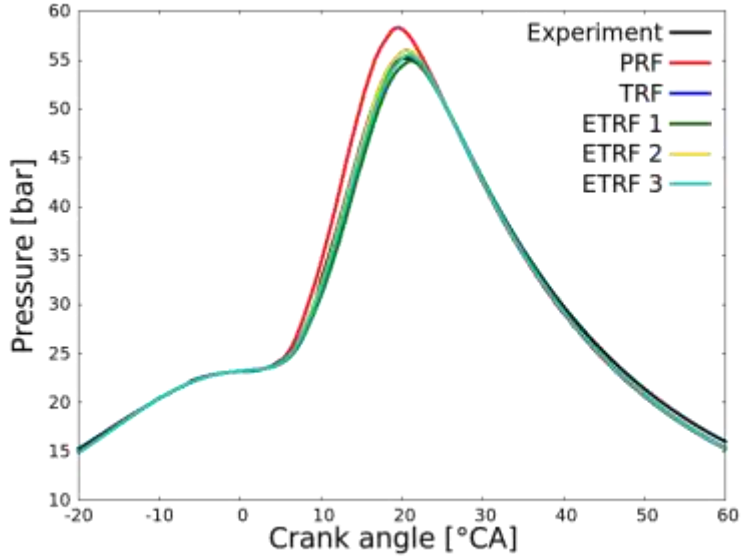
- Surrogate components



- Surrogates



- Combustion Prediction



	ΔCA_{50}	Δp_{max}
Surrogates	1.5°CA	3.5 bar

AUTO-IGNITION PREDICTION

Auto-Ignition Prediction – Same Fuel Mass

- Same fuel and air mass
- Different H:C:O-ratios

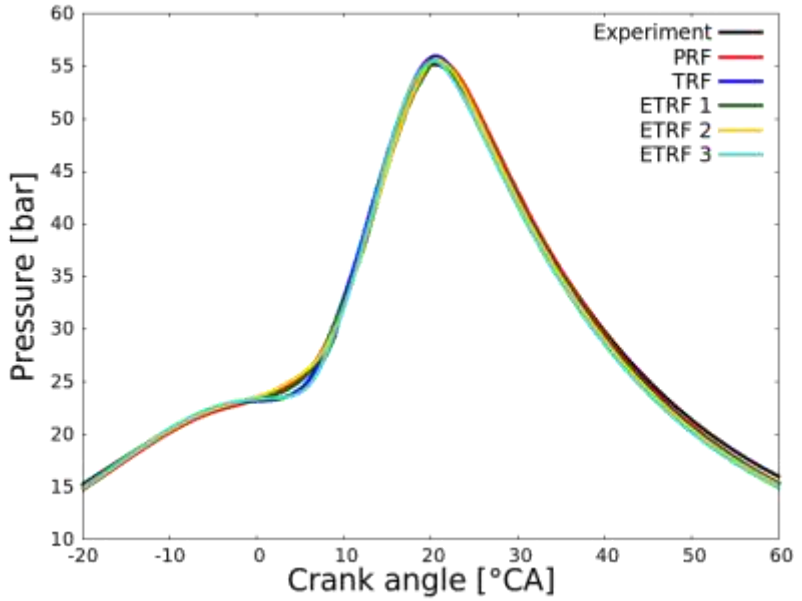
→ ϕ = 1+/- 0.05

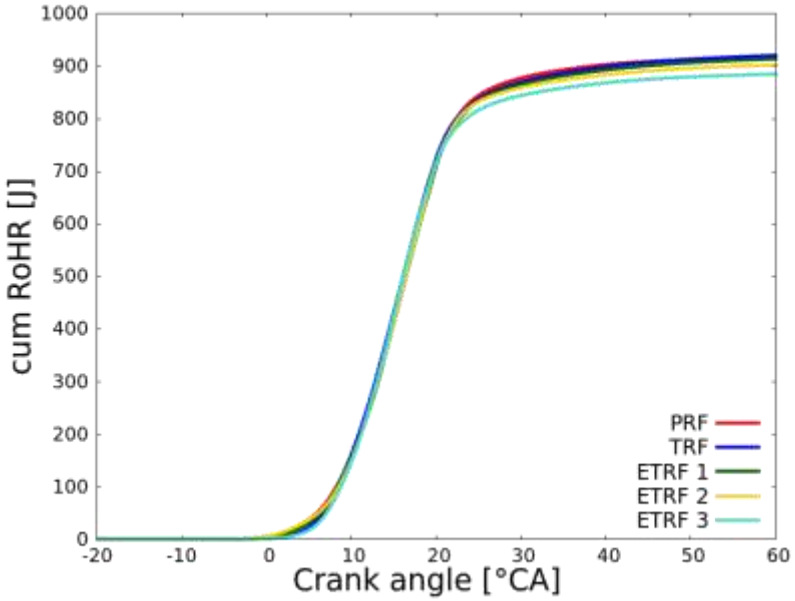
→ Different trapped energy at IVC

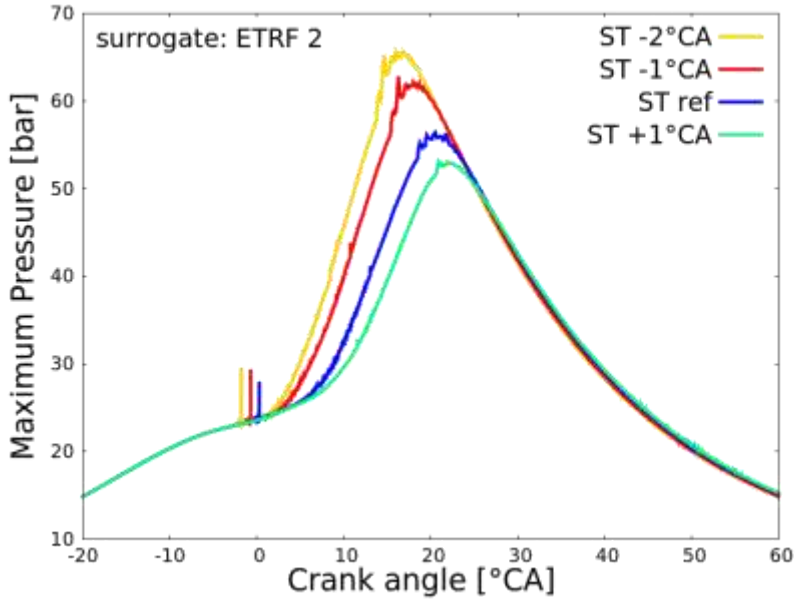
- Same flame speed table

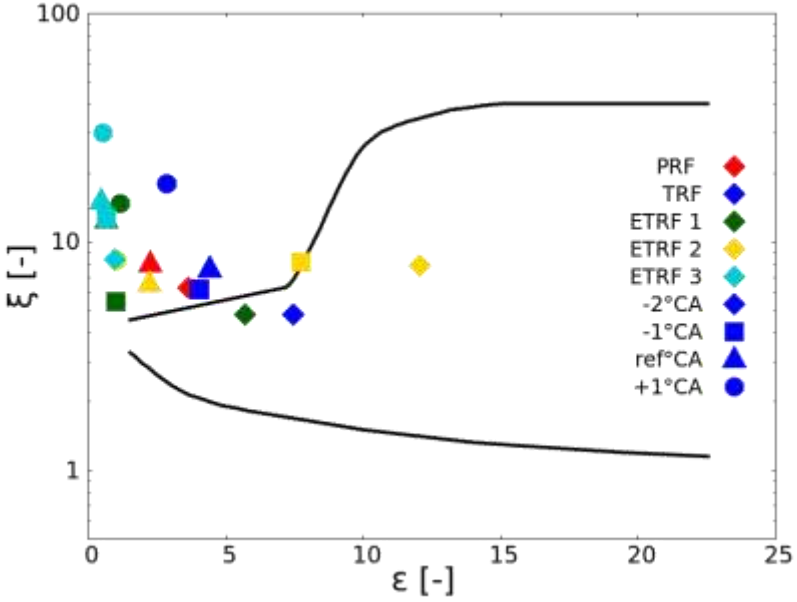
→ Similar flame propagation and location of the hotspots

- Spark timing sweep
- Auto-igniton evaluation using the detonation diagram

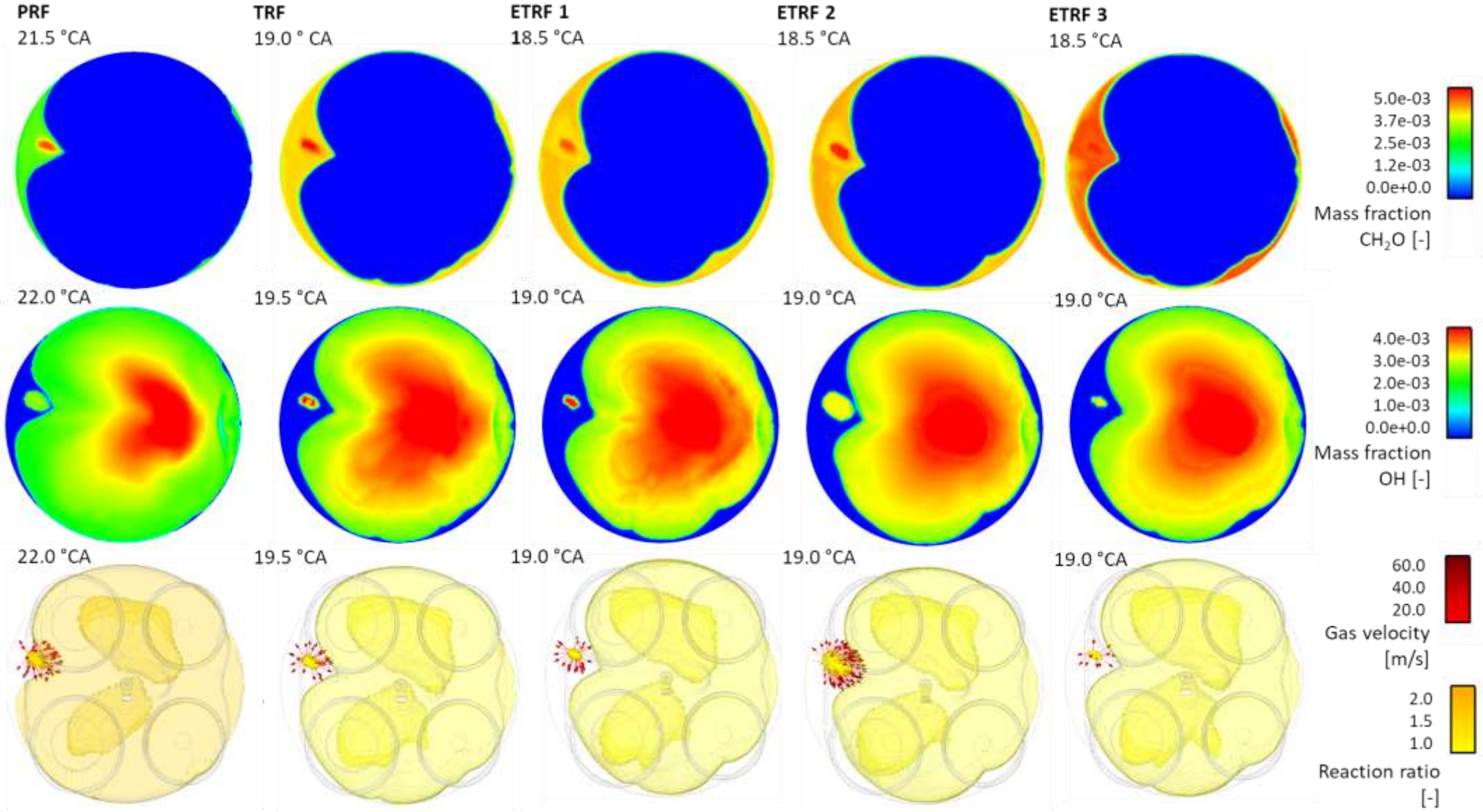






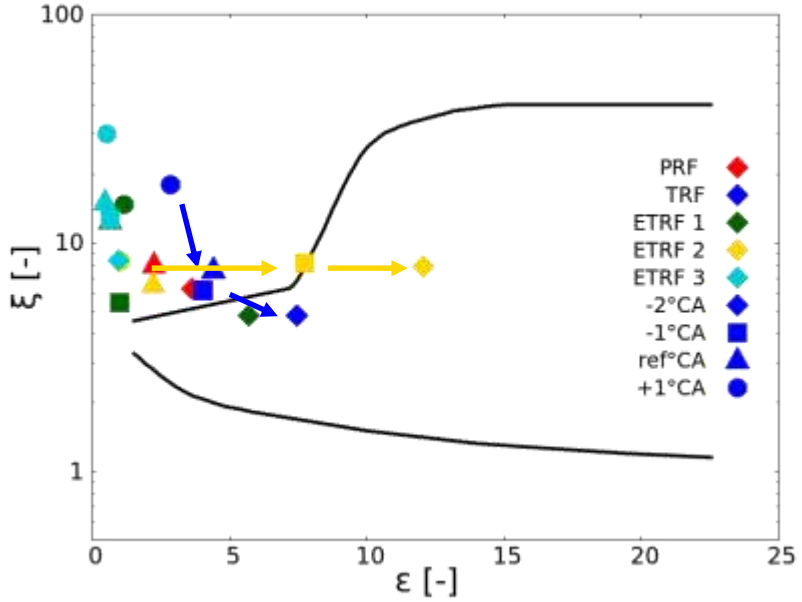


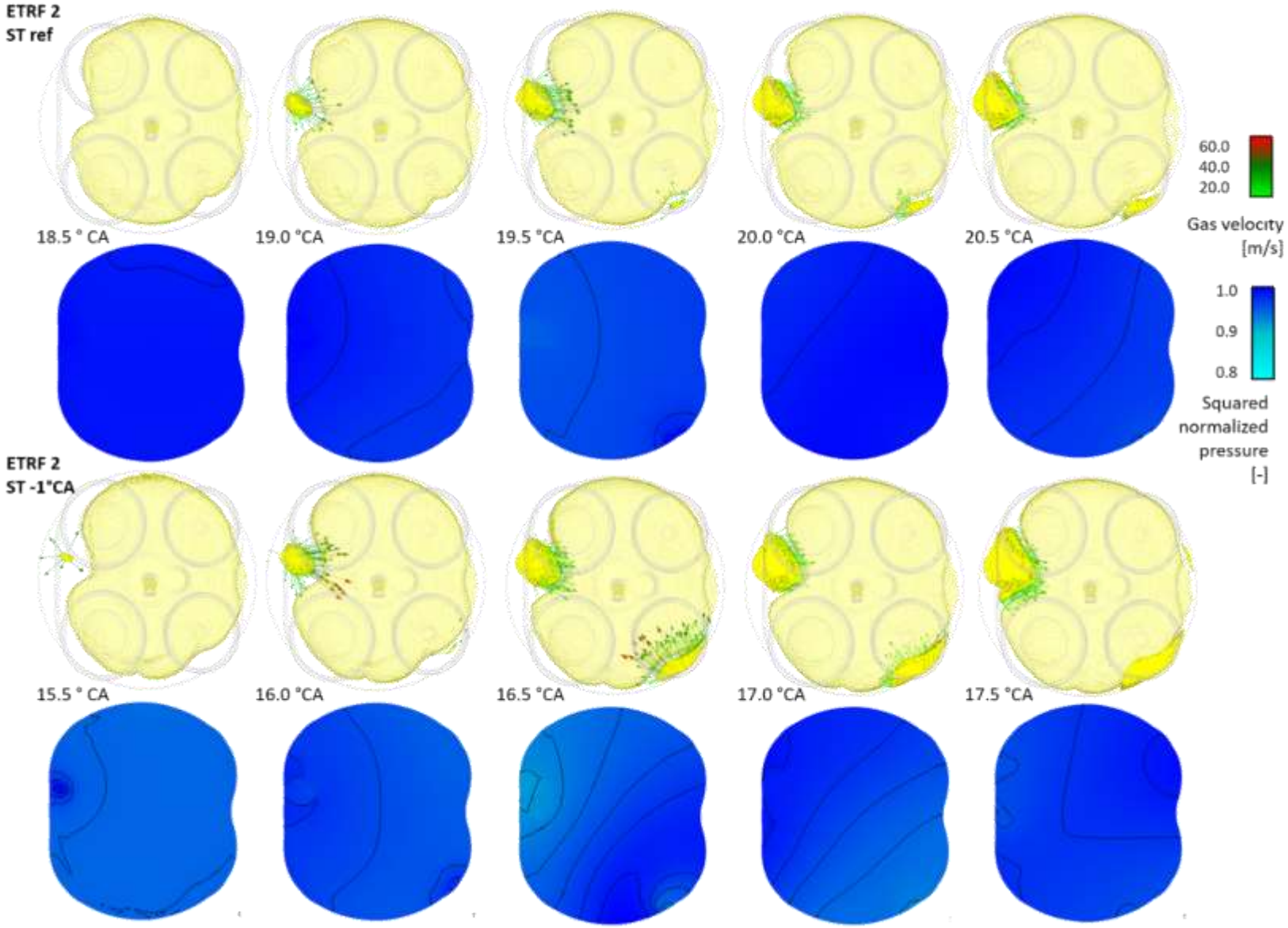
Auto-Ignition Prediction – Same Fuel Mass



Auto-Ignition Prediction – Same Fuel Mass

- Transition from Deflagration to Developing Detonation





Auto-Ignition Prediction – Same Fuel/Air Equivalence Ratio

- Same fuel/air-equivalence ratio

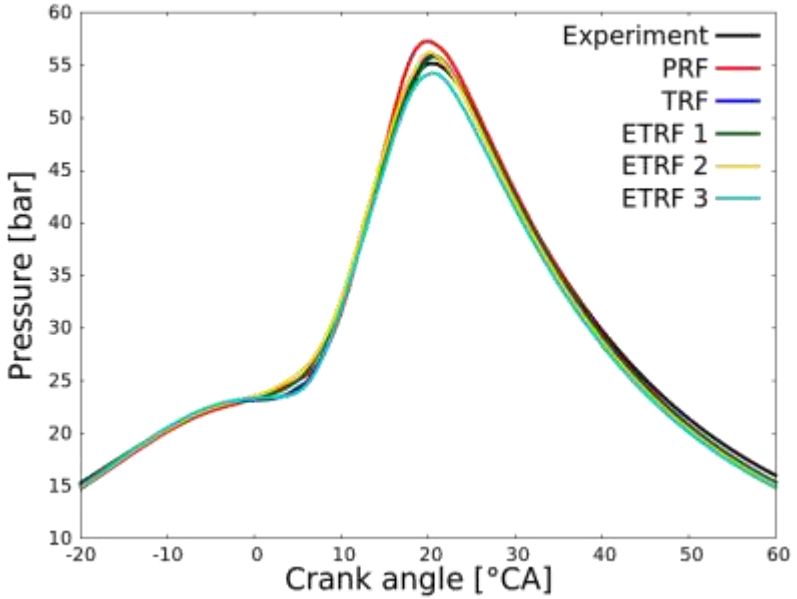
→ ϕ = 1+/- 0.01

- Surrogate specific flame speed table

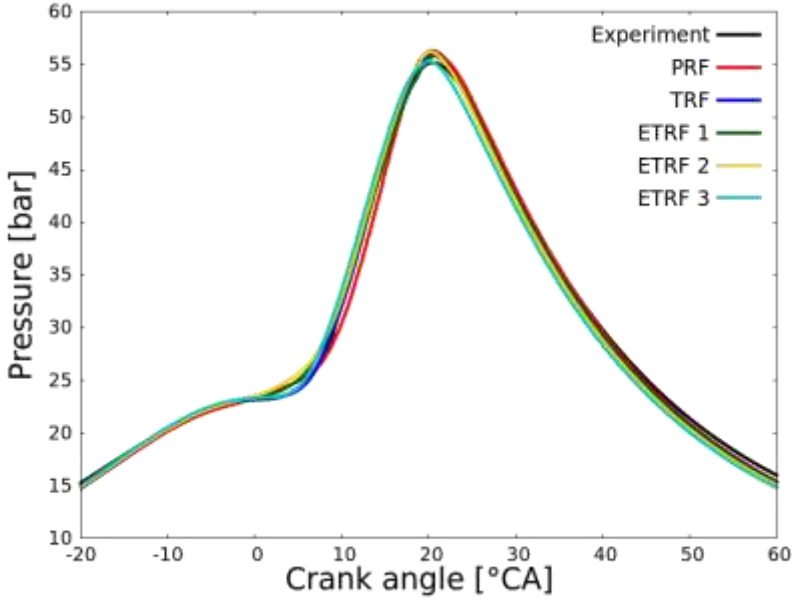
→ Spark timing calibration

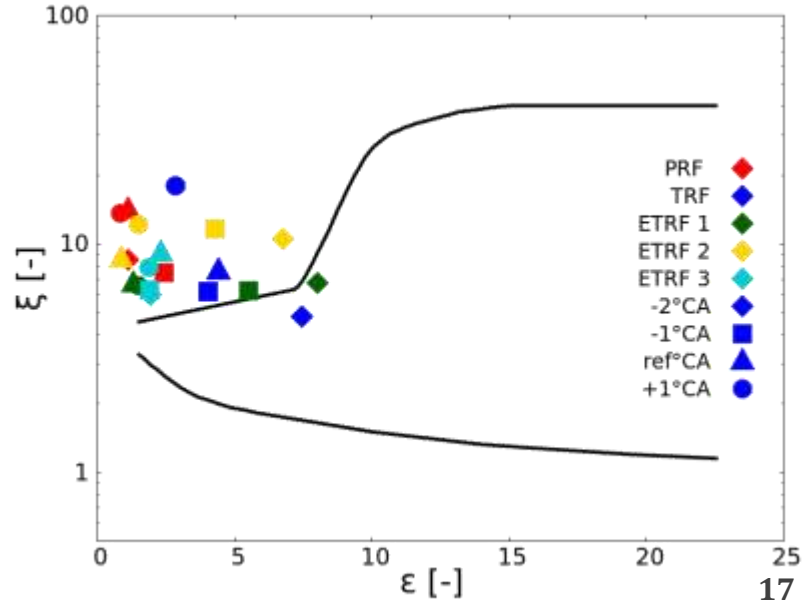
	PRF	ETRF 3
ΔST	+2°CA	-0.5°CA

- Spark timing sweep
- Auto-ignition evaluation using the detonation diagram

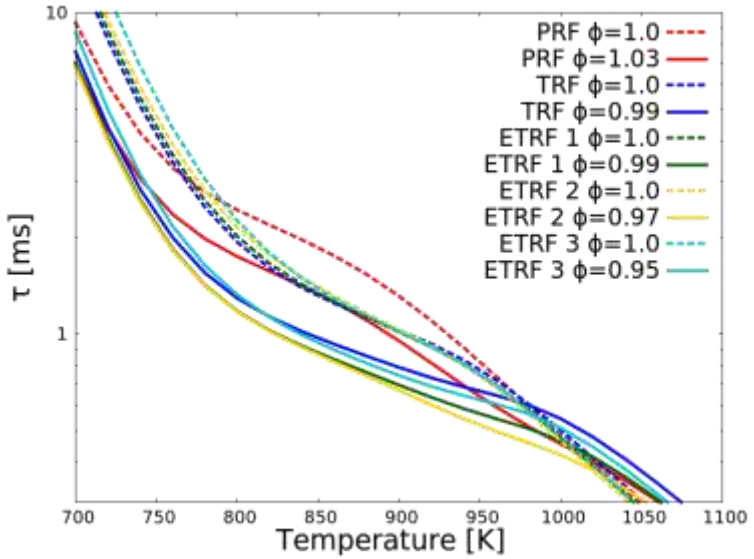


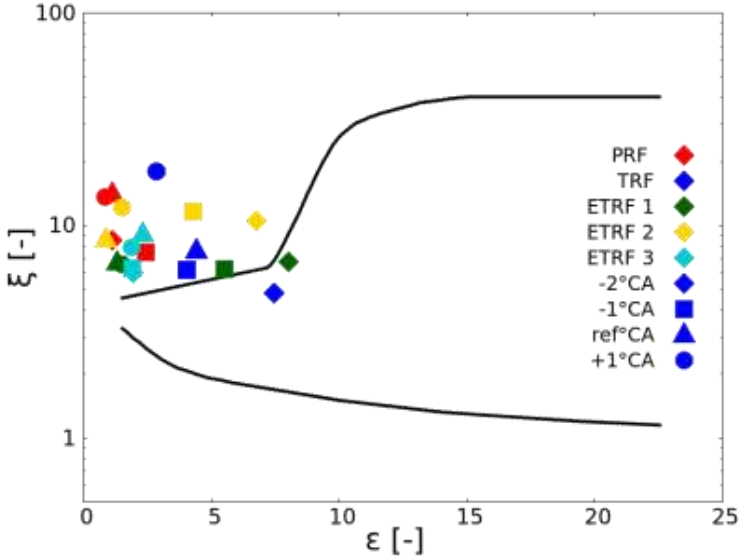
ST





Auto-Ignition Tendency Estimation





Zero-dimensional, homogenous simulations:

- CVR = Constant Volume Reactor
- RCM = Rapid Compression Machine (transient)

MON		ETRF 3 > ETRF 2 > ETRF 1 > TRF >PRF
CVR	1.0	TRF > ETRF 1 > ETRF 2 > ETRF 3 > PRF
CVR	1+/-0.05	ETRF1 | ETRF 2 > TRF > ETRF 3 > PRF
RCM	1+/-0.05 $T_{initial}$ = 600 K	ETRF2 > ETRF 1 > TRF | ETRF 3 > PRF
RCM	1+/-0.05 $T_{initial}$ = 800 K	ETRF2 | PRF > ETRF 1 | ETRF 3 > TRF
CFD	1+/-0.05	ETRF2 > TRF > ETRF 1 > PRF > ETRF 3
CFD	1+/-0.01	TRF > ETRF 1 > ETRF 2 > PRF | ETRF 3

SUMMARY AND CONCLUSIONS

Summary and Conclusion

Summary

1. Surrogates with same RON, but different MON have been composed: PRF, TRF and ETRF
2. Analysis of impact of the laminar flame speed model
3. Air mass and fuel mass constant and similar flame propagation (3d CFD)

   → ignition kernel appearance at the same position (3d CFD)
4. Same fuel/air equivalence ratio and surrogate specific laminar flame speed table

   → Shift in spark timing necessary
5. Comparison to knock tendency in constant volume reactors and rapid compression machine simulations
6. Step 3. and Step 5. have been repeated using the scheme from Cai and Pitsch (2015)

Summary and Conclusion

Flame propagation

- Correlation vs. detailed chemistry $\Delta CA_{50,max}$ = 4°CA, Δp_{max} = 12 bar
- Surrogate impact surrogates $\Delta CA_{50,max}$ = 1.5°CA, Δp_{max} = 3.5 bar

Auto-ignition and knock prediction

- For the same RON, the auto-ignition tendency in the engine simulations is very different
- The found shift in KLSA is >2 °CA and bigger, ETRF 2 and TRF agree with experiment
- No clear connection between MON and knock tendency
- No clear connection between ignition delay time in homogenous reactors and knock tendency
- This finding is irrespective of the used reaction scheme, but may depend on the specific surrogate properties such as density, heat capacity, lower heating value and C:H:O-ratio
- We found that it is not possible to estimate the knock tendency of different surrogates in the CFD simulation solely from homogenous reactor calculations

CONVERGE User Conference–North America

Thank you!

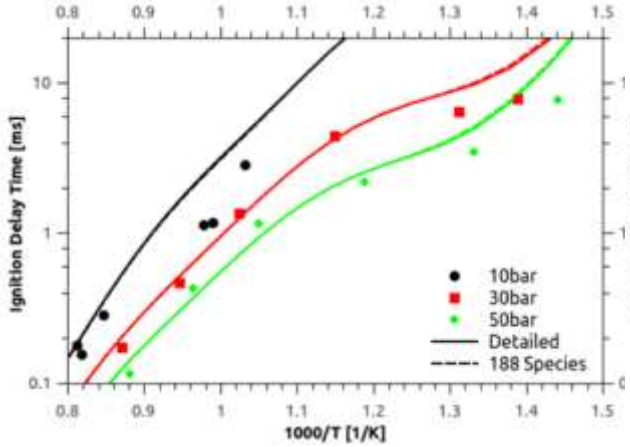
C. Netzer, F. Mauss,
Brandenburg University of Technology, Cottbus, Germany

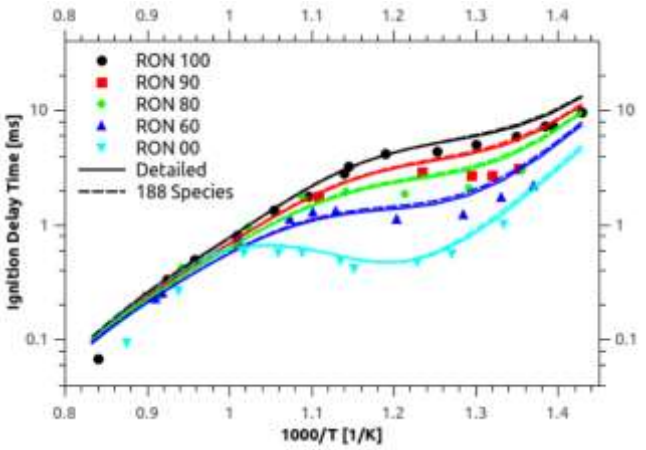
L. Seidel, H. Lehtiniemi
LOGE AB, Lund, Sweden

September 24–28, 2018, Madison, USA

Mechanism Validation

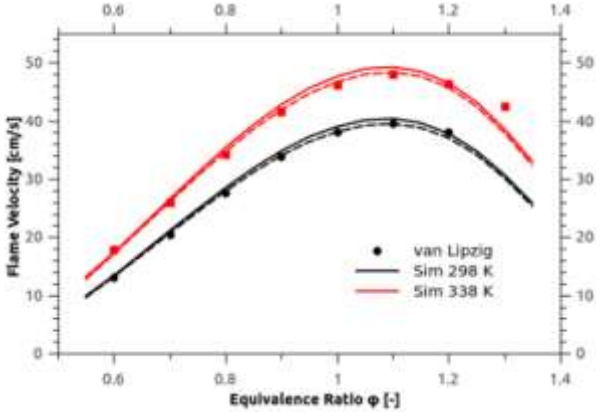
Ignition delay time for a mixture of 0.72 toluene and 0.28 n-heptane (mole fraction) at φ = 0.3, p = 10, 30, 50 bar for the detailed and reduced reaction scheme. Experimental data from Herzler et al.

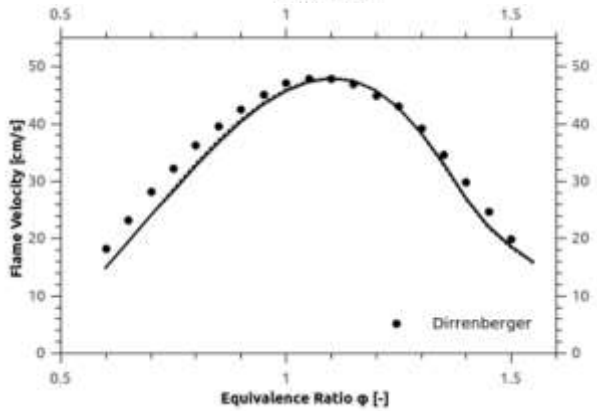




Measured ignition delay time of iso-octane/n-heptane mixtures at 40 ± 2 bar, φ = 1 from Fieweger et al. [11]. Simulation for the detailed and reduced reaction scheme using upper pressure limit.

Laminar flame speeds at 1 atm and 358 K with air as oxidizer for a mixture of 33.3% n-heptane, 33.4% iso-octane, and 33.3% ethanol (liquid volume fraction). Experimental data from van Lipzig et al. Solid line: detailed reaction scheme; Dashed line: reduced scheme.





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, 36.88% toluene and 15.0% ethanol (liquid volume fraction). Experimental data from Dirrenberger et al. Solid line: detailed reaction scheme; Dashed line: reduced scheme.