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Universal Autoignition Models for ‚designer' fuels in HCCI combustion

Vandersickel Annelies, Yuri M. Wright and Prof. K. Boulouchos
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IEA Task Leader Meeting,
Nara, July.2010

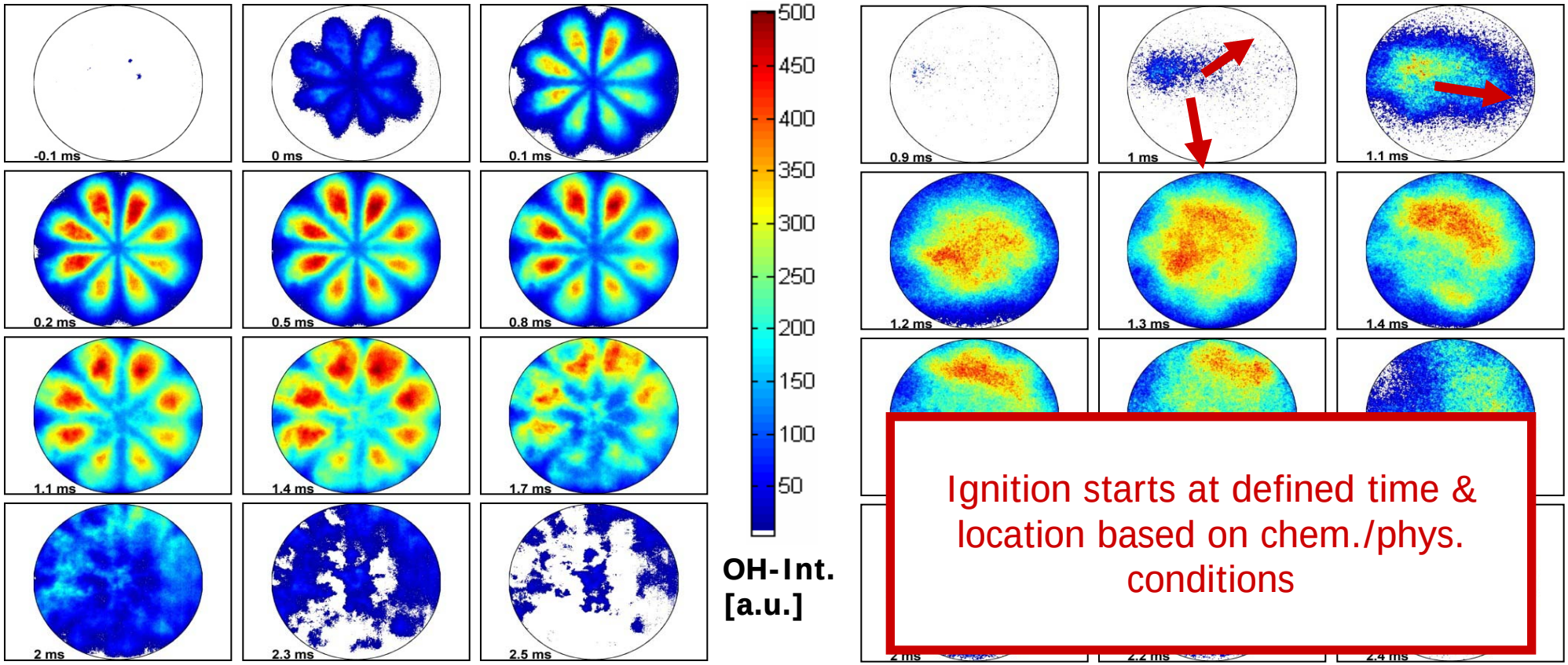
Universal Autoignition Models for ‚designer' fuels in HCCI combustion

CONTENT

- Introduction on HCCI & project
- 2 modeling approaches:
  - ‚3 Arrhenius' Model with Ignition Integral
  - Lumped Reaction Model
- Conclusions & Outlook

HCCI – an alternative combustion mode

- **Diffusion combustion**
- **HCCI combustion**



avg. OH-intensity (11 cycles)

avg. OH-intensity (12 cycles)

Joint Research Project

How do FUEL PROPERTIES affect HCCI ignition ?!??

	1	2	3	4	5	6	7	8	9	10
	CEC-REF	**n-Hept**	**Naptha 1**	**Naptha 2**	**Kero 1**	**Kero 3**	**CCS**	**Diesel 1**	**Diesel 2**	**Diesel 3**
Cetane Number (CN)	54.5	57	35.4	48.2	38.4	50.3	44.2	50.3	56.7	60.4
% normal, iso-parrafins	86.1	100	70.8	53.3	35.91	69.41	79.50	100	100	100
% cyclo-parraffins	-	-	29.3	46.7	51.93	31.22	-	-	-	-
% aromatics	9.4	-	-	-	12.16	-	20.50	-	-	-
% olefins	4.5	-	-	-	-	-	-	-	-	-
Initial Boiling Point (IBP °C)	209.8	98	87.0	92.2	153.3	150.2	158.7	192.2	205.7	229.8
Final Boiling Point (FBP °C)	365	98	157.7	178.1	275.2	315	212.1	327.1	334.1	327.1

- 5 universities and ≥15 automotive & related companies (incl. Shell) participating in a large cluster
- Systematic chain of experiments & simulations: pure chemistry → real engines

Kinetics !

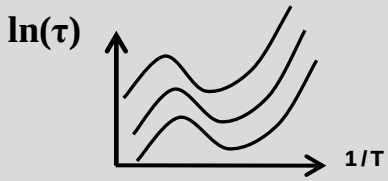
Evaporation

Joint Research Project

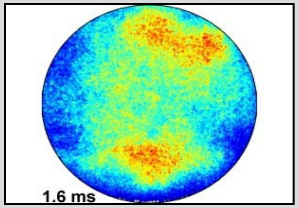
- Develop a chemical reaction mechanism suitable for such fuels
- Validate by experiments
- Employ in 3D-CRFD of 'real' systems

TP 2 - Development / Application of Chemical Reaction mechanism
Zürich / LAV

TP 1
Shock Tube
Duisburg / IVG



TP 3
Single Stroke Engine
Zürich / LAV



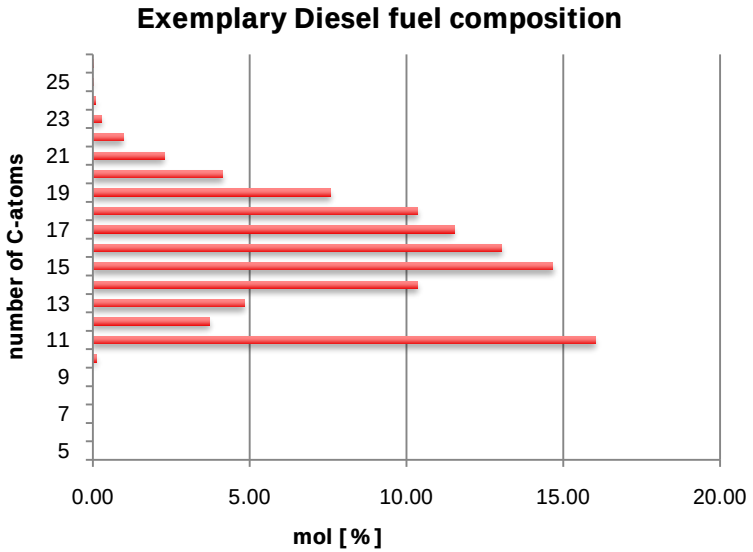
TP 5
Passenger Car Engine
Stuttgart / IVK

TP 5
Passenger Car Engine
Stuttgart / IVK

Chemistry Modeling

Detailed mechanisms

- Not available for the larger components



- Applicability to complex fuel blends ?
- Reduction potential limited for use in CFD

Simplified approaches

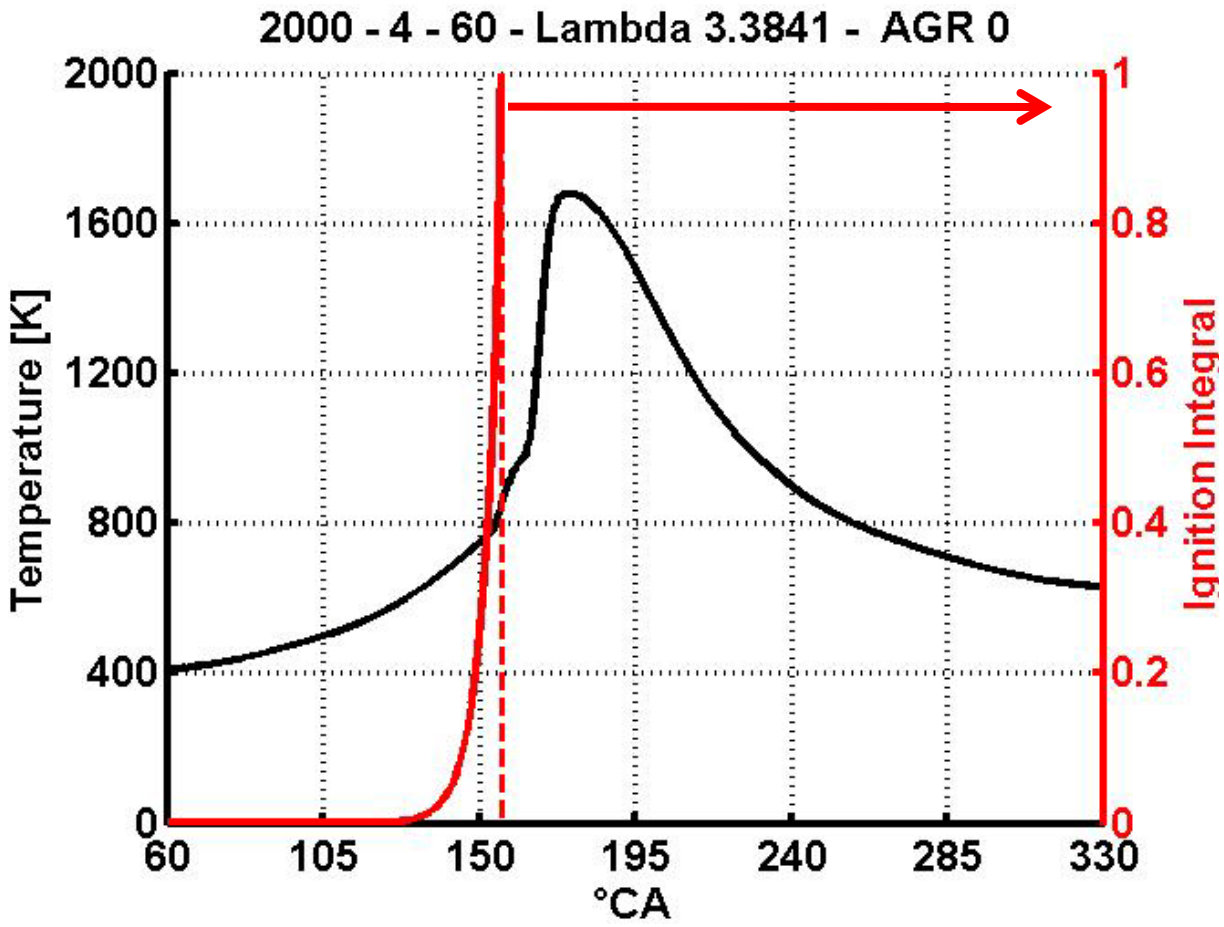
- Ignition models/knock integral
- Shell & derivatives
- Müller – Schreiber – Zheng
  - less than 10 species & reactions
  - Reflect typical NTC-behaviour
  - Employ ‘generic’ species

adaptable to other fuels

Image Source: Fuel data analysis: FVV Project „Kraftstoffkennzahlen“; BSc Thesis Simon Weihers, ETH Zürich

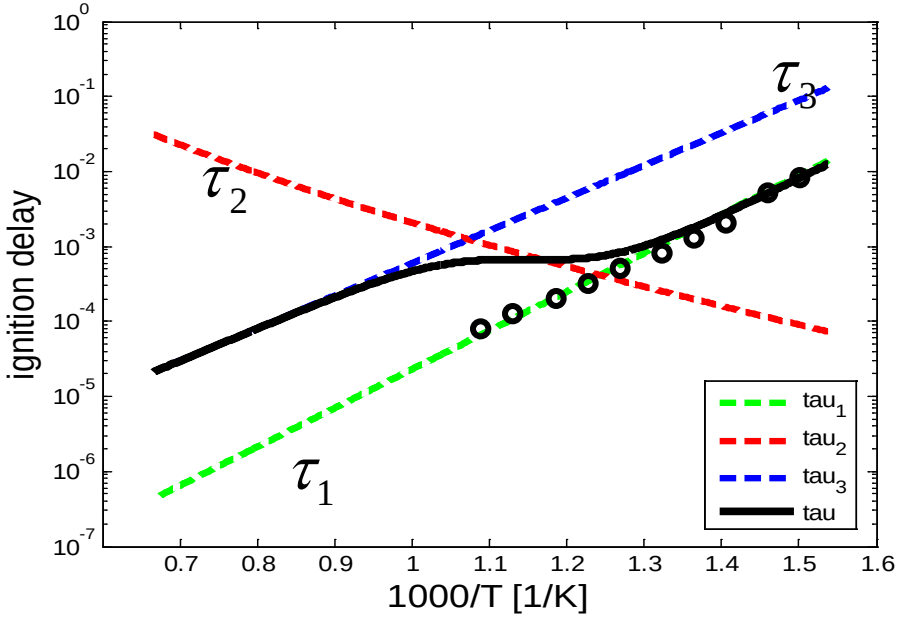
Ignition Integral Model

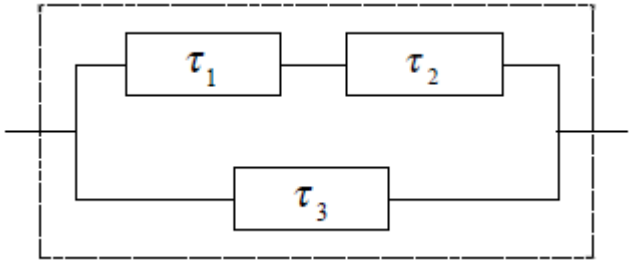
$$\int_{t_0}^{t_0+\tau_{id}} \left(\frac{1}{\tau(p, T, \varphi, EGR)} \right) dt = 1$$



Ignition Integral ~ Livengood and Wu

‚3-Arrhenius' Ignition Delay Model



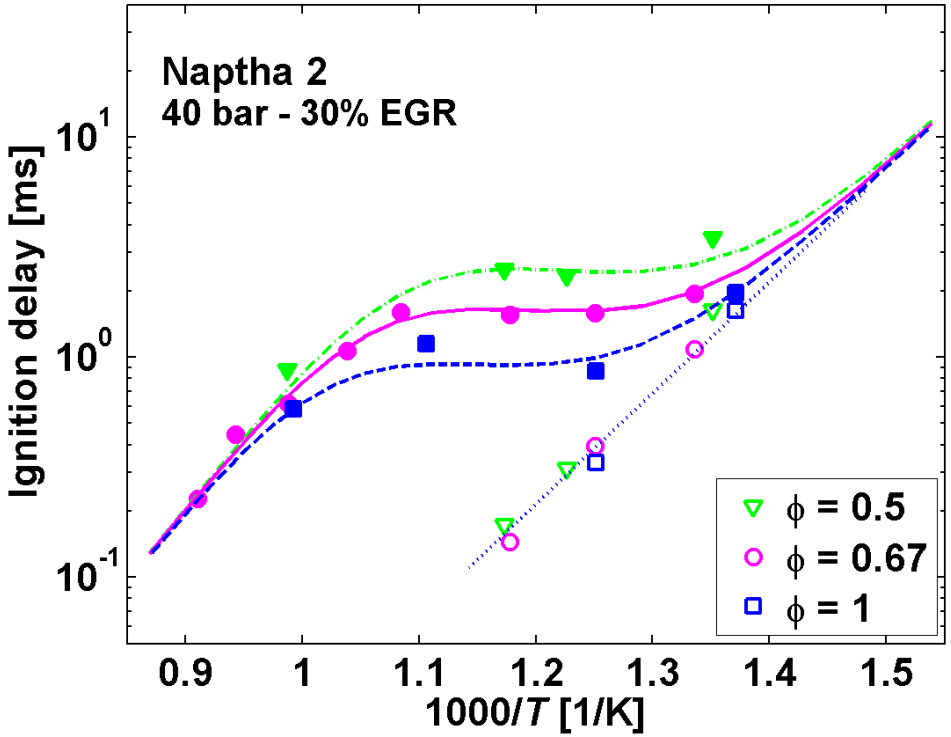


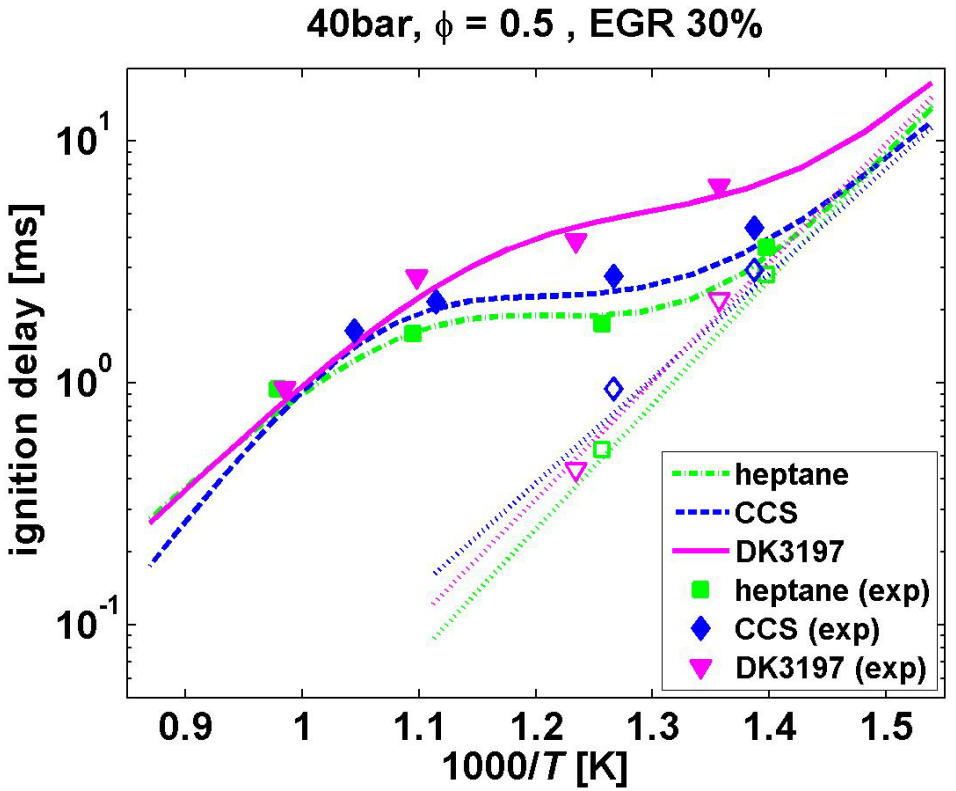
$$\frac{1}{\tau} = \frac{1}{\tau_1 + \tau_2} + \frac{1}{\tau_3}$$

Original: G.A..Weisser, Diss. ETH No. 14465

$$\tau_i = A_i \cdot \left(\frac{p}{p_{ref}}\right)^{\beta_i} \cdot T^{b_i} \cdot \exp\left(\frac{T_{Ai}}{T}\right) \cdot \varphi^{\gamma_i} \cdot \left(\frac{[N_2]}{[O_2]}\right)^{d_i} \cdot \exp\left(\frac{[N_2]}{[O_2]} \cdot \frac{e_i}{T}\right)$$

‚3-Arrhenius' Ignition Delay Model



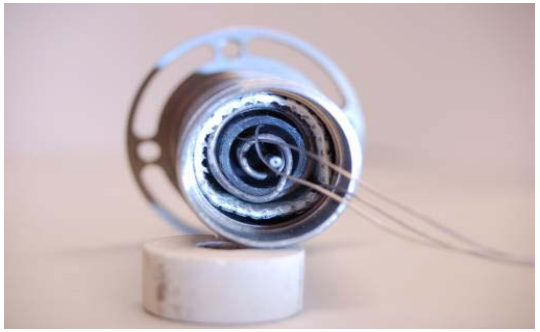


PARAMETER SET for each project fuel

Excellent agreement of both low & high T ignition delay

- Typical **R^2 > 90 %**
- Typical **RMS Error ≈ 0.2 – 0.4 ms**

Validation by TP 5: Single Cylinder PC Engine

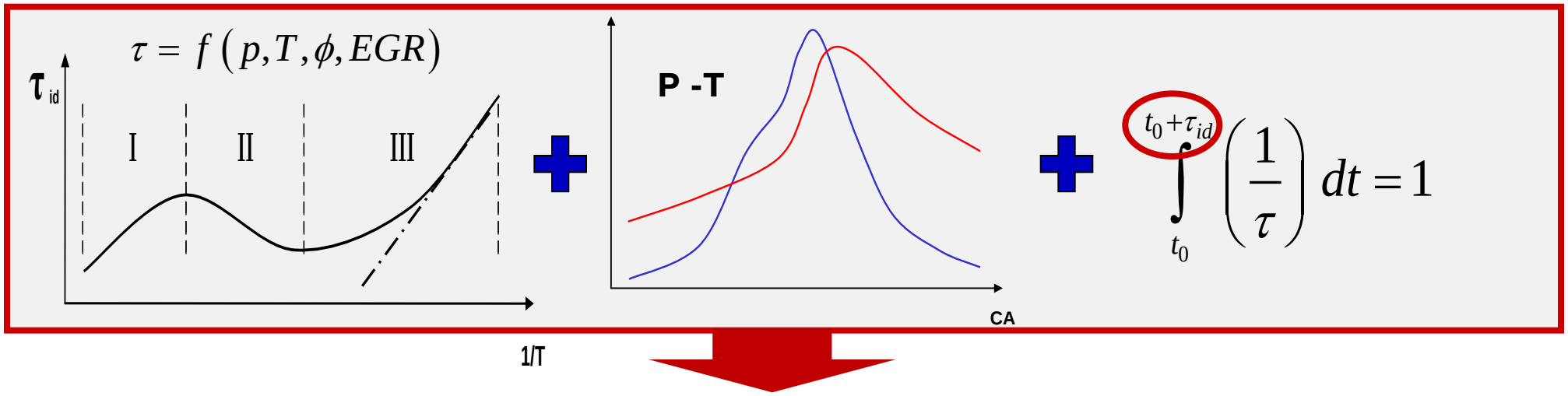


Specifications:

- Displacement: 537 cm³
- Geo. comp. ratio 16.7
- Cyl. peak pressure 145 bar
- Ext. boosting sys. 3 bar
- CRS 2.2 with max 1600 bar

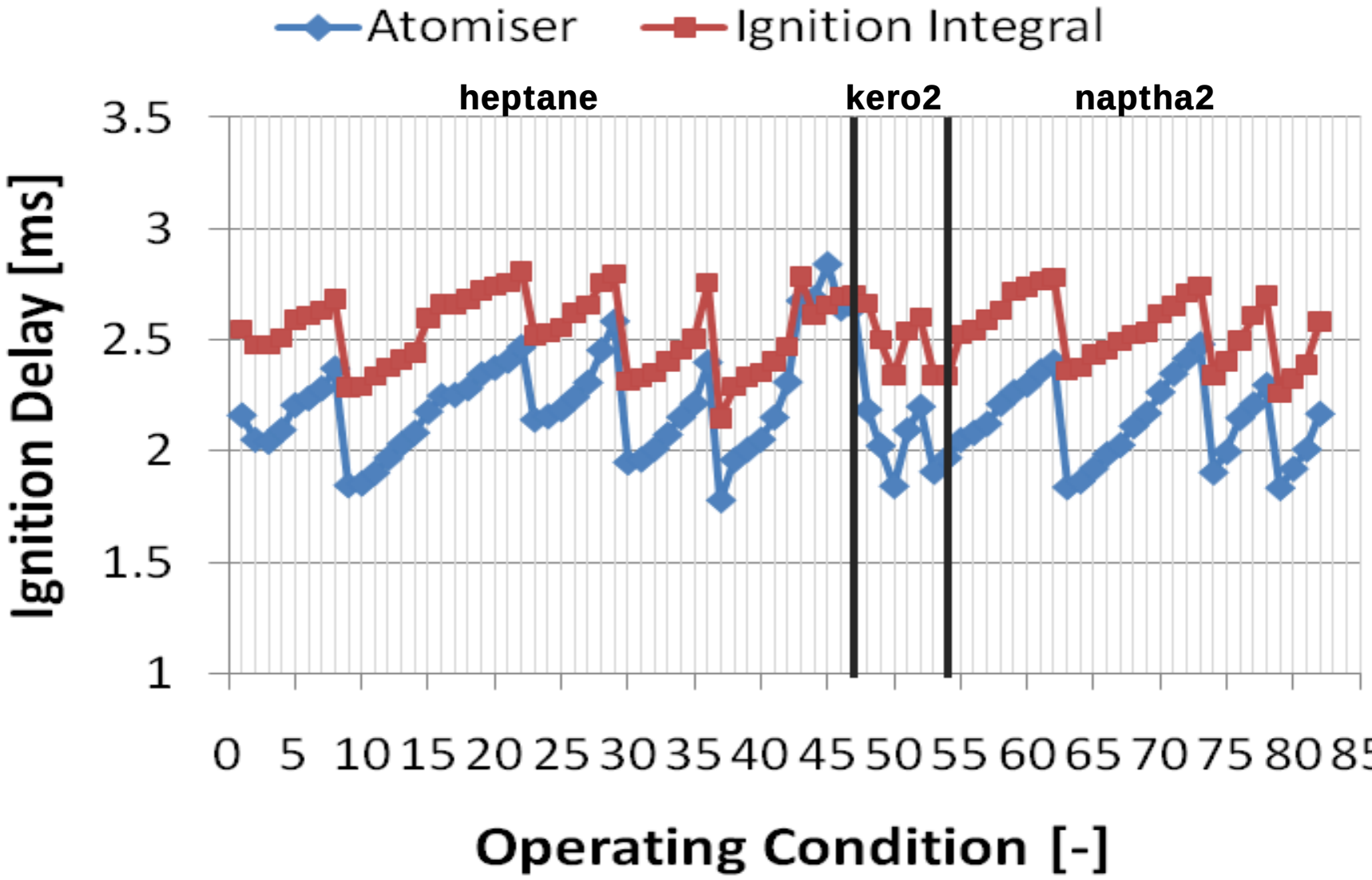
„KraftstoffKennzahlen“, Informationstagung Motoren, Herbst 2009, Dresden

From shock tube to engine ignition delay

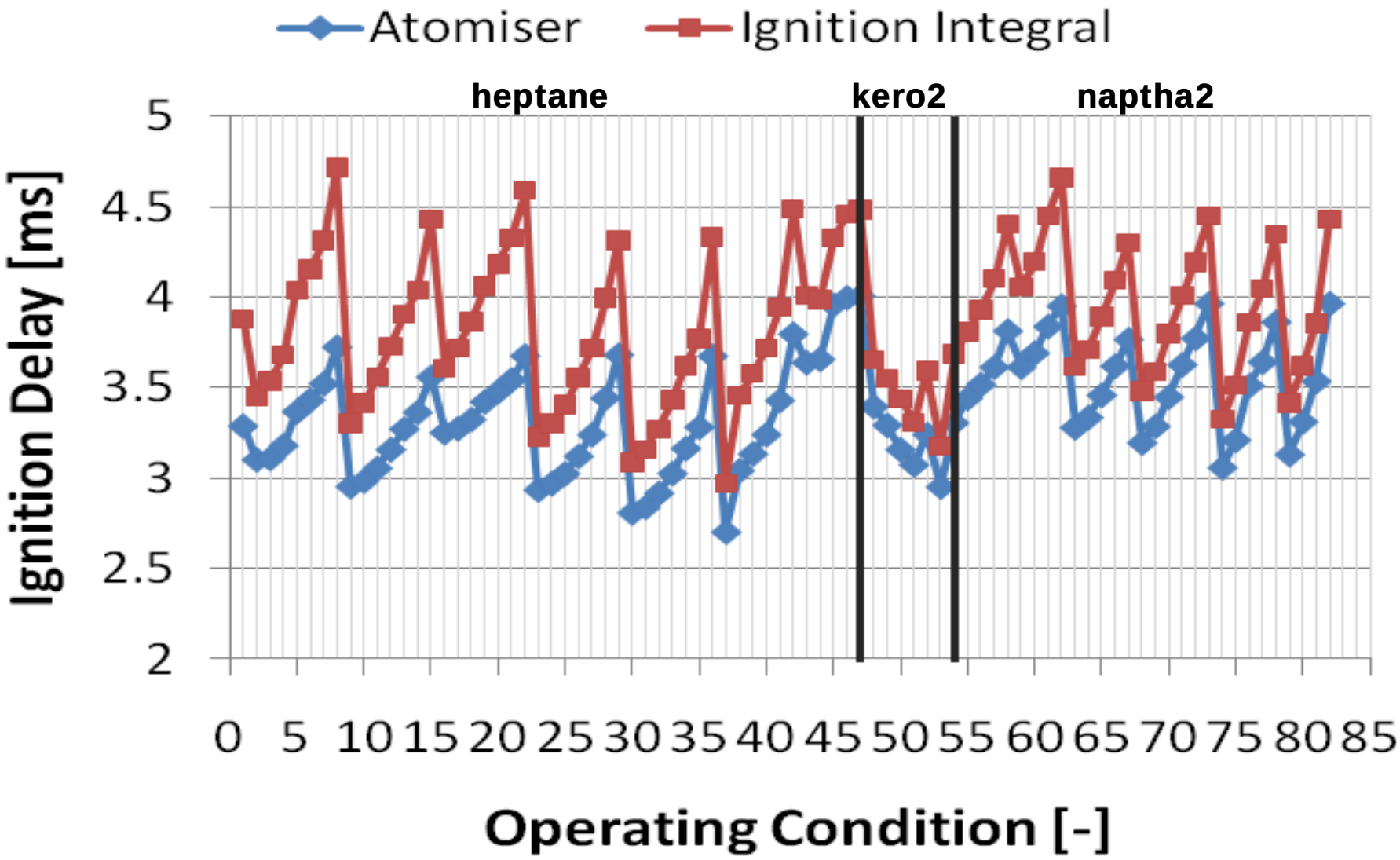


ENGINE IGNITION DELAY

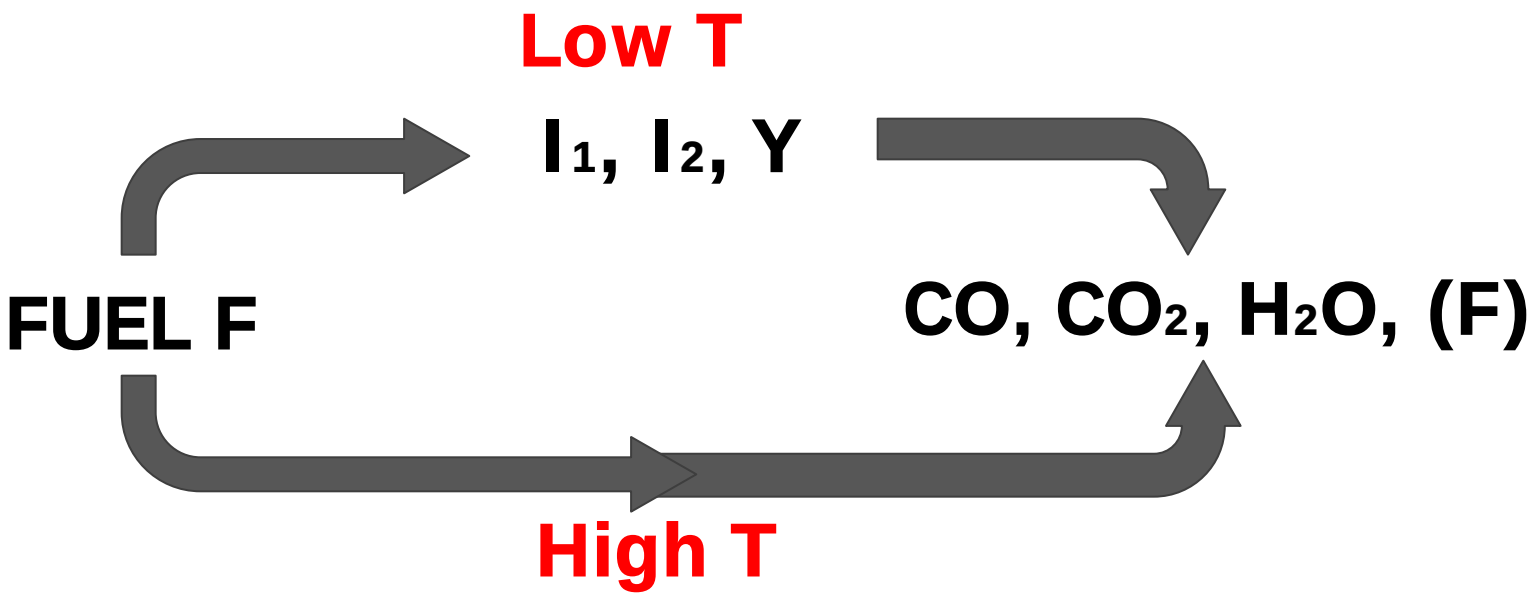
Application to IVK engine – First Stage Ignition



Application to IVK engine - Main Ignition



Lumped Reaction Mechanism



Original Zheng et al. [SAE 2004-01-2950] **- n-heptane**

- 7 Reactions
- $RR = A_i \exp(-E_i/RT) \ [X_i]^{y} (p/p_{ref})^{a}$

Lumped Reaction Mechanism

1. $F + 7.5O_2 \Rightarrow 8H_2O + 7CO$
2. $CO + 0.5O_2 \Leftrightarrow CO_2$
3. $F + 2O_2 \Leftrightarrow I_1$
4. $I_1 \Rightarrow 2Y$
5. $Y + 0.5F + 6.5O_2 \Rightarrow 8H_2O + 7CO$
6. $I_1 \Rightarrow I_2$
7. $I_2 \Rightarrow 2Y$

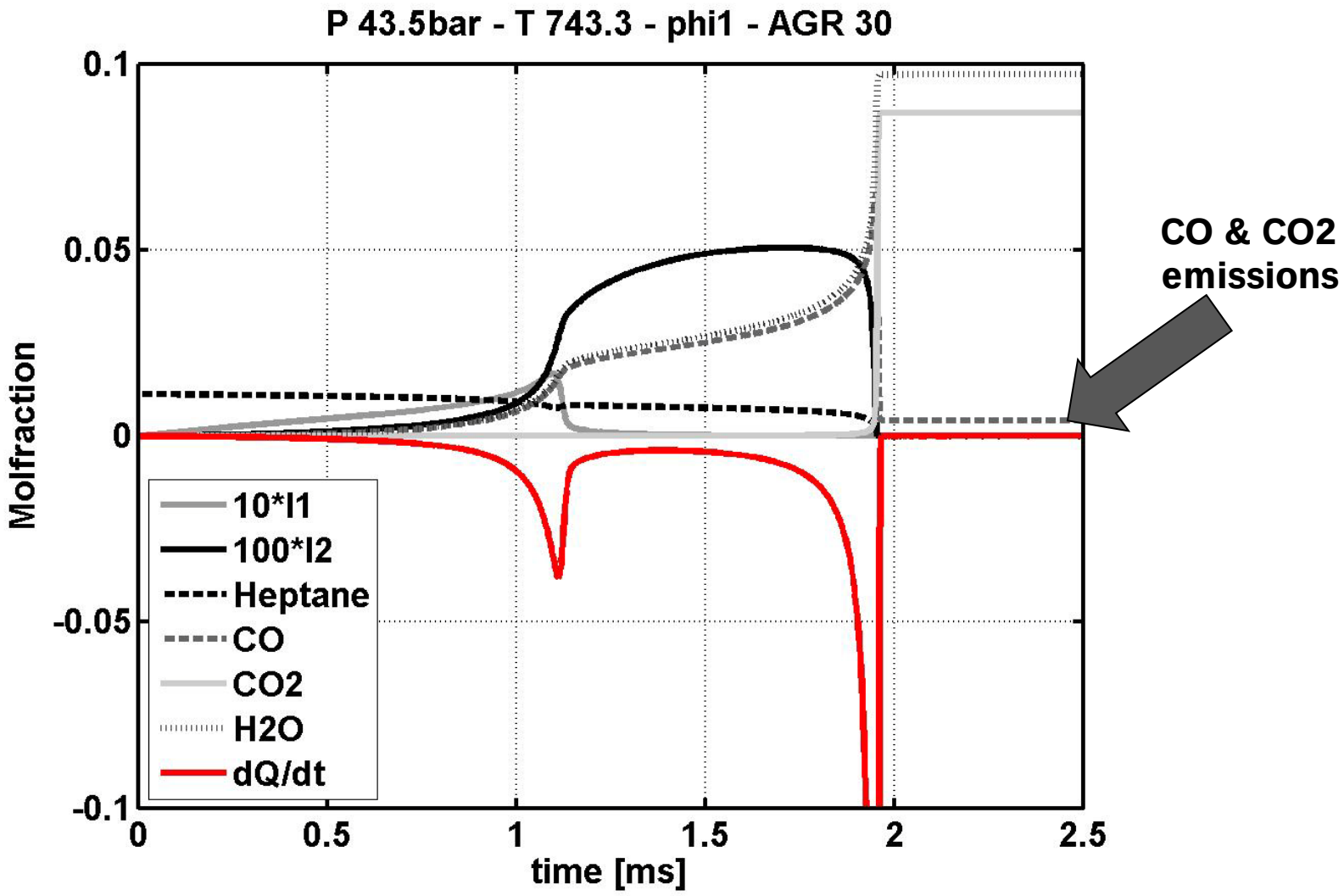
MODIFICATIONS

- Extended validity for n-heptane
- Extension towards other project fuels
  1. Representative Fuel Molecule C_xH_y
  2. Stoichiometric coefficients
  3. Fuel & Generic enthalpy & C_p
  4. Genetic Algorithm Optimization of the rate parameters (A_i, E_i, a)

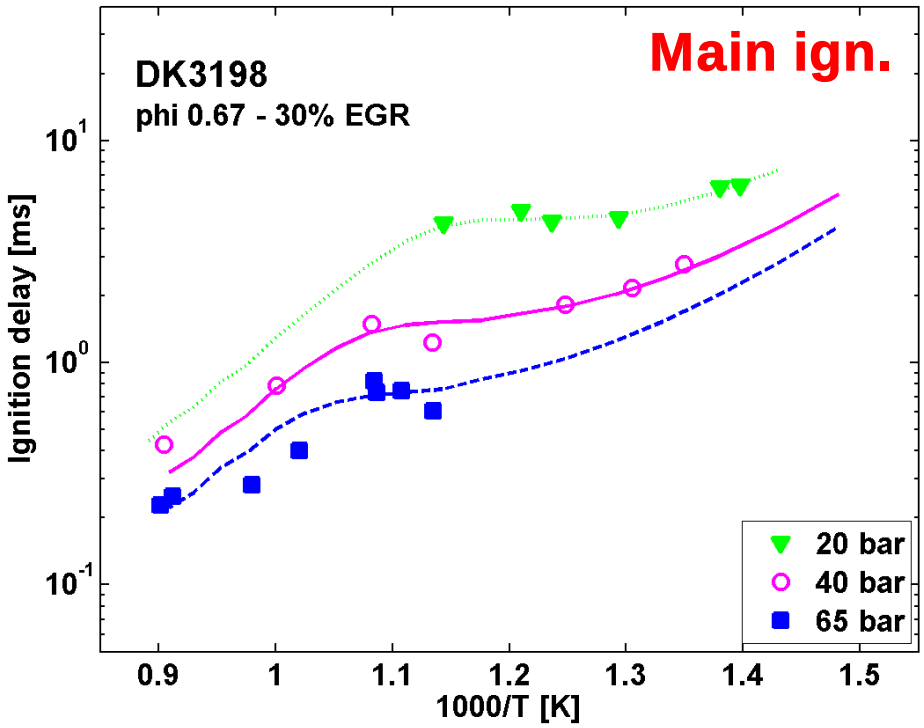
SET MODELPARAMETERS for each fuel

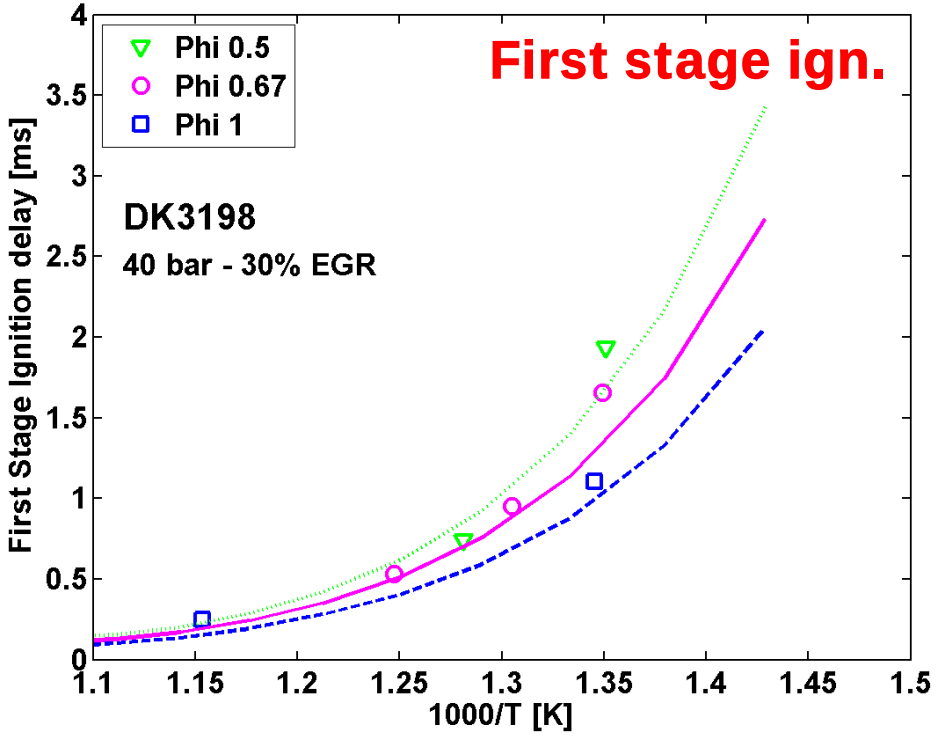
Vandersickel et al., Global reaction model for practical fuels in HCCI Applications, THIESEL 2010

Optimization Criteria and Results



Optimisation based on shock tube data





Optimised for 3 project fuels

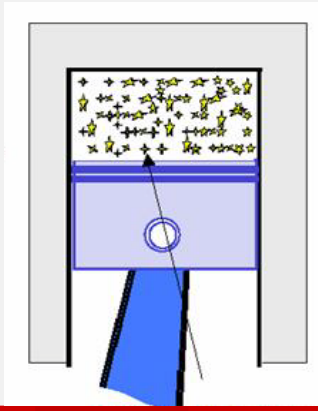
Excellent agreement of both low & high T ignition delay

- Typical **R^2 > 90 %**
- Typical **RMS Error ≈ 0.3 – 0.4 ms**

From shock tube to the engine

Lumped model
7 REACTIONS

+

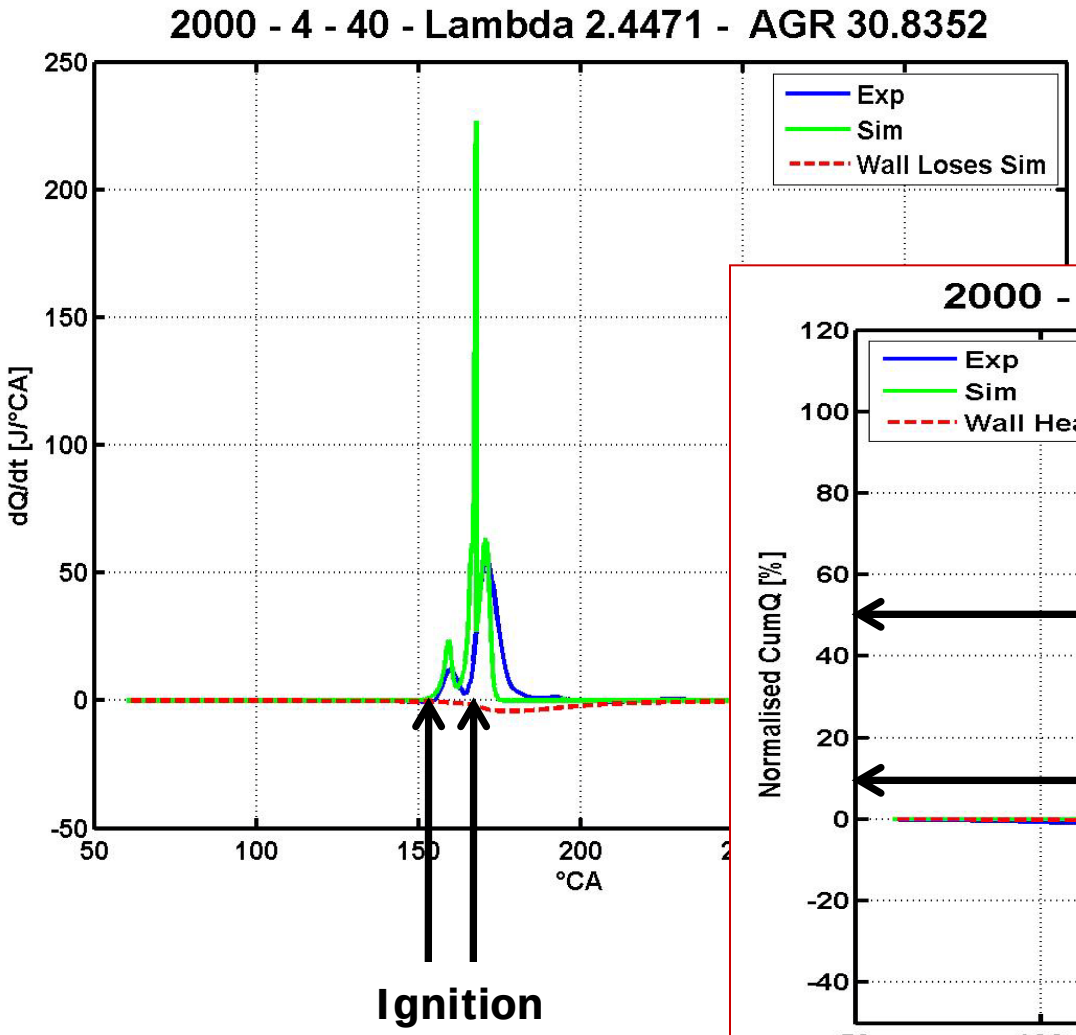


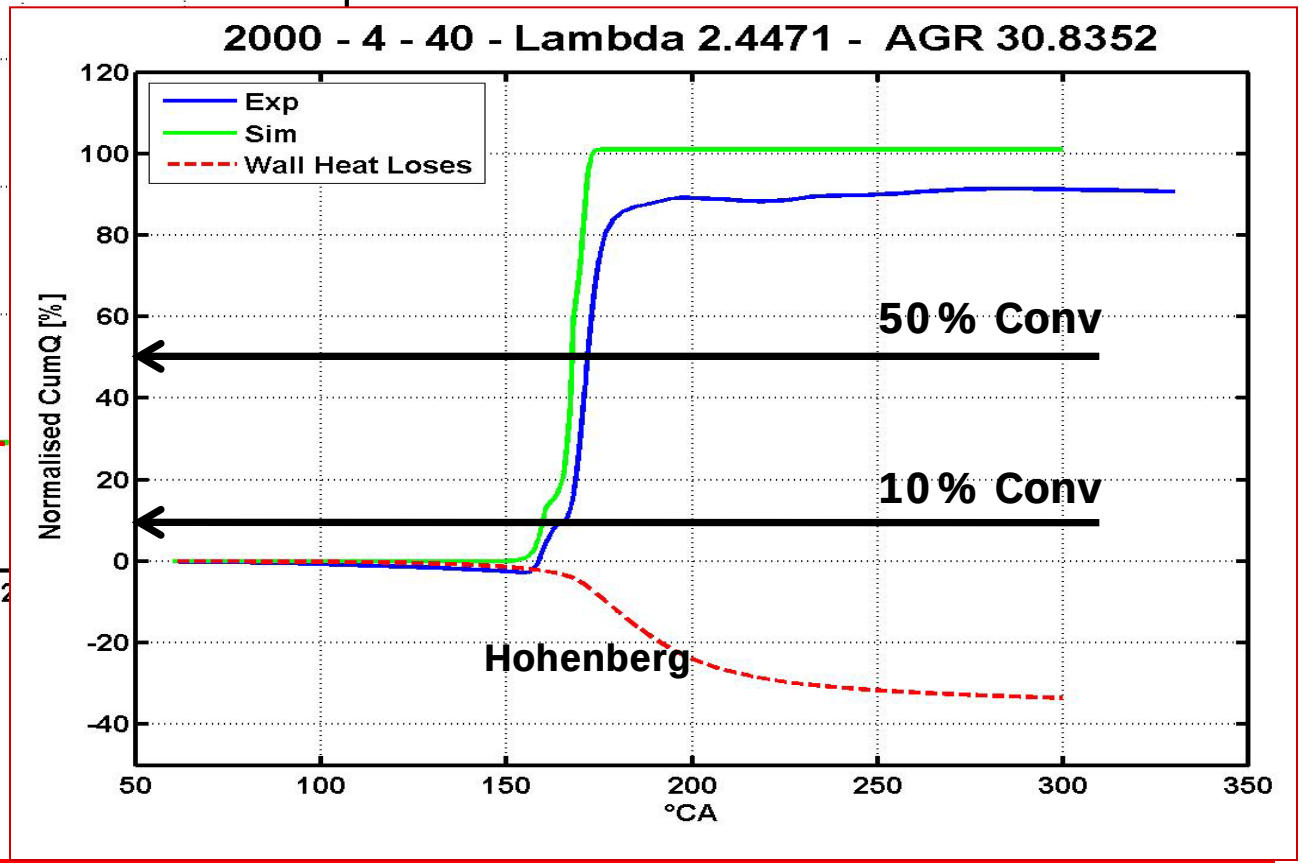
→Homogenous Mixture
& Temperature

→ Wall loses ~ Hohenberg

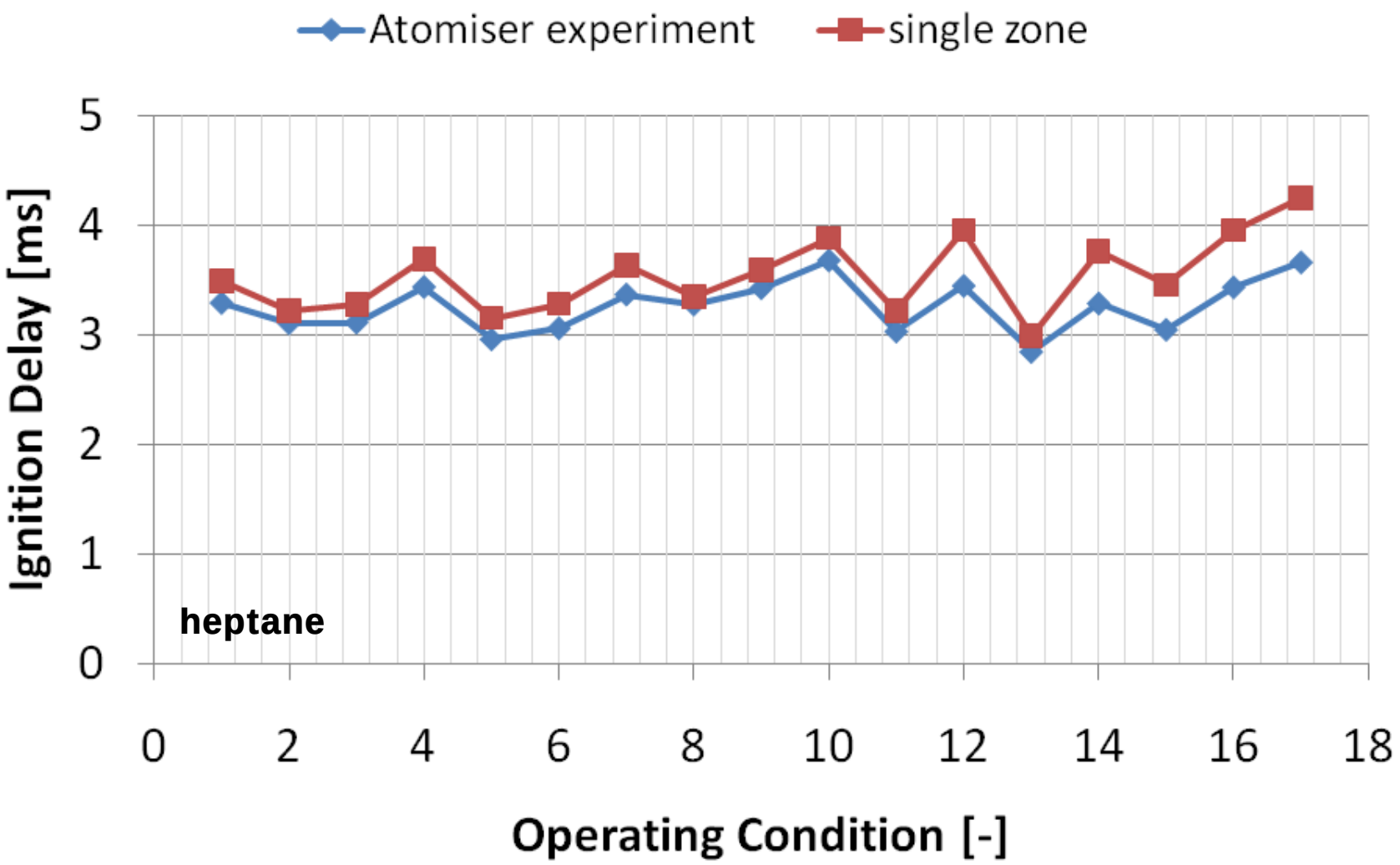
SINGLE ZONE
ENGINE MODEL

Application to IVK engine – Burning Rate

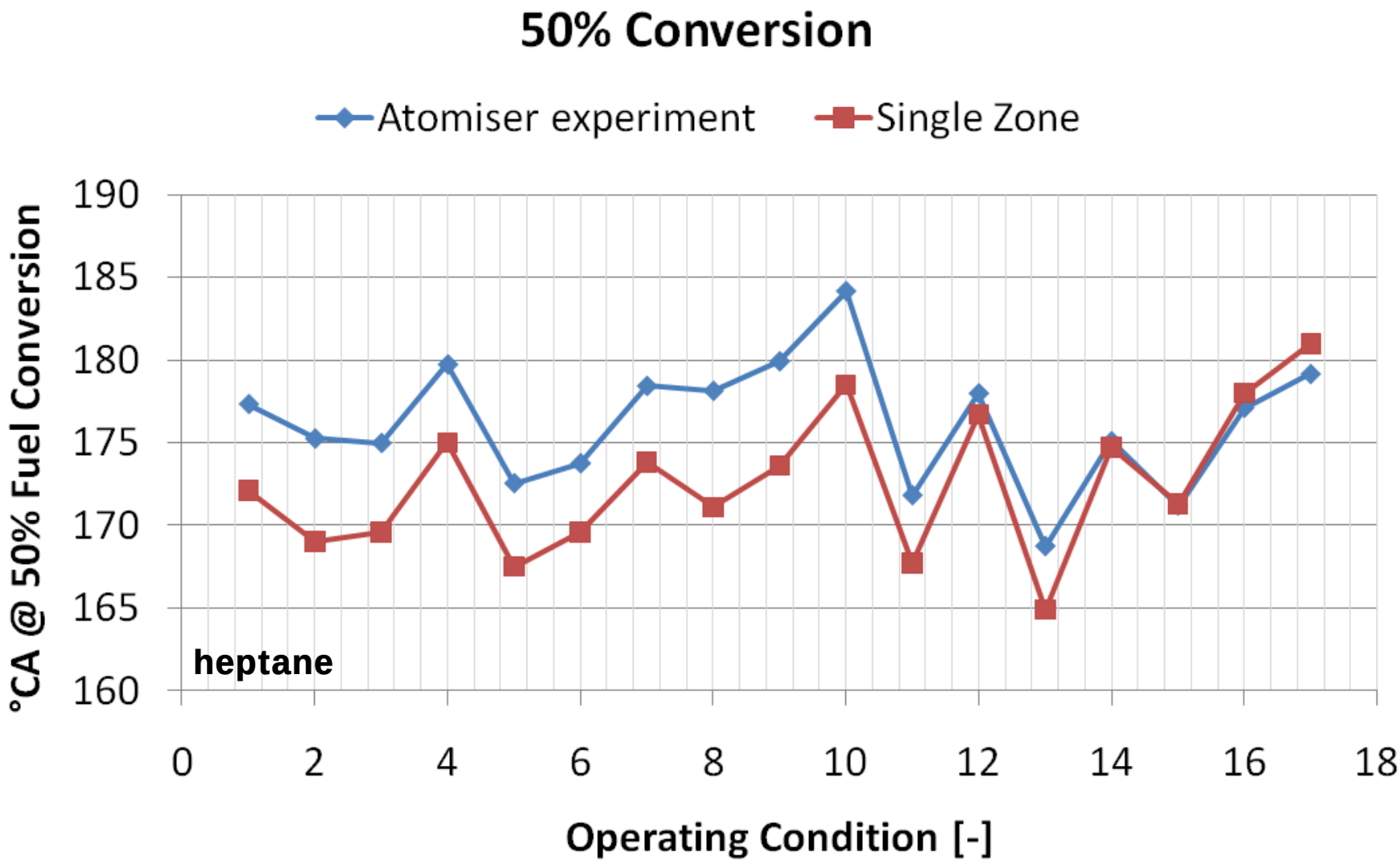




Application to IVK engine – main ignition



Application to IVK engine – Burning Rate



Conclusions

2 Ignition/Combustion Models developed :

- ‚3-Arrhenius' Model combined with Ignition Integral
- Lumped Reaction Model

Applicable to a large range of fuels

Capture influence of changing Operating Conditions on chemistry

Outlook

- **Optimise lumped model parameters for remaining fuels**

- **Employ developed models in 3D-CFD code (Conditional Moment closure based)**
  - ➢ Simulation of a broad range of operating conditions and fuels
  - ➢ Validate with experimental data from partner projects

  - ➢ Investigate influence of fuel properties & interaction with inhomogeneities

Acknowledgements / funding / collaborations

- Forschungsvereinigung Verbrennungskraftmaschinen (FVV)
- Swiss Federal Office of Energy (BfE) – Dres. Hermle & Renz
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IEA Task Leader Meeting,
Nara, July.2010

International Energy Agency Task Leader Meeting, Nara –Japan, July 2010

Universal Autoignition Models for 'designer' fuels in HCCI combustion

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1. Introduction

Homogeneous Charge Compression Ignition (HCCI) has the potential to simultaneously reduce both NO_x and soot emissions, while maintaining diesel-like efficiencies. Its applicability, however, is hindered mainly by the lack of sufficient ignition timing control.

The present project therefore aims at identifying how the HCCI ignition process and operating range can be influenced and controlled by tailoring of fuel properties. To do so, within the framework of a large scale collaboration between 5 universities and more than 15 automotive companies, a large set of technical fuels (see figure 1) is investigated both experimentally and numerically.

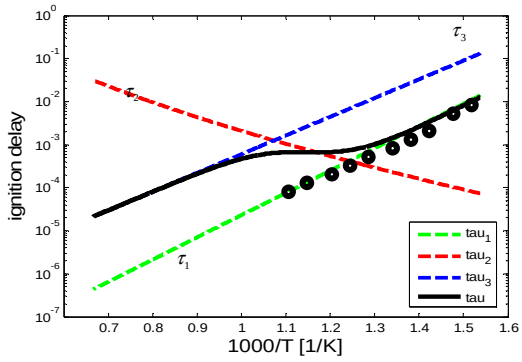
	1	2	3	4	5	6	7	8	9	10
	CEC-REF	n-Hept	Naptha 1	Naptha 2	Kero 1	Kero 3	CCS	Diesel 1	Diesel 2	Diesel 3
Cetane Number (CN)	54.5	57	35.4	48.2	38.4	50.3	44.2	50.3	56.7	60.4
% normal, iso-parrafins	86.1	100	70.8	53.3	35.91	69.41	79.50	100	100	100
% cyclo-parraffins	-	-	29.3	46.7	51.93	31.22	-	-	-	-
% aromatics	9.4	-	-	-	12.16	-	20.50	-	-	-
% olefins	4.5	-	-	-	-	-	-	-	-	-
Initial Boiling Point (IBP °C)	209.8	98	87.0	92.2	153.3	150.2	158.7	192.2	205.7	229.8
Final Boiling Point (FBP °C)	365	98	157.7	178.1	275.2	315	212.1	327.1	334.1	327.1

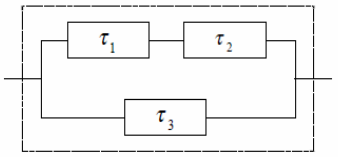
Figure 1: Overview and properties of the fuels investigated

In HCCI engines, ignition no longer depends on an external actuator (spark or injection) but on charge conditions (p, T, EGR), mixture formation and especially on the fuel oxidation chemistry. Despite the major impact of the fuel kinetics itself, one still has to reside to reduced/global ignition models in order to asses the influence of operating conditions and turbulence on the ignition of multi-component fuels in practical combustion systems (3D-CRFD). The present paper presents two such models, adapted for each of the fuels considered based on shock tube data from a partner project at the University of Duisburg and validated with atomizer engine experiments from the University of Stuttgart.

2. ‚3-Arrhenius' Model combined with an ignition integral

In order to quickly assess the impact of engine operating conditions on both first stage and main ignition timings, a compact autoignition model based on an ignition delay integral has been developed and calibrated for each of the project fuels. The shock tube delays used in the integral expression are described using a 3-Arrhenius model, which in the present work has been extended to account for the presence of EGR in the gas mixture. An overview of the final model and the corresponding model equations is given in figure 2. First stage ignition delay times (circles in fig.2) are given by τ_1, whereas





$$\frac{1}{\tau} = \frac{1}{\tau_1 + \tau_2} + \frac{1}{\tau_3}$$

Original: G.A..Weisser, Diss. ETH No. 14465

$$\tau_i = A_i \cdot \left(\frac{p}{p_{ref}}\right)^{\beta_i} \cdot T^{b_i} \cdot \exp\left(\frac{T_{Ai}}{T}\right) \cdot \varphi^{\gamma_i} \cdot \left(\frac{[N_2]}{[O_2]}\right)^{d_i} \cdot \exp\left(\frac{[N_2]}{[O_2]} \cdot \frac{e_i}{T}\right)$$

Figure 2: Overview of the 3-Arrhenius shock tube ignition delay model (pressure *p* [bar], p_{ref} = 1 bar, temperature *T* [K], equivalence ratio [-])

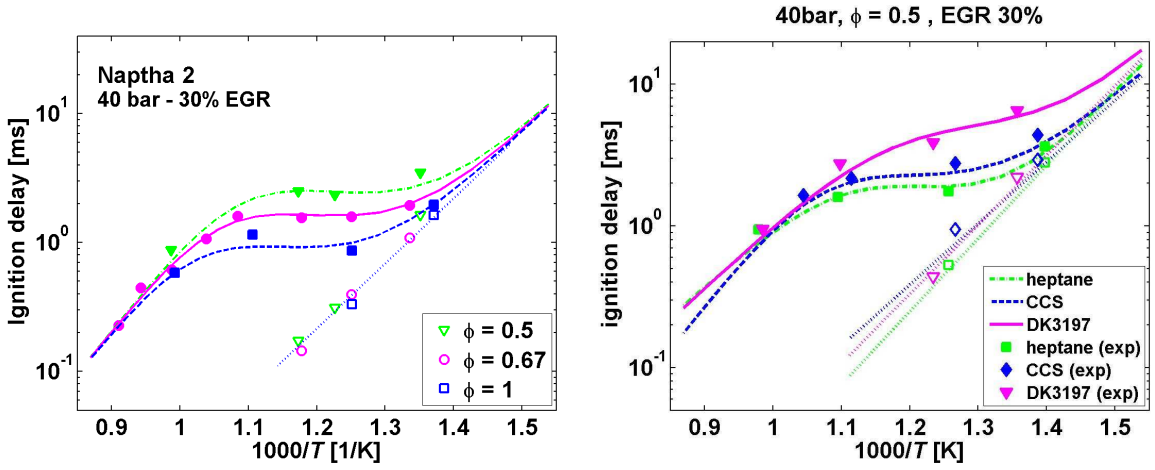


Figure 3: Comparison of measured (symbols) and simulated (line) ignition delays: Left – influence of shock tube conditions – right - influence of the fuel

the main ignition delay times τ are described as a combination of the three ignition delays τ_1, τ_2 and τ_3 representing respectively the low, medium and high temperature chemistry.

After calibration of the model parameters indicated in red, an excellent agreement with the measured shock tube data could be achieved, as illustrated in figure 3. The complete ignition model, using the ignition integral given by the equation below, has been validated based on atomizer engine data obtained form a partner project at the University of Stuttgart. As can be seen in figure 4, the model successfully captures the influences of changing operating conditions on ignition delay times. For brevity only the main ignition delays are shown, but similar results were obtained for the first stage ignition delays as well.

$$\int_{t_0}^{t_0+\tau_{id}} \left(\frac{1}{\tau(p, T, \varphi, EGR)}\right) dt = 1$$

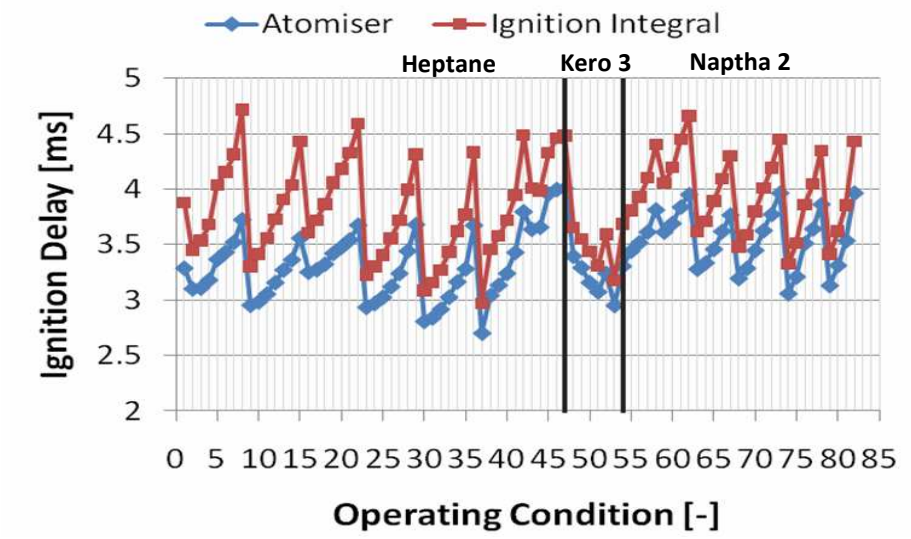


Figure 4: Comparison of measured (blue) and calculated (red) main engine ignition delay times

3. Lumped reaction model

The second model is based on the global n-heptane reaction mechanism previously developed by Zheng et al. [1]. The model consists of 7 global reactions and 7 seven active species. Its basis structure is shown in table 1. The high temperature chemistry is embodied in the first two reactions, whereas the low and intermediate temperature phenomena are described by global reactions 3 to 5. The low temperature scheme is controlled by the interaction of the three generic species I1, I2 and Y and represents the alkyl radical chemistry typical for the low temperature oxidation of alkanic fuels. Reaction rates are expressed as the product of the rate constant (Arrhenius expression), the species concentrations and for reaction 3, an additional pressure correction term.

Reaction	$Log_{10}A^+$	E^+	$Log_{10}A^-$	E^-
1. $F + 7.5O_2 \Rightarrow 8H_2O + 7CO$	12.36	39.70		
2. $CO + 0.5O_2 \Leftrightarrow CO_2$	14.0	40.00	7.08	40.00
3. $F + 2O_2 \Leftrightarrow I_1$	C_3^+20.17	37.62	31.64	88.11
4. $I_1 \Rightarrow 2Y$	6.38	3.96		
5. $Y + 0.5F + 6.5O_2 \Rightarrow 8H_2O + 7CO$	18.00	32.67		
6. $I_1 \Rightarrow I_2$	10.45	13.86		
7. $I_2 \Rightarrow 2Y$	19.18	53.46		

Table 1: global reaction mechanism for n-heptane – Reaction Rates = f (ki , [Xi]yi , pai)
Arrhenius parameters for the rate constants, units: cc, mole, s, kcal)

Motivated by the similarity in their ignition behaviour, we generalized the above 7-step model for application to practical gasoline and diesel fuels. Scope of the generalization is to accurately predict global quantities like ignition delay timings as well as pressure, temperature and important tracer species evolutions, using the same overall scheme for each of the fuels considered. To this end, for each of the fuels, the following set of modifications was undertaken.

1. Based on the chemical composition of the fuel, a representative fuel molecule $F = C_xH_y$ is defined.
2. The stoichiometric coefficients of reaction 1 and 5 are adjusted to obtain a correct CO_2/H_2O-ratio in the post combustion gas.

3. The thermodynamic properties of both the fuel molecule F and the generic species are adapted to ensure that the overall heat release corresponds to the heating value of the fuel under consideration.
4. Using a genetic algorithm optimisation algorithm, the reaction rate parameters are calibrated to match the measured shock tube ignition delay times, both first stage and main ignition, and capture the evolution of the main tracer species.

More detailed information about the model optimisation will be presented at the THIESEL 2010 Conference (Sept. 14-19 in Valencia) and published in the Conference Proceedings. The optimization has been completed successfully for n-heptane and one of the kerosenes, and is ongoing for the remaining project fuels. The optimized model has been implemented in a single zone engine model and shows a very good agreement with the measured heat release and pressure/temperature data from the atomizer engine experiments in Stuttgart. Due to the simplifications of a single zone model, the absolute value of ignition delays and fuel conversion rates are deviating. The influence of changing operating conditions on both quantities, however, is very well captured, as illustrated in figure 5.

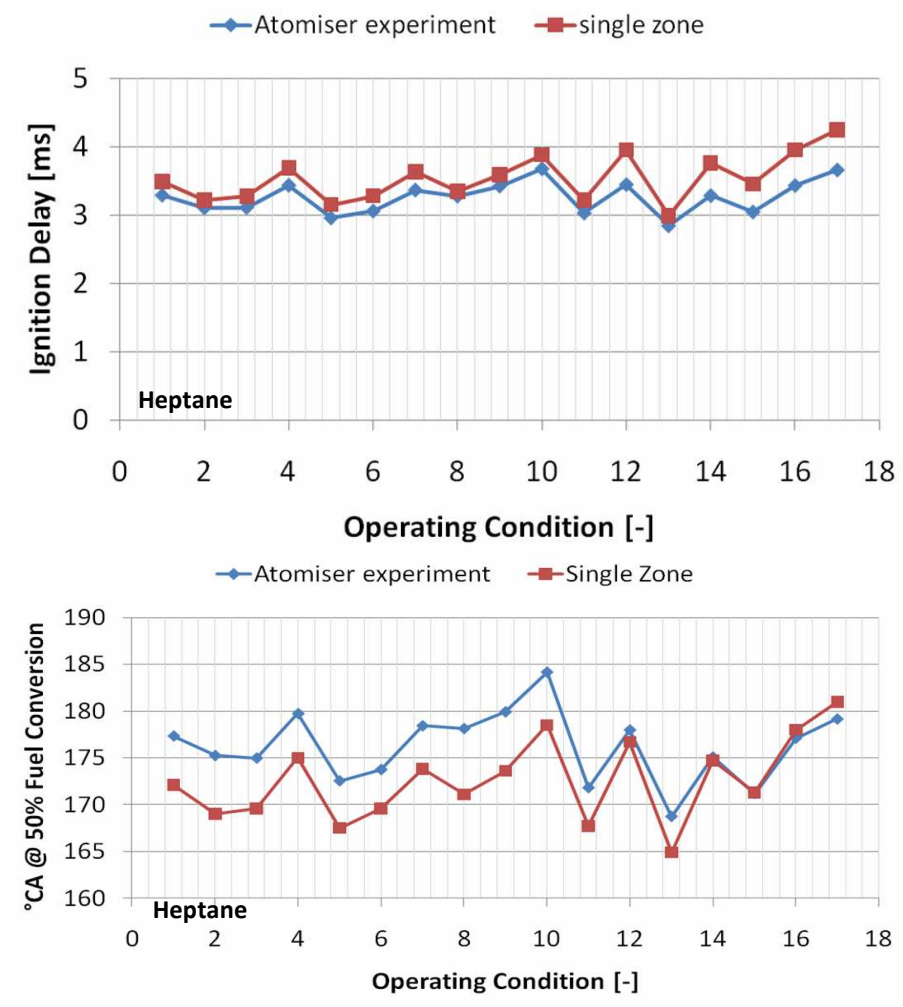


Figure 5: Comparison of measured (blue) and simulated (red) main engine ignition delay times (top) and 50% Conversion point (bottom)

4. Conclusions and outlook

In the present paper, two global ignition models have been adapted in order to describe the ignition behavior of each of the project fuels. Both models are calibrated based on shock tube data from a partner project and have been successfully validated with atomizer engine experiments. Especially the influence of the engine operating conditions (p, T, lambda, EGR, rpm, load) on the autoignition and combustion chemistry is very well captured.

In the next step, the optimization of the 7-step reaction mechanism will be completed for the remaining process fuels. Both models will then be implemented into a 3D-CFD code in order to assess the additional influence of temperature/mixture inhomogeneities and the physical fuel properties on the HCCI ignition and combustion event.

5. References

[1] Zheng et al., SAE 2004-01-2950