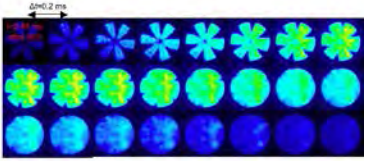
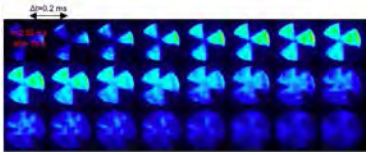
Bundesamt für Energie BFE
Forschungsprogramm Verbrennung

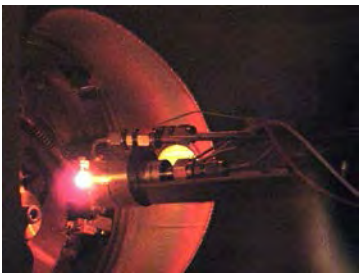
Tagung

Verbrennungsforschung in der Schweiz

28. Oktober 2011
Semper Aula an der ETH in Zürich







Schweizerische Eidgenossensc
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Bundesamt für Energie BFE

PAUL SCHERRER INSTITUT
PSI

ETH LAV
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Verbrennungsforschung in der Schweiz

28. Oktober 2011 09:00 bis 17:00 Uhr Semper Aula HG G 60 ETH Zürich

Die **Verbrennung** ist anteilmässig der **wichtigste Prozess** zur Umwandlung verschiedener Energieträger in die nutzbaren Energieformen Kraft und Wärme. Alternative Brennstoffe, ein möglichst hoher exergetischer Wirkungsgrad und geringe Emissionen sind Ziele und **Herausforderungen der Forschung**, um den Anforderungen der Zukunft zu genügen. Dafür braucht es hochqualifizierte Forschende sowie technologische und wirtschaftliche Erfolge der Industrie.

Die **Schweizer Verbrennungsforschung** ist durch die ansässige weltweit agierende Industrie sowie qualifizierte Forschungszentren der Hochschulen in zahlreichen Themen international gut positioniert oder sogar **führend**.

Die öffentliche Hand aber auch private Organisationen unterstützen die Verbrennungsforschung in der Schweiz auch finanziell. Damit sollen Themen, welche den **energiepolitischen Zielen** entsprechen erforscht oder neue Produkte zur Marktreife entwickelt werden können.

Ziele der Tagung sind der Informationsaustausch über aktuelle **Forschungsprojekte** aus den **Hochschulen** und der **Industrie**, Neuigkeiten über Forschungsschwerpunkte der Industrie und Rahmenbedingungen von Förderinstitutionen. Neues wird auch über die Ziele **internationaler Organisationen** mit Bezug zur Verbrennung zu erfahren sein. Nicht zuletzt soll die Tagung **Netzwerkaktivitäten** dienen und jungen Forschenden Kontakte zur Industrie ermöglichen.

Der Eintritt ist frei. Anmeldung bitte bis 14. Oktober 2011

Kontaktadresse und Anmeldung
ETH Zürich – Institut für Energietechnik, Sekretariat Prof. K. Boulouchos
Laboratorium für Aerothermochemie und Verbrennungssysteme
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Organisatoren
•Prof. Dr. K. Boulouchos, Institut für Energietechnik - Laboratorium für Aerothermochemie und Verbrennungssysteme, ETH Zürich
•Dr. P. Jansohn, Labor für Verbrennungsforschung, Paul Scherrer Institut (PSI)
•S. Renz & Dr. S. Hermle, Forschungsprogramm Verbrennung, Bundesamt für Energie (BFE)

Programm

08:30	*Registrierung & Kaffee*
09:00	**Begrüssung**
09:15	**Energieforschungskonzept des Bundes** R. Schmitz, Leiter Sektion Energieforschung, Bundesamt für Energie (BFE), Bern
09:30	**Schwerpunkte der Verbrennungsforschung im ETH-Bereich** K. Boulouchos, Labor Aerothermochemie und Verbrennungssysteme, ETHZ, Zürich
Forschungsprojekte aus Industrie und Hochschulen	
09:45	**Auswirkung von Verdampfung, Drall und Brennstoffqualität auf die Einspritzung in grossen 2-Takt-Dieselmotoren** B. von Rotz Wärtsilä Schweiz AG, Winterthur
10:10	**Miller Prozess für niedrige NOx-Emissionen und höhere Effizienz in Grossdieselmotoren** P. Kyrtatos, Labor Aerothermochemie und Verbrennungssysteme, ETHZ, Zürich
10:35	*Kaffeepause –Poster – Networking*
11:00	**Verbrennungseigenschaften von H_2-reichen Brenngasen unter gasturbinen-relevanten Bedingungen** Yu-Chun Lin, Paul Scherrer Institut (PSI), Villigen
11:25	**Verbrennungskonzepte für H_2- reiche Brennstoffe unter Gasturbinenbedingungen** Timothy Griffin, Fachhochschule Nordwestschweiz, Brugg-Windisch
11:50	**Einfluss von reaktiven Oberflächen auf die Verbrennung von H_2-reichen Brenngasen** M. Schultze, Paul Scherrer Institut (PSI), Villigen
12:15	*Mittagessen – Poster – Networking*
13:45	**3D-CFD Simulationen zur Optimierung des Verbrennungssystems und zur Gestaltung des Abgasstranges von Off-Road Dieselmotoren** A. Schilling, Liebherr Machines Bulle SA
14:10	**Modellierung der Russbildung von n-Heptan Sprays bei dieselmotorischen Bedingungen** M. Bolla, Labor Aerothermochemie und Verbrennungssysteme, ETHZ, Zürich
14:35	**Regenerationsvorgänge und Emissionen verschiedener DPF-Systeme mit RME** S. Bürki, AFHB Berner Fachhochschule, Nidau
15:00	*Kaffeepause – Poster – Networking*
15:25	**Mehrzyklen-LE-Simulationen der Verbrennung im direkteinspritzenden Erdgasmotor** Y. Wright, Labor Aerothermochemie und Verbrennungssysteme, ETHZ, Zürich
15:50	**Katalytisch beschichtete Kolben im Benzin- und Erdgasmotor** P. Soltic, Empa, Dübendorf
Forschungsziele der Industrie	
16:15	**Zukünftige Herausforderungen der Auflade- und Motortechnik** D. Brand, ABB Turbo Systems, Baden
16:30	**Dynamic Response of Turbulent Low Emission Flames at Different Vortex Breakdown Conditions** F. Genin, Alstom (Schweiz AG)
16:45	Zusammenfassung, Verabschiedung

Posterausstellung

„Verbrennungsforschung in der Schweiz“

28. Oktober 2011 – ETH Zürich, Semper Aula

Poster-Nr.	Titel	Autor
1	Efficient NO Calculations in Turbulent Non-Premixed Flames Including Consistent Nitrogen Chemistry	B. T. Zoller, J. Allegrini, U. Maas, P. Jenny Institut für Fluiddynamik ETH Zürich
2	A PDF Model to Predict Local Extinction in Turbulent Partially Premixed Flames	B. T. Zoller, P. Jenny Institut für Fluiddynamik ETH Zürich
3	A Joint PDF Closure of Turbulent Premixed Combustion	M. L. Hack, P. Jenny Institut für Fluiddynamik ETH Zürich
4	HCCI Combustion Fuel Index - Experiments in the Single Stroke Machine	D. Mitakos Institut für Energietechnik ETH Zürich
5	HCCI modeling: ‚global‘ reaction model for technical fuels	A. Vandersickel et al. Institut für Energietechnik ETH Zürich
6	Transient simulation of NOx reduction over a Fe-Zeolite catalyst in an NH3-SCR system under non-isothermal operating conditions	L. Sharifian et al. Institut für Energietechnik ETH Zürich
7	Experimental and Numerical Investigations of Dual Fuel Combustion in Gas engines with Pilot Injection	Stéphanie Schlatter et al. Institut für Energietechnik ETH Zürich
8	Soot Formation Modeling of n-Heptane Spray Combustion Under Diesel Engine Conditions Using the Conditional Moment Closure Approach	Michele Bolla et al. Institut für Energietechnik ETH Zürich
9	CLean and Efficent VEhicle Research	Reto Egli et al. Institut für Energietechnik ETH Zürich
10	Spray modeling and analysis by means of experiments with a large 2-Stroke Marine Spray Combustion Chamber CH)	Michel Cattin et al. Institut für Energietechnik, ETH Zürich Beat von Rotz et al. Wärtsilä Schweiz
11	Verbrennungsforschung mit Synchrotron Strahlung	T. Gerber Paul Scherrer Institut
12	Bestimmung von thermo-chemischen Daten verbrennungsrelevanter Moleküle an der SL/VUV beamline	T. Gerber Paul Scherrer Institut
13	Grundlagen zur Erweiterung des Leistungsbereichs und der Brennstoff-Flexibilität von Ölbrennern mit Vorverdampfertechnik	T. Griffin Fachhochschule Nordwestschweiz
14	Turbulence Modulation in Particle Laden Flows	D. W. Meyer, P. Jenny Institut für Fluiddynamik ETH Zürich
15	Modeling Molecular Mixing in Turbulent Flows	D. W. Meyer, R. Deb, P. Jenny Institut für Fluiddynamik ETH Zürich

Abstracts Liste

„Verbrennungsforschung in der Schweiz“

28. Oktober 2011 – ETH Zürich, Semper Aula

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1	**Energieforschungskonzept des Bundes**	**Rolf Schmitz** *Bundesamt für Energie, Bern*
2	**Schwerpunkte der Verbrennungsforschung im ETH-Bereich**	**Konstantinos Boulouchos** *ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory*
3	**Auswirkung von Verdampfung, Drall und Brennstoffqualität auf die Einspritzung in grossen 2-Takt-Dieselmotoren**	**Beat von Rotz** *Wärtsilä Schweiz AG, Winterthur*
4	**Miller Prozess für niedrige NOx-Emissionen und höhere Effizienz in Grossdieselmotoren** *Miller Cycle for Low NOx Emissions and High Efficiency in Medium-Speed Diesel Engines: Potential and Limitations*	**Panayotis Kyrtatos** *ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory*
5	**Verbrennungseigenschaften von H2-reichen Brenngasen unter gasturbinen-relevanten Bedingungen**	**Yu-Chun Lin** *Paul Scherrer Institut (PSI), Villigen*
6	**Verbrennungskonzepte für H_2- reiche Brennstoffe unter Gasturbinenbedingungen**	**Felipe Bolaños, Felipe Piringer, Dieter Winkler und Timothy Griffin** *Fachhochschule Nordwestschweiz, Brugg-Windisch*
7	**Einfluss von reaktiven Oberflächen auf die Verbrennung von H2-reichen Brenngasen** *Catalytic combustion of rich hydrogen mixtures*	**Marco Schultze** *Paul Scherrer Institut (PSI), Villigen*
8	**3D-CFD Simulationen zur Optimierung des Verbrennungssystems und zur Gestaltung des Abgasstranges von Off-Road Dieselmotoren**	**Alexander Schilling** *Liebherr Machines Bulle SA*
9	**Modellierung der Russbildung von n-Heptan Sprays bei dieselmotorischen Bedingungen** *Soot Formation Modelling of n-Heptane Spray Combustion Under Diesel Engine Conditions Using the Conditional Moment Closure Approach*	**Michele Bolla, Yuri M. Wright and Konstantinos Boulouchos** *ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory*
10	**Regenerationsvorgänge und Emissionen verschiedener DPF-Systeme mit RME**	**Samuel Bürki** *AFHB Berner Fachhochschule, Nidau*
11	**Mehrzyklen-LE-Simulationen der Verbrennung im direkteinspritzenden Erdgasmotor** *Multiple cycle LES simulations of a direct injection methane engine*	**Martin Schmitt, Yuri M. Wright, Christos E. Frouzakis, Konstantinos Boulouchos** *ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory*
12	**Katalytisch beschichtete Kolben im Benzin- und Erdgasmotor**	**Patrick Soltic** *EMPA, Dübendorf*
13	**Zukünftige Herausforderungen der Auflade- und Motortechnik**	**Daniel Brand** *ABB Turbo Systems, Baden*
14	**Validierung von Neu-Entwicklungen künftiger Gasturbinen**	**Franklin Genin** *Alstom (Schweiz AG)*

Energieforschungskonzept des Bundes

Rolf Schmitz
Leiter Sektion Energieforschung, Bundesamt für Energie, Bern

ABSTRACT

Die Commission fédérale pour la recherche énergétique (CORE) wurde 1986 als beratendes Organ für die Energieforschung durch den Bundesrat eingesetzt. Sie erarbeitet alle vier Jahre das Energieforschungskonzept des Bundes, prüft die schweizerische Energieforschung, äussert sich zur energiebezogenen Ressortforschung des Bundes und sorgt für eine angemessene Information über die Erkenntnisse und Entwicklungen der Energieforschung. Bisher wurde das Konzept der CORE in über 20 Forschungsbereiche gegliedert und diente vorab den Forschenden als Informationsbasis. Um die Ziele und beabsichtigten Wirkungen der Forschung konzentrierter darstellen zu können, hat die CORE für das Konzept 2013 -16 vier Schwerpunkte definiert, denen sich im Wesentlichen alle Bereiche der Energieforschung zuordnen lassen.

Wohnen und Arbeiten der Zukunft
Mobilität der Zukunft
Energiesysteme der Zukunft
Prozesse der Zukunft

Sie widerspiegeln das tägliche Leben und den damit verbundenen Bedarf an Energie. Die vier Schwerpunkte sind auch im Ausland als wichtigste Ansatzpunkte für verstärkte Effizienz und Reduktion von Emissionen erkannt worden. Mit der Festlegung dieser Schwerpunkte sollen die Schlüsselthemen für die Forschung «top-down» her leitbar sein, und das Systemdenken soll gefördert werden.

Am 28/29.11.2011 führt die CORE eine Energieforschungskonferenz durch und präsentiert das Konzept Fachkreisen aus Politik, Wirtschaft und Wissenschaft. Nach einer Vernehmlassungsphase wird das Konzept per 1.1.2013 in Kraft treten.

Die Rahmenbedingungen und Ziele des CORE-Konzepts dienen als Vorgabe für das Energieforschungskonzepts des Bundesamts für Energie. Darin werden die Forschungsziele für die einzelnen Forschungsprogramme abgeleitet, so auch für die Verbrennungsforschung. Wichtige Ziele sind in Verbrennungssystemen einen möglichst hohen exergetischen Wirkungsgrad zu erzielen und die Umwelt minimal mit Schadstoffen zu belasten. Die Anpassung der Verbrennungssysteme für neue Brennstoffe – aus Biomasse aber auch synthetisch erzeugte – wird in der Zukunft eine wichtige Rolle spielen. Neben der Forschung an Motoren oder Turbinen unterstützt das BFE auch die Verbesserung der Forschungsinstrumente wie die Weiterentwicklung der Simulationsmodelle oder die Vertiefung der Kenntnisse über die chemisch/physikalischen Vorgänge im Verbrennungsprozess.

Jedes Forschungsprogramm des BFE wird durch eine Begleitgruppe, die sich aus Personen aus Wissenschaft und Wirtschaft sowie einem Mitglied der CORE zusammensetzt, unterstütz. Damit wird der Kreis zur CORE als Planungsgremium wiederum geschlossen.

Schwerpunkte der Verbrennungsforschung im ETH-Bereich

Konstantinos Boulouchos
ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory

ABSTRACT

Current Status and Future Perspectives

- The Swiss Combustion Community is well established, diverse and strong, both in fundamental and applied research.
- Given the size of the country, the international visibility is certainly good. In addition future scientific challenges are abundant.
- However: There is a widespread opinion among funding agencies (etc.!), that combustion is a mature technology, where no revolutionary developments can be expected.
- Therefore the community must sharpen its profile and concentrate on few areas of strategic importance for the future energy system.

Auswirkung von Verdampfung, Drall und Brennstoffqualität auf die Einspritzung in grossen 2-Takt-Dieselmotoren

Beat von Rotz
Wärtsilä Schweiz AG, Winterthur

ABSTRACT

The acquisition of fundamental reference data with regard to the spray and combustion characteristics in large marine diesel engines is an absolute prerequisite for the systematic application of existing computational models. For this purpose, a novel experimental test facility has been realized to reproduce the operational characteristics of marine diesel engines at start of injection with respect to the thermo- and fluid dynamic conditions as well as regarding the physical dimensions. First reference data generated on the spray evolution (penetration, cone angle) by means of shadow-imaging contribute to the generally improved understanding of in-cylinder processes and allow the validation of simulation models. Based on preceding analyses of measurements at evaporating conditions, additional experiments have been performed to study the spray evolution in a non-evaporating environment at different gas densities. Moreover, the effect of the swirl level on the injected fuel spray has been investigated in order to obtain a better understanding of the interaction of the spray and the gas flow. Finally, the influence of fuel quality variations has been assessed by comparing data from first tests, where heavy fuel oil was used instead of light fuel oil.

Miller Prozess für niedrige NOx-Emissionen und höhere Effizienz in Grossdieselmotoren

Miller Cycle for Low NOx Emissions and High Efficiency in Medium-Speed Diesel Engines: Potential and Limitations

Panayotis Kyrtatos
ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory

ABSTRACT

In recent years, the main aim in internal combustion engine development has been the reduction of emissions, in order to satisfy ever stricter emission regulations. In the marine diesel engine sector in particular, there has been a significant push for lower NOx emissions, with successive reductions in the NOx emissions allowed. In order to maintain the same level of operating cost, the marine diesel engine industry aims to lower NOx, while maintaining similar levels of efficiency, power density and reliability.

A leading concept used to lower NOx emissions in diesel engines is advanced Miller valve timing, whereby the inlet valve is closed before the gas exchange TDC, allowing the inlet charge to expand before compression. This concept, coupled to high charge pressures achieved using two-stage turbocharging, has been proven to lower NOx emissions and increase engine efficiency by lowering cycle temperatures. The high inlet pressures allow power density to remain at similar levels without a reduction in air-to-fuel ratio, in spite of the shorter inlet valve opening.

In the past, the effects of Miller valve timing to diesel combustion and emission formation have been thoroughly investigated using test-bench measurements and simulations. In publications of such studies, reports of a positive relationship between adiabatic flame temperature and NOx emissions are commonplace. It is argued that an increase in Miller degree and thus a resulting decrease in cycle temperatures and a lower adiabatic flame temperature will cause a decrease in NOx emissions.

However, as shown in the present experimental work amongst others, the NOx reduction benefits obtained through the reduction of cycle temperature are limited. The experiments with increasing Miller timing showed:

- A limit in the NOx-SFC tradeoff benefit offered by increasing Miller degree at high load, and an eventual deterioration of the tradeoff at lower loads
- A correlation between ID (obtained through changing cycle temperature) and NOx emissions for constant charge pressure and injection conditions, with a clear NOx minimum at a certain level of ID and an increase in NOx with reducing temperature/increase in ID
- High cycle to cycle variability with increasing ID

- A connection between high ID and acoustic excitation of the cylinder gases, in the form of higher frequency of ringing cycles and higher pressure fluctuation magnitudes resulting from higher ID
- An increase of apparent mixing levels as a result of increased ID and pressure fluctuations, observed through in-cylinder pressure measurements
- A reduction in soot present in the cylinder as a result of increased ID and pressure fluctuations, observed through in-cylinder soot luminosity measurements using an optical probe

The above experimental observations, coupled to literature review and 3D-CRFD investigations resulted in the following suggestions as possible causes for the NOx trend reversal:

- The increased mixing rate observed during high ringing cycles causes and increase in flame temperature, as well as an increase in the oxygen availability of the NOx producing post-flame gases, contributing to the increase of the NOx emissions. The increased mixing rate observed is further supported by the reduction in measured soot density, which is understood to be caused by increased soot oxidation during combustion due to mixing.
- The increased ID due to lower charge temperatures creates higher proportions of premixed combustion as well as lean premixed combustion zones, resulting in increased thermal NO production during premixed combustion. Additionally, the long ID allows the spray to travel further before ignition, covering a larger part of the combustion chamber and creating a larger and leaner burning zone.
- The reduction in soot density due to increased soot oxidation result in lower radiation cooling of the flame, increasing the flame temperature and as a result NO reaction rate
- The lower temperatures and the increased proportion of premixed combustion could result in an increase in the contribution of NO through prompt NO production in the total NOx emissions
- Due to the Arrhenius nature of reactions, the local pressure and resulting temperature fluctuations result in higher HC and NO reaction rates when compared to rates at the mean temperature. This causes both higher flame temperatures due to higher HC reaction rates and higher rates of NO production locally.

Overall, in terms of its applicability to future engine applications, the Miller cycle coupled to two-stage turbocharging is a technology which could aid in the reduction of NOx emissions and SFC, up to a point. Beyond this point, the Miller cycle will have to be employed in parallel with additional NOx reduction technologies. In terms of in-cylinder measures, based on the present observations, multiple injections could provide a further improvement in the NOx-SFC tradeoff, especially in combination with extreme Miller timing.

Verbrennungseigenschaften von H2-reichen Brenngasen unter gasturbinen-relevanten Bedingungen

Combustion properties of hydrogen-rich fuel gases at gas turbine relevant conditions

Yu-Chun Lin
Paul Scherrer Institut (PSI), Villigen

ABSTRACT

Gasification of solid fuels is considered as an option for mitigating pollutant (e.g. NO_x and CO) and CO_2 emissions when combined with carbon capture technologies. The derived fuel mixtures consist mainly of H_2 and CO (syngas) with various diluents (N_2 and CO_2) based on the feedstock and gasification process. The volume composition of fuel gas can vary from a H_2-CO ratio of 0.5 to almost 100% H_2 if pre-combustion carbon capture is implemented. Such integrated gasification combined cycle (IGCC) plants present new challenges for premixed gas turbine engines conventionally fuelled with natural gas. Accordingly, a “fuel-flexible” gas turbine engine capable of operating with various fuels and fulfilling emission requirements simultaneously becomes essential. A detailed description and understanding of both combustion and emission characteristics for hydrogen-containing fuels are thus imperative.

In this paper, characteristics of turbulent combustion and NO_x emission for high hydrogen-content fuel gases (H_2 > 70 vol. %; “hydrogen-rich”) are addressed. An experimental investigation is performed in a perfectly-premixed axial-dump combustor under gas turbine relevant conditions. Fundamental features of turbulent combustion for these mixtures are evaluated based on OH-PLIF diagnostics. On the other hand, NO_x emissions are measured with an exhaust gas sampling probe positioned downstream the combustor outlet.

Compared to syngas mixtures (H_2 + CO), the operational limits for hydrogen-rich fuel gases are found to occur at even leaner conditions concerning flashback phenomena. With respect to effects of operating pressure, a strongly reduced operational envelope is observed at elevated pressure. Only with decreasing the preheat temperature a viable approach to further extend the operational range is seen. Evaluation of the averaged turbulent flame shape shows that the profile of the flame front is generally approaching that of an ideal cone. Thus a simplified approach for estimating the turbulent flame speed only via the location of the flame tip can be applied.

The level of NO_x emission for the hydrogen-rich fuel mixtures is generally above that of syngas mixtures them showing already higher NO_x emission values than natural gas. Distinct features are found specifically at elevated pressure. While the pressure effects are weak for syngas, a non-monotonic behavior is observed for the hydrogen-rich fuels. Reaction path analysis is performed to complement and provide more insight to the findings from the measurements. From chemical kinetic calculations a distinct shift in NO_x formation pathways (thermal NO_x vs. NO_x through N_2O/NNH reaction channels) can be observed for the different fuel mixtures.

Verbrennungskonzepte für H_2- reiche Brennstoffe unter Gasturbinenbedingungen

Felipe Bolaños, Felipe Piringer, Dieter Winkler und Timothy Griffin
Fachhochschule Nordwestschweiz, Brugg-Windisch

ABSTRACT

Die Verwendung von wasserstoffreichen Brennstoffen in heutigen Gasturbinenbrennern ist wegen der Rückschlaggefahr und hoher NOx-Emissionen nicht einfach umsetzbar. Um Auslegungskriterien für Brenner zu gewinnen, die eine emissionsarme Verbrennung wasserstoffreicher Brennstoffe erlauben, wurden verschiedene Eindüsungs- und Mischkonzepte in einem Laborprüfstand unter gasturbinen-typischen Bedingungen untersucht. Die Versuche führten in der Regel zu dem Ergebnis, dass schlechte Vormischung die Rückschlaggefahr vermindert, aber die NOx-Emission erhöht, was sich für bessere Vormischung umkehrt. Optische Untersuchungen mit einem Glasmischrohr zeigten, dass die Flamme an der Wandgrenzschicht entlang zurückschlägt. Um dies zu vermeiden wurde die Wand des Mischrohrs mit einem Wandluftfilm frei von Brennstoff gehalten. Dieses Konzept ergab bezüglich NOx-Emissionen und Rückschlaggefahr gute Ergebnisse.

Als zweiter Ansatz wurde ein Konzept mit zweistufiger Verbrennung ausgelegt und getestet. In diesem Brenner wird die eintretende Luft in zwei Strömungskanäle aufgeteilt. Im ersten Kanal, welcher als Vorstufe funktioniert, wird der gesamte Brennstoff zugeführt, so dass mit dem dort vorhandenen Luftanteil ein fettes Gemisch mit einem Verbrennungsluftverhältnis λ von 0.3 bis 0.5 erzeugt wird. Das Gemisch wird mittels einer katalytischen Beschichtung gezündet. Durch die Verbrennung unter Sauerstoffmangel entsteht ein Wasserstoff/Stickstoff/Wasserdampf-Gemisch ohne nennenswerte NOx-Produktion. Am Ende der Vorstufe wird das Gemisch mit dem zweiten Luftstrom vermischt und kann dann vollständig ausbrennen. Da keine ausgeprägte Mischzone mehr vorhanden ist, besteht keine Rückschlag-gefahr. Mit dem zweistufigen Konzept wurden mit 100% Wasserstoff bei einem Druck von 8 bar und einer adiabaten Flammentemperatur von 1750 K NOx-Emissionen von unter 50 ppm gemessen.

Einfluss von reaktiven Oberflächen auf die Verbrennung von H2-reichen Brenngasen *Catalytic combustion of rich hydrogen mixtures*

Marco Schultze
Paul Scherrer Institut (PSI), Villigen

ABSTRACT

The hetero-/homogeneous combustion of fuel-rich hydrogen-air mixtures over platinum is investigated at pressures up to 5 bar (relevant for atmospheric pressure burners and microturbine-based portable reactors),fuel-to-air equivalence ratios ranging from j = 2 to 7, and laminar flow conditions (Re ≈1200 to 1400). Experiments are performed in a high-pressure, optically accessible, channel flow catalytic reactor and involve in situ planar laser induced fluorescence (LIF) of the OH radical for the assessment of the homogeneous ignition and 1-D Raman measurements of the major gas-phase species concentrations in the boundary layer for the evaluation of the catalytic processes. Numerical simulations are carried out with an elliptic 2-D model that includes detailed heterogeneous and homogeneous chemical reaction schemes. Hetero-/homogeneous reaction schemes capable of reproducing the onset of homogeneous ignition and the catalytic processes preceding the onset of ignition have been identified. It is shown that the resulting flame structure is markedly different from the corresponding one at fuel-lean conditions, with direct implications for the reactor thermal management.

3D-CFD Simulationen zur Optimierung des Verbrennungssystems und zur Gestaltung des Abgasstranges von Off-Road Dieselmotoren

Alexander Schilling
Liebherr Machines Bulle SA

ABSTRACT

Die zunehmenden Anforderungen der Emissionsgesetzgebung unter Berücksichtigung der im Off-Road Bereich vorhanden applikationsspezifischen Besonderheiten und deren Vielfalt, sowie die limitierten Entwicklungsressourcen, führen zu einem Zielkonflikt, welcher nur durch den vermehrten Einsatz von Simulationswerkzeugen entschärft werden kann. Die dreidimensionale Strömungssimulation, gekoppelt mit der 1D-Simulation, bietet ein geeignetes Mittel um auch Abschätzungen hinsichtlich lokaler Strömungsphänomene zu treffen bzw. diese zu optimieren. Die in diesen Beitrag dargestellten Methoden geben einen Einblick in die Optimierung mittels CFD-Simulationen, wie diese erst in den letzten Jahren aufgrund der hohen Rechenleistungen möglich wurde. Exemplarisch werden die folgenden zwei Anwendungen behandelt: 1) Einspritzung- und Verbrennungsprozess sowie die 2) HC-Eindüsung für die aktive DPF-Regeneration.

Modellierung der Russbildung von n-Heptan Sprays bei dieselmotorischen Bedingungen

Soot Formation Modelling of n-Heptane Spray Combustion Under Diesel Engine Conditions Using the Conditional Moment Closure Approach

Michele Bolla, Yuri M. Wright and Konstantinos Boulouchos
ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory

ABSTRACT

Methodology

First results of numerical simulations of soot formation of n-heptane spray in a constant-volume vessel under Diesel engine conditions are presented for a broad range of conditions, including five different ambient oxygen molar concentrations (8-21 % O_2 range) and two ambient pressures (42 and 85 bar) for a total of nine tested conditions. The results are validated against high-fidelity measurements from the Sandia constant-volume combustion chamber facility [1, 2], which consists of a cubic shape with 108 mm side length. The experimental gas temperature was for all cases 1000 K.

The numerical flow field was solved with the commercial computational fluid dynamics (CFD) solver STAR-CD [3] coupled with an elliptic conditional moment closure based combustion model [4, 5]. The conditional chemical source terms are closed at first order; the reduced n-Heptane chemical mechanism by Liu et al. [6] consisting of 22 species and 18 global reactions is used. Standard modeling approaches for conditional velocity, conditional scalar dissipation rate and conditional turbulent fluxes as proposed in [5]. The high Reynolds number k-□-RNG turbulence model [3] is used. Fuel spray droplets are treated in an Eulerian-Lagrangian way with STAR-CD built-in primary and secondary breakup models [7, 8].

Soot formation is modeled with the semi-empirical two-equations model of Leung [9], where simultaneous soot particle inception, surface growth, coagulation and oxidation by O_2 and OH are considered. In the current implementation, particle inception rate is a first order function of acetylene concentration only. Transport equations for the soot mass fraction and soot number density were solved with unity Lewis number assumption, neglecting differential diffusion effects of soot particles, whose size distribution was assumed as mono-dispersed. Radiation of soot particles was modeled with an optical-thin formulation after [10] using soot mean absorptivity values from [11].

Results

Ignition delay times at 85 bar were well predicted for all ambient oxygen concentrations considered, while at 42 bar they were slightly overestimated for all ambient oxygen concentrations considered. The discrepancy became larger with lower oxygen presence; however the increase in ignition delay by diminishing oxidizer content was correctly described. The same trend for lift-off heights was observed, i.e. increased lift-off heights by reducing ambient oxidizer amount and fair agreement of the predictions with the experiment was found. The influence of the ambient oxygen mole fraction on the flame structure is analyzed on the basis of the 21 % and 10 % O_2 cases at 42 bar. Flame characteristics relevant for soot behaviour (mixture fraction, temperature, mass fractions of OH, O_2 and C_2H_2) are illustrated for the two

different cases at 5 ms after start of injection during the quasi steady-state period of the flame. The main difference consists in the lower value of the stoichiometric mixture fraction for the 10 % O_2 case. As a consequence the stoichiometric region becomes larger and therefore the entire flame becomes broader. Maximal stoichiometric axial distances were approximately 75 mm and 105 mm for 21 % and 10 % O_2, respectively. With a lower ambient O_2 concentration, as expected, a lower flame temperature was observed due to the reduced oxidizer availability. All chemical processes are shifted farther downstream from the injector. Mass fractions of C_2H_2 and OH are roughly one order of magnitude lower compared to the 21 % O_2 case.

The soot volume fraction during quasi-steady spray behavior between 3-6 ms was compared with experiment [1] which was performed with laser induced incandescence methodology. The experimental soot distribution was measured up to approximately 90 mm axial distance from the injector tip through quartz glass windows; soot was observed in the fuel rich zone. In the 21 % O_2 case, the entire soot-loaded region was visualized in the experiment, instead for the 10 % case peak soot concentration was only partially within the observable domain.
The soot volume fraction distribution with the higher oxygen content was well predicted. For the lower oxidizer concentration the peak soot volume fraction was overpredicted, although the measured peak soot concentration was not in the observation region. A lower soot amount and a farther downstream location from the injector with lower oxygen concentration were both predicted correctly.

First results suggest that the conditional moment closure combustion model approach can be considered a highly promisinyg framework for soot modeling due to the accurate flame structure predictions, which are essential for soot predictions.

References

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Regenerationsvorgänge und Emissionen verschiedener DPF-Systeme mit RME

Samuel Bürki
AFHB Berner Fachhochschule, Nidau

ABSTRACT

The fatty acid methyl esters (FAME'S) - in Europe mostly RME (Rapeseed methyl ester) - are used in several countries as alternative biogene Diesel fuels in various blending ratios with fossil fuels (Bxx). Questions arise often about the influences of these biocomponents on the modern exhaust aftertreatment systems and especially on the regeneration of Diesel particle filters (DPF).
Different regeneration procedures of DPF systems were investigated with biofuels B0, B20 & B100.
The tested regeneration procedures were:

- passive regenerations: DOC + CSF; CSF alone,
- active regenerations: standstill burner; fuel injections & DOC.

During each regeneration on-line measurements of limited and unlimited emission components (nanoparticles & FTIR) were conducted.
It can be stated that the increased portion of RME in fuel provokes longer time periods to charge the filter with soot. This is due to the lower PM-emissions of the engine, as well as to the higher reactivity and higher SOF-portion of the particle mass from RME.

With the passive regeneration system with stronger catalytic activity (DOC + CSF) there is a stronger NO_2-production with Bl00 and due to the NO_2-supported oxidation of PM the balance point temperature is approx. 20°C lower, than with B0.
For the active regenerations the time courses of emissions and temperatures are closely connected with the chosen regeneration strategy - switching, timing and intensity (of burner, or fuel aerosol generator).

A higher portion of biocomponent causes usually a stronger break-down of the instantaneous DPF filtration efficiency during the regeneration procedure - this is an effect of stronger artefact of spontaneous condensation after DPF.

In summary there is no negative short term effect of bio-blend-fuels on the investigated regeneration procedures.

Mehrzyklen-LE-Simulationen der Verbrennung im direkteinspritzenden Erdgasmotor Multiple cycle LES simulations of a direct injection methane engine

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ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory

ABSTRACT

In an internal combustion engine, turbulence and physical effects like wall heat losses, flame propagation and cycle-to-cycle variations can be better accounted for using Large Eddy Simulations (LES) instead of the traditional unsteady RANS (URANS) modeling. In this study, the flow field solver STAR-CD v4.14 was employed to perform single as well as multiple cycle simulations of a direct injected (DI) turbocharged four-stroke 1.4l four-cylinder engine to assess the influence of the resolved turbulence in the flow field and the reasons for multiple cycle fluctuations. The engine is derived from a state of the art gasoline DI engine which has been modified for CH_4 DI by means of prototype injectors.

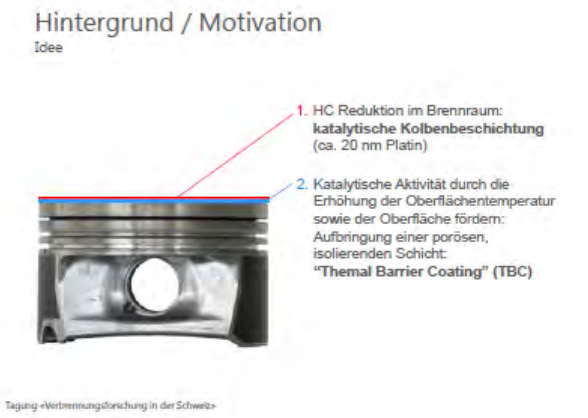
The plugin es-ice has been used to treat the time varying geometry which accounts for valve and piston movement and hence allows for multiple cycle simulations. Three meshes with increasing resolutions have been employed, namely a coarse mesh with 650,000 cells, an intermediate resolution with close to 1 million cells and a fine mesh with 1.5 million cells with corresponding mean sizes of 0.65, 0.55 and 0.45 mm, respectively. Pressure boundary conditions were imposed at the inlet and outlet using tabulated data obtained from a separate 1-D GT-Power simulation. For LES turbulence was modeled with a one equation LES k-l turbulence model and the boundary layers at the wall were calculated with low Reynolds damping. The RANS calculations use a standard $k - \varepsilon$ turbulence model and a wall function for the simulation of the near wall region. Combustion was treated by means of the G-equation as implemented in STAR-CD, which accounts for partial stratification due to the imperfections in mixture homogeneity resulting from the direct injection of the gaseous CH_4 during the intake/compression stroke. For the fuel admission, a Lagrangian-Eulerian approach has been adopted. Further details concerning turbulence, combustion and the injection models can be found in [1].

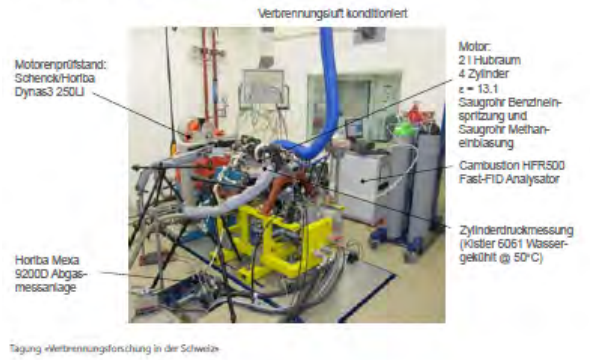
In a first step, the results of the LES and URANS simulations were compared in a single-cycle calculation. Typical vector fields computed with the two approaches are compared in Fig. 1. As expected, the LES can resolve a lot more details of the flow field.

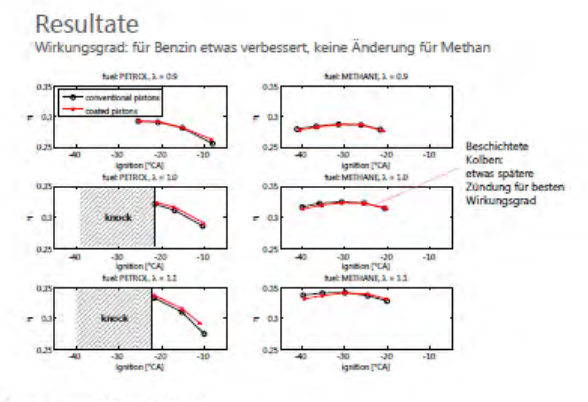
Katalytisch beschichtete Kolben im Benzin- und Erdgasmotor

Patrick Soltic
EMPA, Dübendorf

ABSTRACT

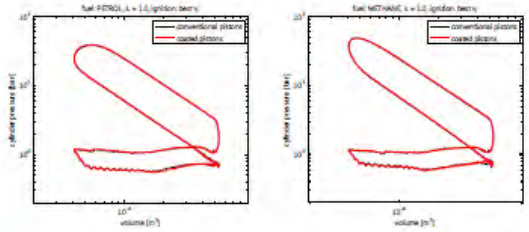






Resultate

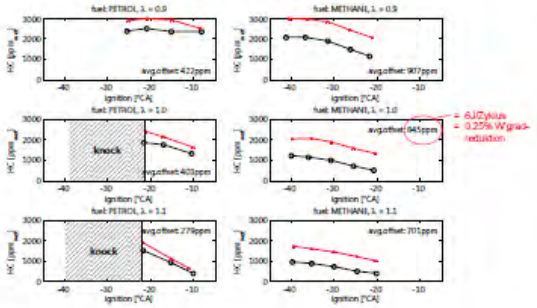
Zylinderdruckverläufe (λ=1, bester η): minimale Unterschiede



- No difference in the gas exchange process
- Coated pistons: slightly higher pressure in the high pressure part of the process for petrol (leads to better efficiency)

Resultate

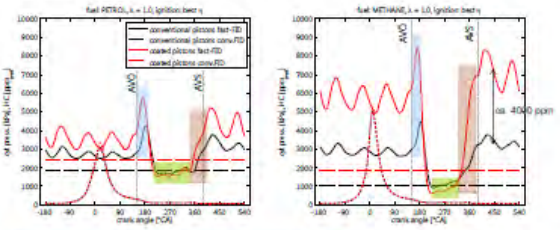
HC Emissionen: Steigen durch die Beschichtung!



Resultate

HC Emissionen ca. 10cm nach Auslassventil (Fast-FID Messungen)

Gemittelt über 200 aufeinanderfolgende Zyklen



Phase 1 (Auslassventil öffnet): ähnliche HC Peaks unbeeinflusst / beschichtet

Phase 2 (Blik Flow): Tiefere HCs bei beschichteten Kolben

Phase 3 (Auslassventil schliesst): höhere HC Peaks für beschichtete Kolben (viel höher bei Methan)

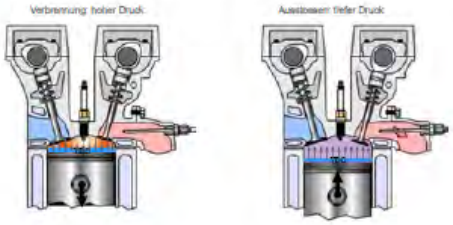
da muss ein methan-selektiver Prozess eine Rolle spielen

Picture source: www.cambustion.com (pictures modified)

Resultate

Methan-selektiver Prozess

- Hypothese: Methan Adsorpion / Desorption in der TBC Schicht



Resultate

Methan Adsorption

TBC Sample der gelaufenen Kolben

Adsorptionsmessung
(Sorptionsisotherme, thermogravimetrische Analyse)

Methan-Adsorption bei 250 °C
- 1.74 10^{-3} g pro Kolben
- Ergibt 1.08 10^{-4} mol CH_4 pro Kolben und Zyklus

Abschätzung des Einflusses:

$$\frac{\text{adsorbierter } CH_4}{\text{Geometrie-Inderladung}} = \frac{1.08 \cdot 10^{-4}}{2.186 \cdot 10^{-1}} \approx 5 \cdot 10^{-3} = 5000\,ppm$$

→ Eine bedeutende CH_4-- Menge kann im TBC Layer gespeichert werden

Diskussion / Ausblick

- TBC/Pt-beschichtete Kolben widerstehen der mechanischen und thermischen Belastung eines Ottomotors (getestet bis 3000 min^{-1} und einem Spitzendruck bis 70 bar)
- Die TBC/Pt Beschichtung erhöht im Benzinbetrieb den Wirkungsgrad im betrachteten Betriebspunkt leicht, im Methanbetrieb führen die erhöhten Methanemissionen nicht zu diesem Effekt
- HC Emissionen steigen mit der TBC/Pt Beschichtung deutlich, die anderen Schadstoffe werden davon nicht beeinflusst
- Die Betrachtung des HC-Verlaufes deutet darauf hin, dass die HC Emissionen der Zylinder-Hauptladung reduziert werden können
- Die Methanadsorption in der TBC Schicht erhöht die HC Emissionen schlussendlich
- Empfehlung: eine poröse Zirkonoxyd-Schicht ist nicht zielführend, eine alternative Isolationsschicht muss gefunden werden
- Bemerkung: Es gibt es theoretische Arbeiten welche vorhersagen, dass Zirkonoxyd im Brennraum eine katalytische Wirkung hat[1]. Adorptions-phänomene wurden dort nicht berücksichtigt.

[1] Nedunchezhian N, Dhandapani S. Study of flame quenching and near-wall combustion of lean burn si-fuel mixture in a catalytically activated spark-ignited lean burn engine. Combustion and Flame 144 (2006), 407-409

Zukünftige Herausforderungen der Auflade- und Motortechnik

Daniel Brand
ABB Turbo Systems, Baden

ABSTRACT

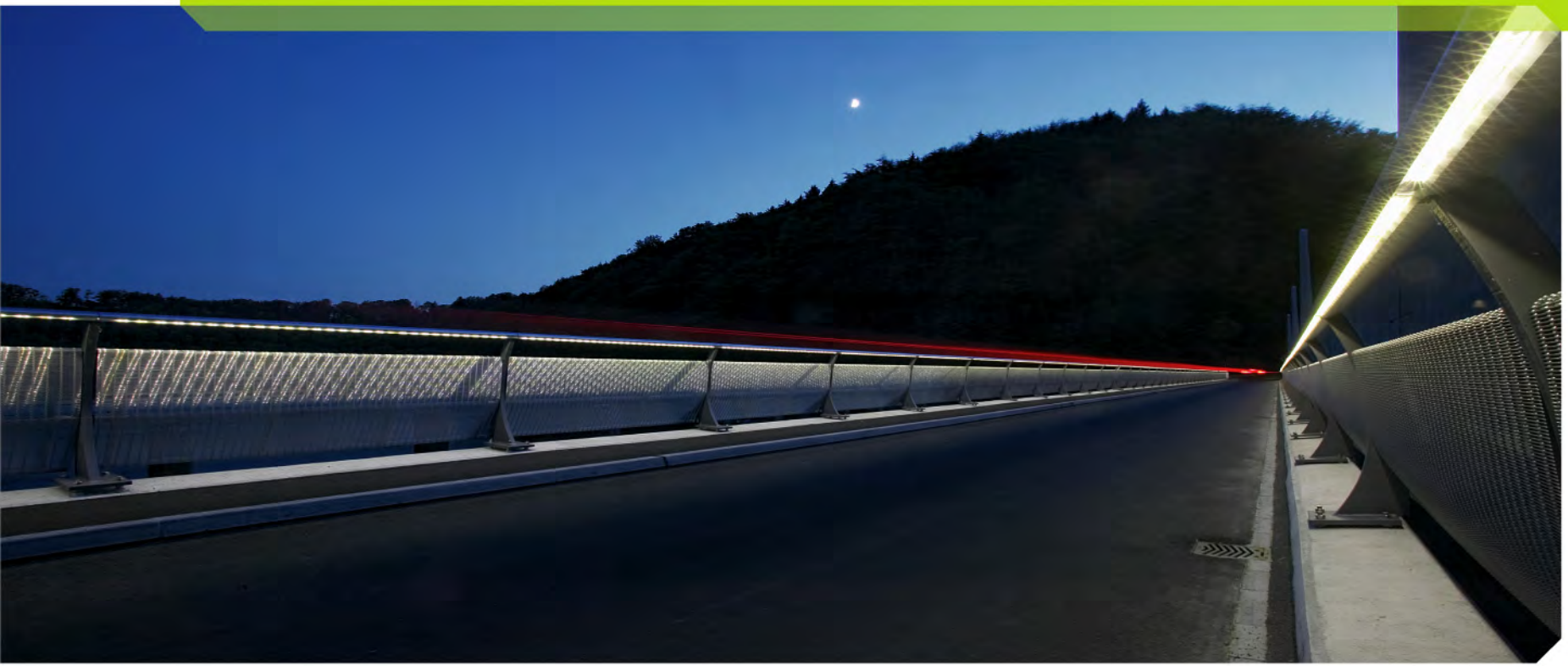
ABB Turbo Systems ist der führende Anbieter von Turboladern für die Aufladung von grossen Gas- und Dieselmotoren mit einer Leistung von mehr als 500 kW. Die so aufgeladenen Motoren finden Anwendung in Schiffen (Hauptantrieb und Hilfsgeneratoren), in Kraftwerken sowie in grossen Off-Road Fahrzeugen und Lokomotiven. Die Motoren decken einen Bohrungsbereich von ca 17 cm bis 98 cm ab.
Es werden 4-Taktmotoren ebenso wie 2-Taktmotoren ausgerüstet.

ABB Turbo Systems AG hat Forschungs- und Entwicklungsbedarf in allen Disziplinen des Strömungsmaschinenbaus. Darüber hinaus, und darauf bezieht sich dieser Beitrag, hat ABB Turbo Systems AG auch einen Bedarf, die Motorenentwicklung via F&E Aktivitäten frühzeitig zu antizipieren und, da wo angezeigt, die notwendigen Trends zu setzen. Die wesentlichen Beiträge der Motorenentwicklung kommen heute und zukünftig aus den Feldern Luft- und Abgasmanagement, inner-zylindrischer Prozessführung, Abgasnachbehandlung und der zugehörigen Steuer- und Regeltechnik. Die ABB Aktivitäten konzentrieren sich auf die Produktentwicklung (neue Turbolader, variabler Ventiltrieb), auf ein erweitertes Verständnis von Potenzial und Grenzen der inner-zylindrischen Vorgänge bei neuen Brennverfahren und auf die Möglichkeiten der Abgasnachbehandlung.

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

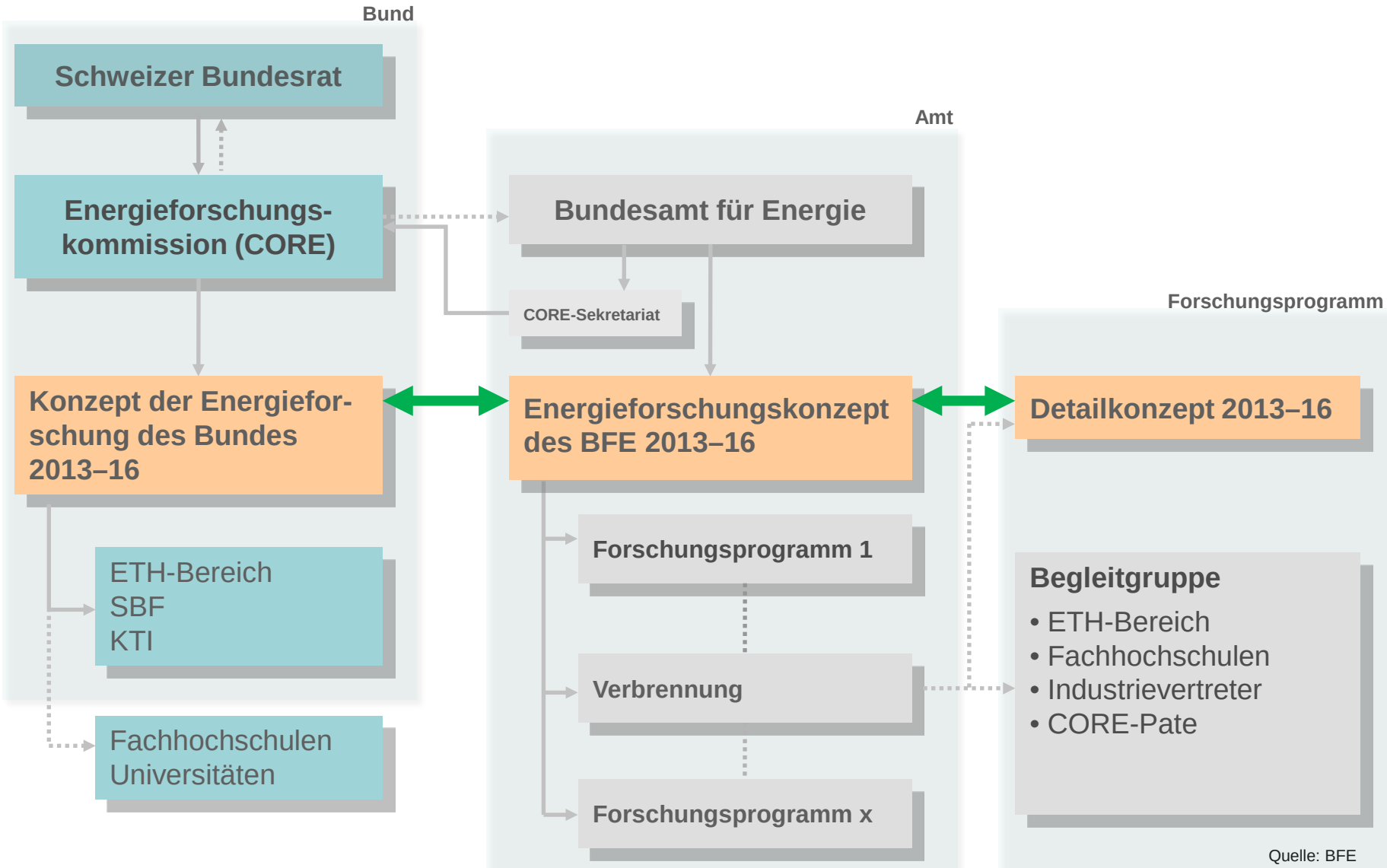
Bundesamt für Energie BFE
Office fédéral de l'énergie OFEN
Ufficio federale dell'energia UFE
Swiss Federal Office of Energy SFOE

Das Energieforschungskonzept des BFE



Dr. Rolf Schmitz, 28.10.11

Organisation der Energieforschung in der Schweiz



Altes und neues Konzept

Altes und neues Konzept

Schwerpunkte 2008–2012

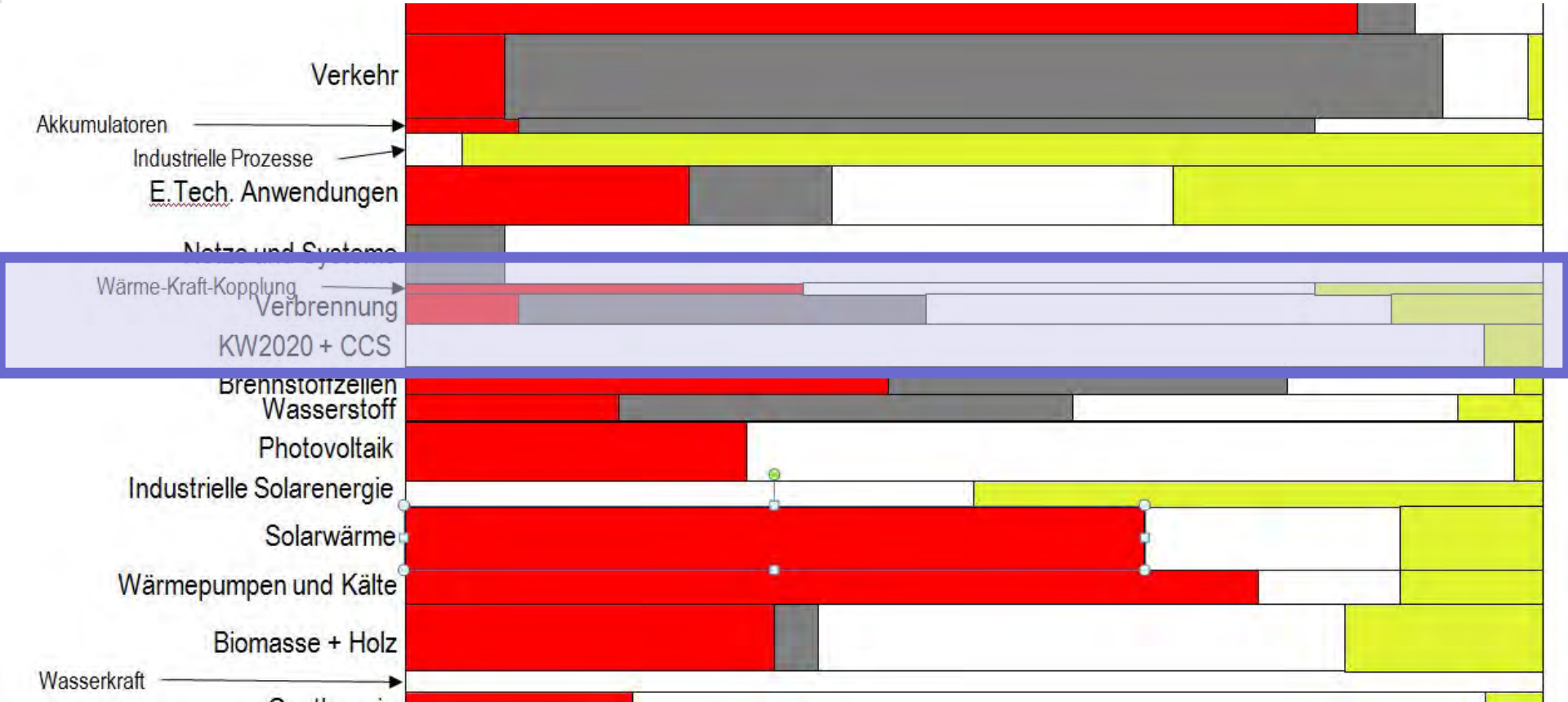
Energie in Gebäuden
Verkehr
Batterien und Supercaps
Elektrizitätstechnologien und -anwendungen
Netze
Wärme-Kraft-Kopplung
Verbrennung
Kraftwerk 2020
Brennstoffzellen
Verfahrenstechnische Prozesse
Solarthermie
Fotovoltaik
Industrielle Solarenergienutzung
Wasserstoff
Umgebungswärme
Biomasse
Wasserkraft
Geothermie
Windenergie
Kernspaltung und Nukleare Sicherheit
Regulatorische Sicherheitsforschung
Kernfusion
Energiewirtschaftliche Grundlagen

Schwerpunkte 2013–2016

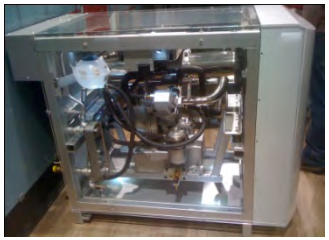
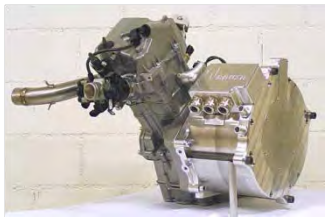
Wohnen und Arbeiten der Zukunft
Mobilität der Zukunft
Energiesysteme der Zukunft
Prozesse der Zukunft

Zuordnung der Programme des BFE zu den Schwerpunkten

Wohnen und Arbeiten	17 FP / 23% Mittel	Energiesysteme	26 FP / 52% Mittel
Mobilität	13 FP / 14% Mittel	Prozesse	21 FP / 11% Mittel



Verbrennungsrelevante Ziele aus CORE-Konzept

Wohnen & Arbeiten	• WKK für Gebäudeheizung (η_{el} > 50%, η_{gesamt} > 95%) • keine Heizkessel	
Mobilität	• Nahverkehr ohne fossil • Schwere Dieselfhz: red. Verbrauch • Biotreibstoffe 2. und 3. Generation • Energieträger und Antriebe flexibel	
Energiesysteme	• Brenngase aus Biomasse • GuD η_{el} 62–63 % • CO_2-Abscheidung • Strom-Wärme-Kälte kombinieren	
Prozesse	• Effiziente Antriebe (off road) • Verbesserte Verbrennung Industrie (Zement, Ziegelei, KVA) plus CO_2-Abscheidung	

Ziele BFE Forschungsprogramm Verbrennung

Was ist wichtig	• Hoher exergetischer Wirkungsgrad • Geringe Schadstoffemissionen (NO_x, Russ)
Neuartige Brennstoffe	• Verbrennung biogener Brennstoffe optimieren • Variabler Brennstoffeinsatz • Neue Brennstoffe nach Anforderung der Verbrennung
Forschungs-bereiche	• Verbrennungsprozess, Versuchsträger, Simulationsmodelle • Teilsysteme: Brennstoffaufbereitung, Einspritzung, Zündung, Verbrennung, Abgasbehandlung • Gesamtsysteme: Modell-basierte Abstimmung, transienter Betrieb
Anwendungen	• Grosse Gas- und Dieselmotoren (off road, stationär, Marine) • Motoren in hybriden Systemen • kleine, mittlere und grosse WKK-Systeme • Industriefeuerungen

Nächste Schritte: Konzepte CORE und BFE

CORE

Konzept der Energieforschung des Bundes

– Energieforschungskonferenz 28./29.11.11

– Vernehmlassung 1.12.11–28.2.12

– Frühling 2012: Einarbeiten Vernehmlassung und Ergebnisse der interdepartementalen Arbeitsgruppe Energie

– 1.1.2013: Inkrafttreten

BFE

Energieforschungskonzept des BFE

– Februar 2012: Druck für ParlamentarierInnen

– Frühling 2012: Einarbeiten Anpassungen CORE

Vielen Dank

für Ihre

Aufmerksamkeit

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

LAV

Schwerpunkte der Verbrennungsforschung im ETH-Bereich

Tagung «Verbrennungsforschung in der Schweiz», 28. Oktober 2011

Konstantinos Boulouchos, Institut für Energietechnik, ETH Zürich

Combustion Research in Switzerland

- Industry Companies (incl. SME's)
- Fachhochschulen (steady and unsteady combustion)
- ETH-Domain: major activities at:
  - Paul Scherrer Institut
  - EMPA
  - ETH Zürich
  - (..... ?)

Research Focus 2011

Thermal Process Engineering
Serge Biollaz

(biomass) gasification & fuel gas processing
- **hot gas filtration, S-resistant methanation**

Combustion Technologies
Peter Jansohn

Chemical processes (@ high pressure)
- **soot formation** (in syngas production)

Internal combustion / **large diesel engines**
- fuel distribution & mixing

Gas turbines
- **H_2-rich fuels/CO_2** mitigation

Combustion Fundamentals
Ioannis Mantzaras

Modeling of high temperature reactors
- heterogeneous/homogeneous coupling
- **microreactors & porous media**

Molecular Dynamics
Thomas Gerber

Molecular states of reactive species
- Integration: **laser lab + SLS/VUV**

Laser based diagnostics

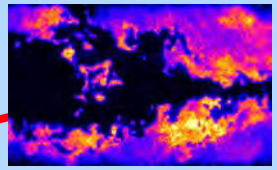
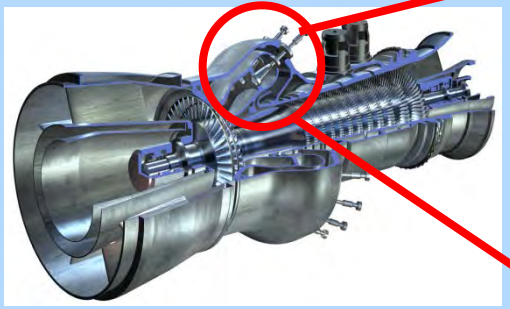
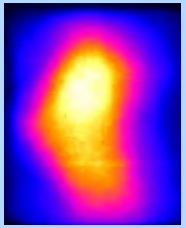
Pilot demonstration units

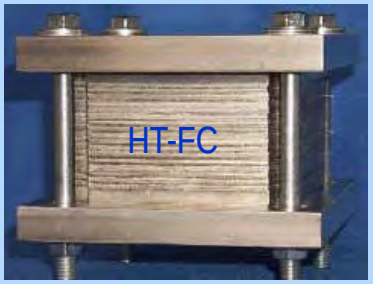
Low emission / high efficiency energy conversion technologies




gasification &
(catalytic) gas processing




spray & soot
diagnostics

turbulent
premixed
flames

combustion
dynamics


catalytic combustion


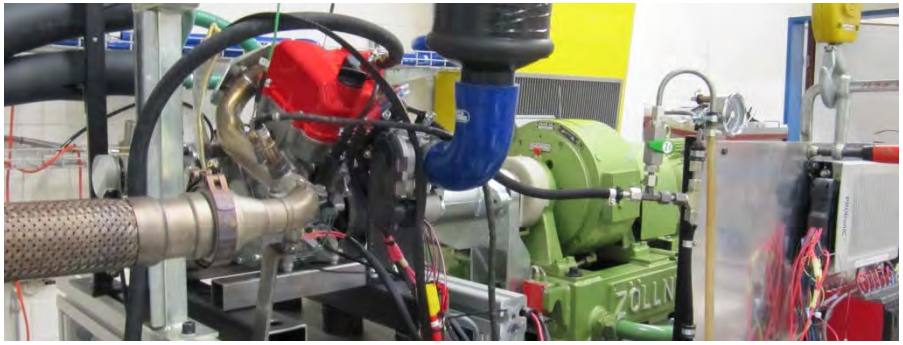
Schwerpunkte der Empa Abteilung Verbrennungsmotoren

EMPA
Materials Science & Technology

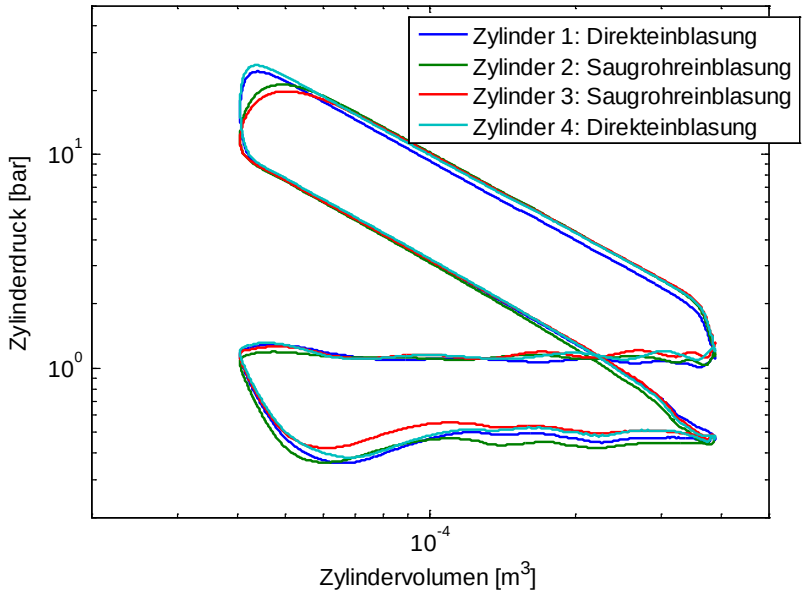
- Experimentelle Verbrennungsforschung an seriennahen Motoren mit dem Schwerpunkt **gasförmige Kraftstoffe (Erdgas/Biogas**) **für PKW und Stationäranwendungen**
- Experimentelle Verbrennungsforschung an **LKW Dieselmotoren** (NO_x-Partikel-Verbrauch Tradeoff für verschiedene Einspritz- und Brennverfahren sowie verschiedene Kraftstoffe), **Zündstrahlbrennverfahren**
- **Zündverbesserung bei gasförmigen Kraftstoffen**, insbesondere durch den Einsatz von Zündbeschleunigern wie Wasserstoff
- Forschung an der **Schnittstelle Verbrennung/Materialien** (Katalyse im Brennraum sowie Abgasnachbehandlung)
- Flexible **Gaswechsel- und Laststeuerungsverfahren** zur Ermöglichung neuer Brennverfahren (Aufbau variabler hydraulischer Ventiltrieb)

Empa Abteilung Verbrennungsmotoren: Aktuelle Beispiele

- Cohyb Projekt: Brennverfahren (direkt- und saugrohreingeblasen) für Methan mit Wasserstoff als Zündbeschleuniger.
  Foto: 1-Zylinder Swissauto Motor auf dem Prüfstand



- Clever Projekt: Potenzialauslotung für Direkteinblasung von Methan.
  Abbildung: Zylinderdruckverläufe in einem 1.4 Liter 4 Zylindermotor mit Zylinder 1+4 DI sowie Zylinder 2+3 Saugrohreingeblasen, alle Zylinder mit identischem Zündwinkel.
  Erkenntnis: Direkteinblasung von Methan kann die Verbrennung massiv beschleunigen.



Combustion Research Group of Prof. P. Jenny

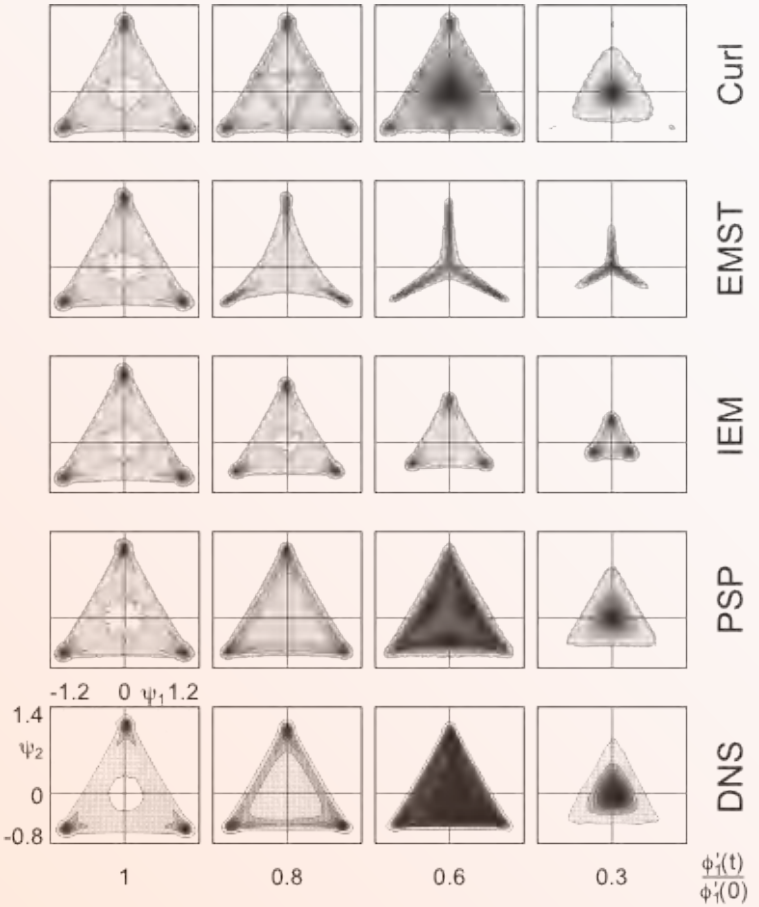
- **Probability Density Function (PDF) Code Development:**
  particles represent joint velocity-concentration PDF, more particles = better statistics, development of efficient & accurate numerical schemes and algorithms

- **Premixed / Partially Premixed Combustion:**
  modeling molecular mixing & flame propagation with statistical methods based on quantities extracted from flamelets and other conceptual representations of the fine-scale physics

- **NO-Formation:**
  NO source term parametrization based on flamelet approach (including radiation) with consistent Nitrogen chemistry

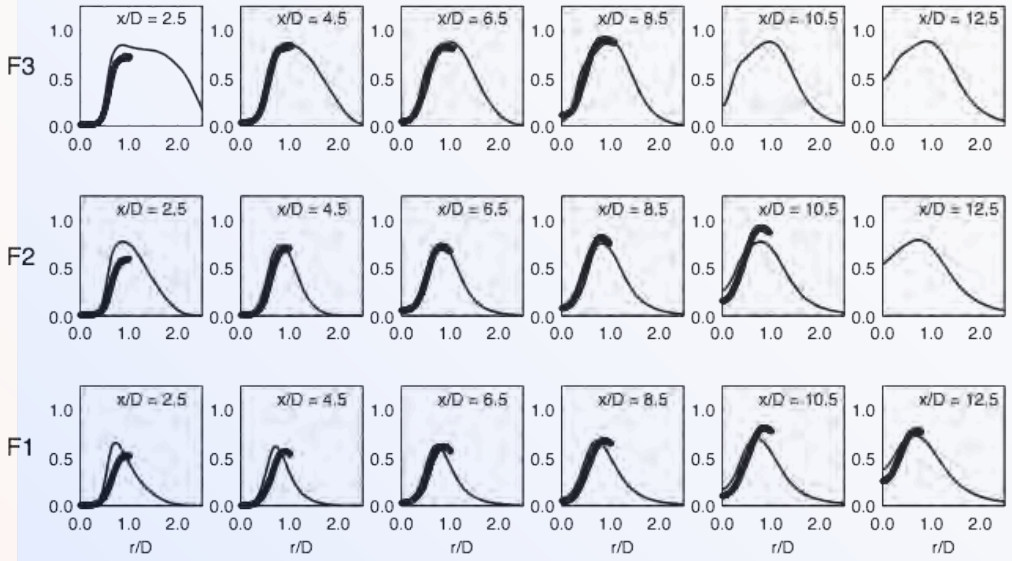
- **Spray Combustion:**
  modeling of turbulence/droplet interaction in dilute sprays in RANS and PDF context, modeling of droplet evaporation and mixing with Lagrangian particle techniques

PDF Modeling molecular mixing in turbulent flows: validation of parametrized scalar profile (PSP) model with DNS and standard mixing models



mixing of joint concentration PDF of two inert scalars in homogeneous isotropic turbulence
rows: DNS and different models
columns: PDF evolution stages over time

BML/PDF calculations of Aachen bunsen flames F1-3:
radial Favre-averaged temperature profiles at different downstream locations



measurements (thick lines), simulation (thin lines)
premixed piloted bunsen flames
very good agreement over a wide range of jet velocities:
flame F1: U_b=65m/s, thin reaction zones regime
flame F3: U_b=30m/s, corrugated flamelets regime

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

LAV

Laboratorium für Aerothermochemie und Verbrennungssysteme

Experiments

WEG
P. Obrecht

Simulation

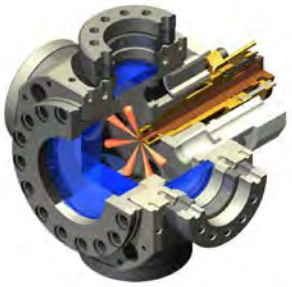
Generic
B. Schneider

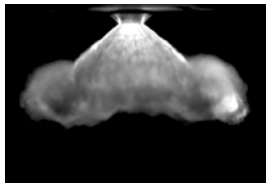
Engines
P. Obrecht

Engines
Y.M. Wright

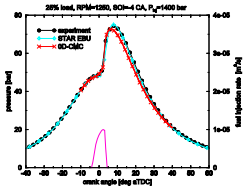
DNS / LES
C. Frouzakis

ELB
I. Karlin

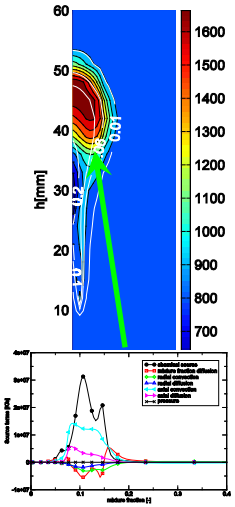




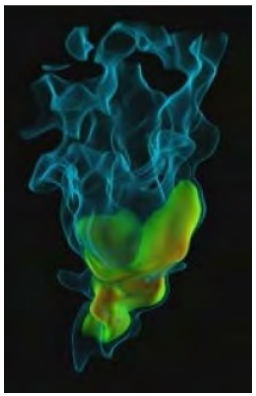
Hollow-cone spray A. Schmid, *LAV 2011*



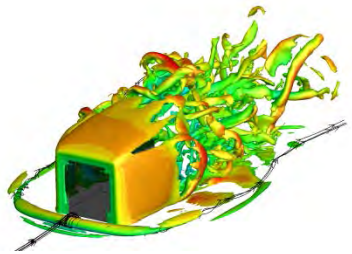
A. Bertola, LAV – *Diss. ETH 15373*



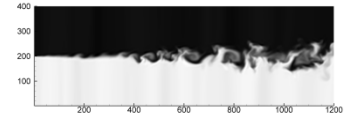
Wright, De Paola, Boulouchos & Mastorakos, *Comb. & Flame* (2005)



Auto-ignition of H_2 plume in tur-bulent hot air co-flow. Kerkemeier, Markides, Frouzakis, Boulouchos. *submitted for J. Fluid Mech. 2011*



S.Chikatamarla, *High Resolution simulation of flow past a cube placed in a wind tunnel*



S. Arcidiacono, S. Ansumali, J. Mantzaras, I. Karlin, C. Frouzakis,
K. Boulouchos, *Phys. Rev. E* (2006)

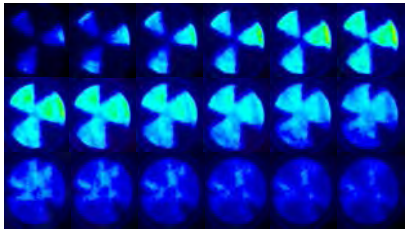
'engine' CRFD

LAV

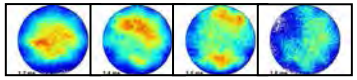
premixed

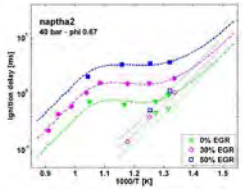
non-premixed

dual fuel
Stéfanie Schlatter
RANS/CMC+Weller3

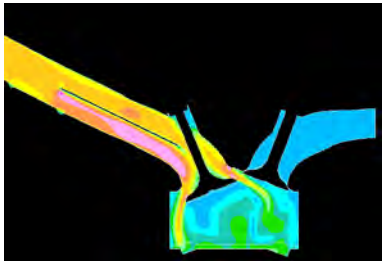


HCCI
Annelies Vandersickel
Global reaction model

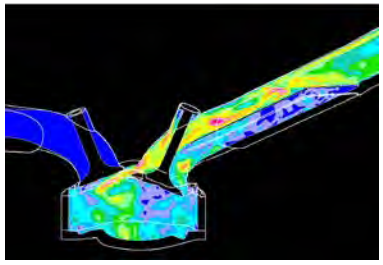




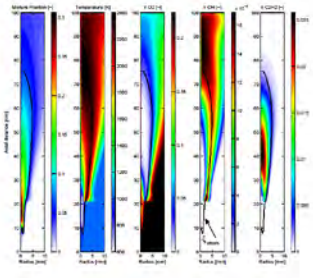
CH_4-DI
Reto Egli
RANS/G-egn



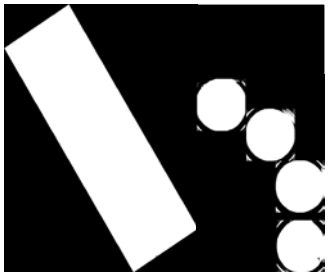
CH_4-DI
Martin Schmitt
LES/G-egn



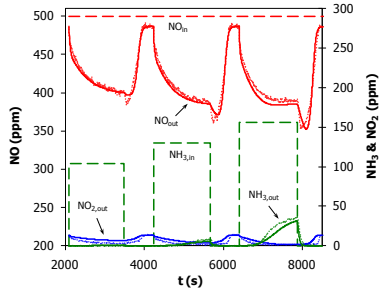
Soot
Michele Bolla
RANS/CMC



Marine
Michel Cattin
RANS/CMC



SCR
Leila Sharifian
1D-1D code

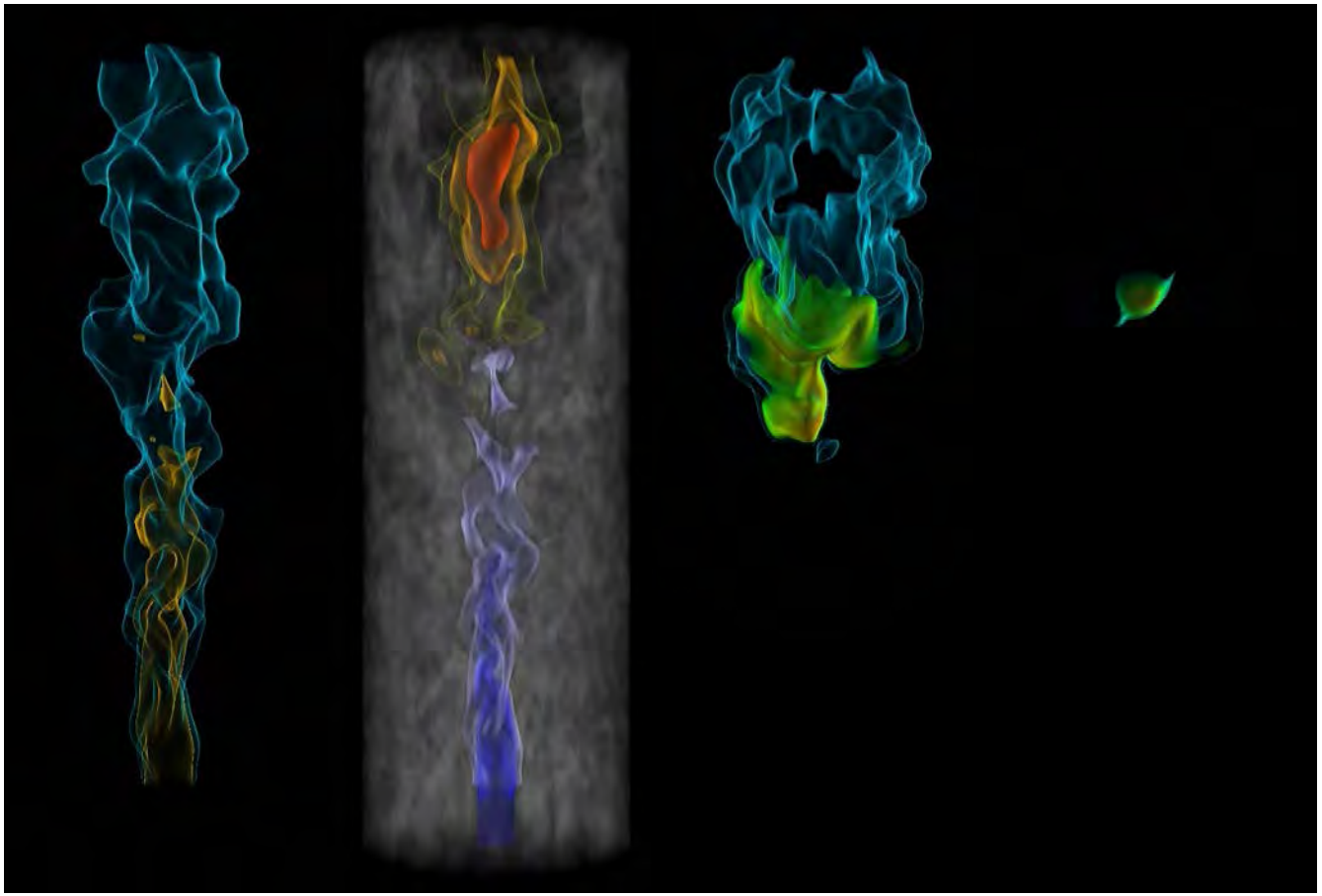


Direct Numerical Simulation (DNS)

- **Accurate *numerical* experiments to provide complete description**
  - Understanding of the complex interplay of flow and combustion
  - Detailed parametric studies
  - Data for model development/validation

- **DNS code**
  - Parallel, spectral element code
  - Low Mach number formulation
  - High-order method/complex geometries
  - Detailed gas-phase and surface chemistry/transport
  - Conjugate heat transfer
  - Excellent scalability up to 10^5 CPUs

Recent applications: Turbulent H2 autoignition



- Laboratory-scale DNS of autoignition
- Cylinder D=16mm, h=55mm
- 300 million grid points
- 11 ms simulation time (δt=100 ns)
- $U_{fuel} = U_{air} = 26$ m/s
- $T_f = 855$K, $T_{air} = 950$K
- detailed H_2/O_2 mechanism (9 species / 21 rxns) and transport
- Synthetic turbulent inflow
  - $Re_{turb} \sim 110$
  - Turbulence intensity: 15% and 25%

- 12M CPUh on ALCF's IBM BG/P using 32k-64k cores
- 100TB of raw data

Mixture fraction (ξ) ξ_{MR} ξ_{st} Temperature Y_{HO_2} $\dot{\omega}_{OH}$ (zoom in)

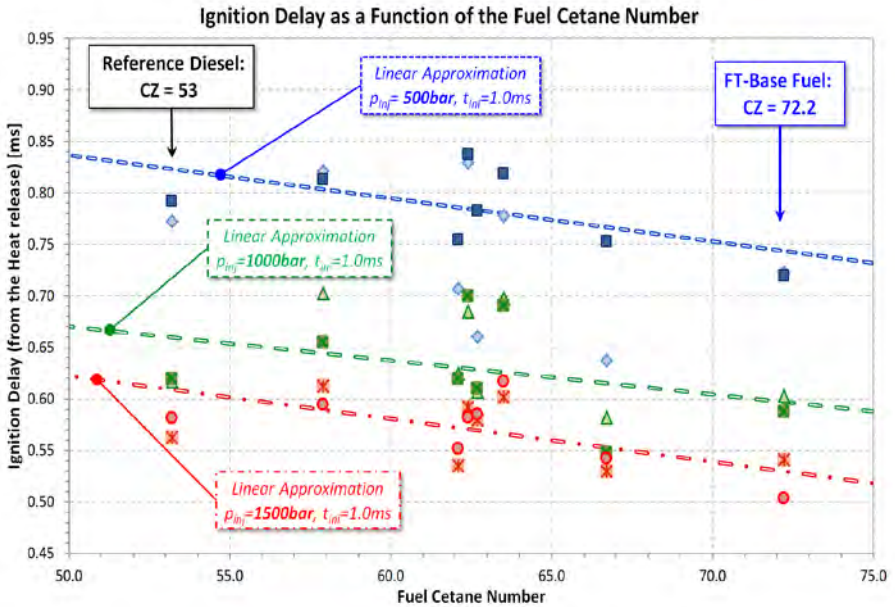
FVV Forschungsvorhaben Nr. 940 : „Future Fuels for Diesel Engines"

- ***Synthetic Diesel Fuels or Fuel Additives offer new opportunities to improve Diesel Engines,***

  but….

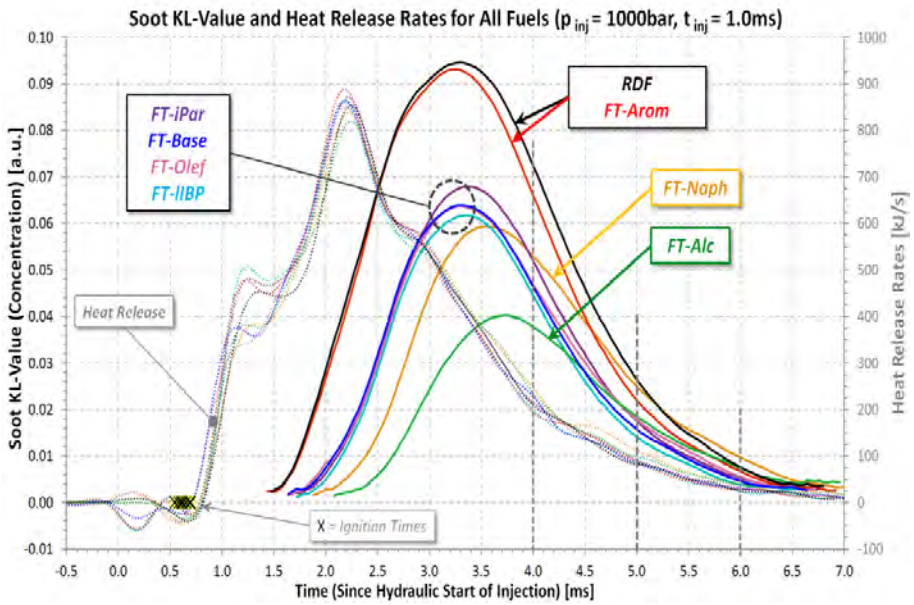
- ***How Will Different Fuel Compositions Affect the Ignition and Diesel Combustion***

Ignition Delay



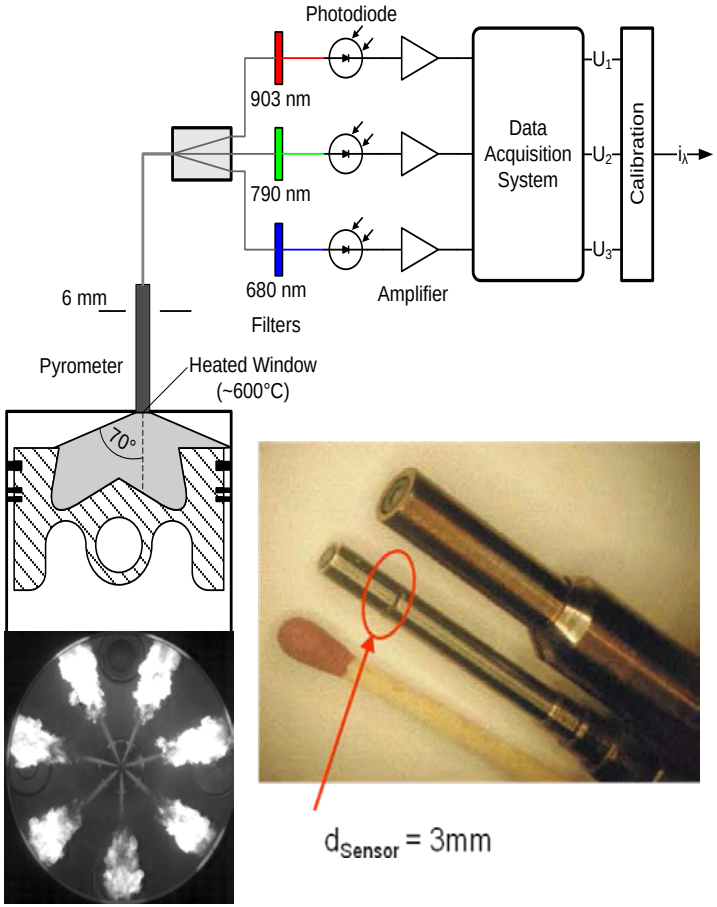
- Injection pressure has a higher influence on the ignition delay than the fuel composition / Cetan number range

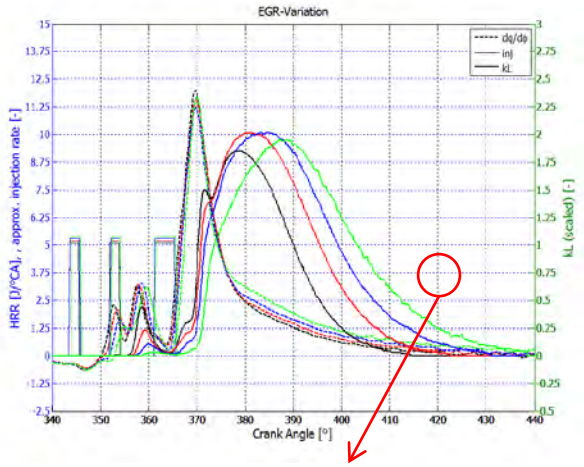
Soot-Development During



- Very different start of soot production and maximum KL-levels (soot concentrations)
- Some fuels show a much slower soot oxidation process than the others

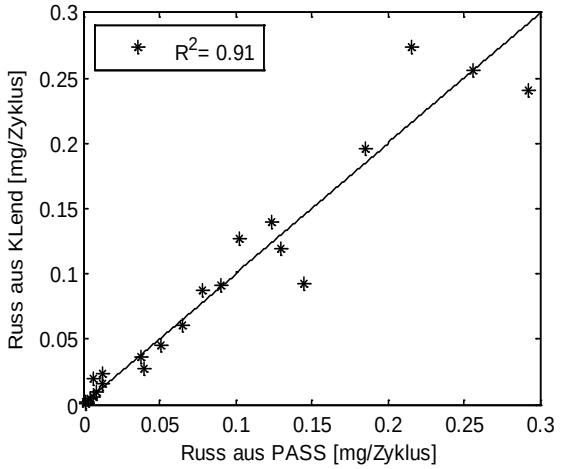
In-Cylinder Soot Measurement – Concept – Application





- EGR 0% Soot: 4 mg/m³
- EGR 10% Soot : 9 mg/m³
- EGR 20% Soot : 41 mg/m³
- EGR 30% Soot : 215 mg/m³

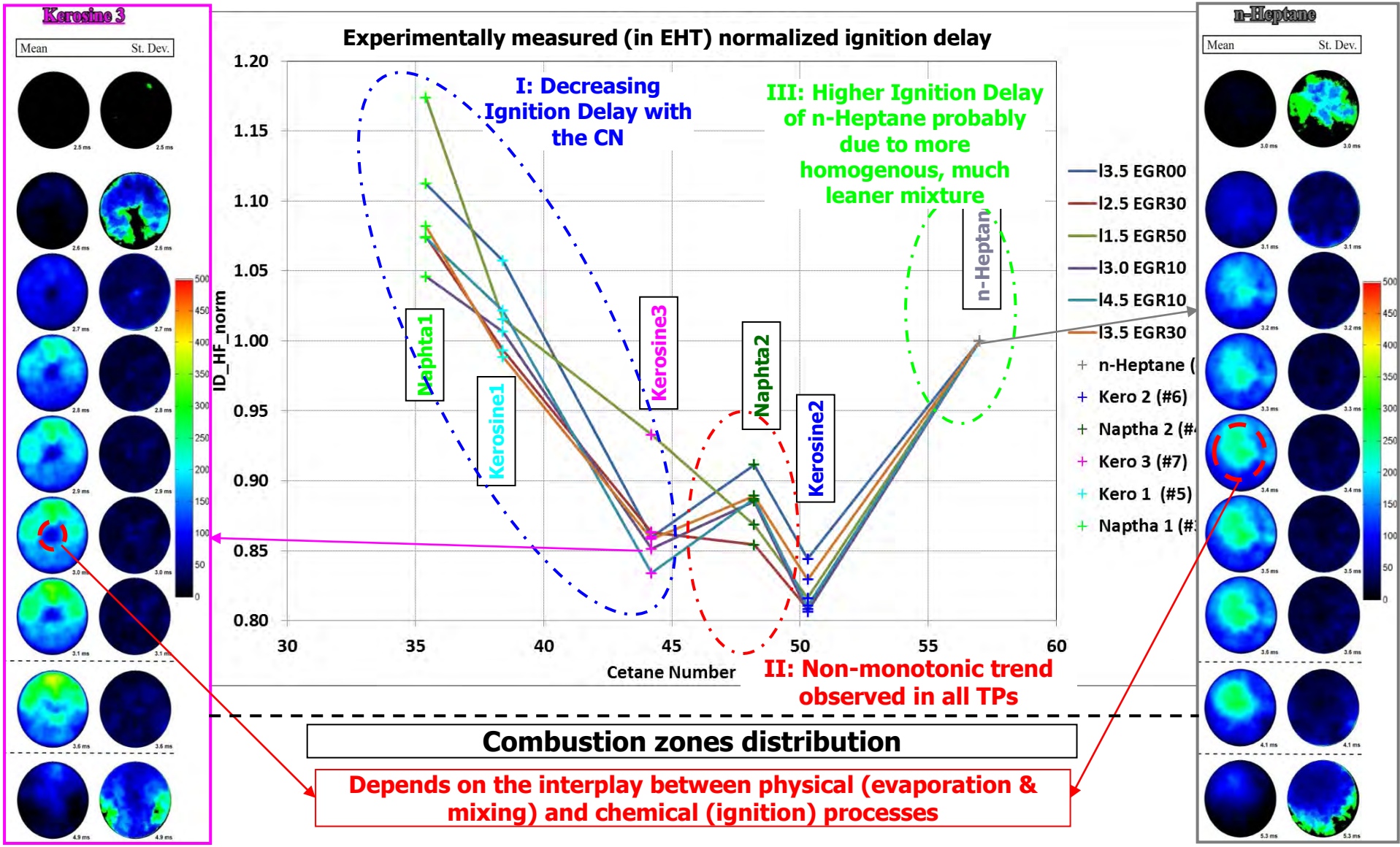
Different **soot evolutions** at „similar" heat release rates under different EGR conditions



24 measurements

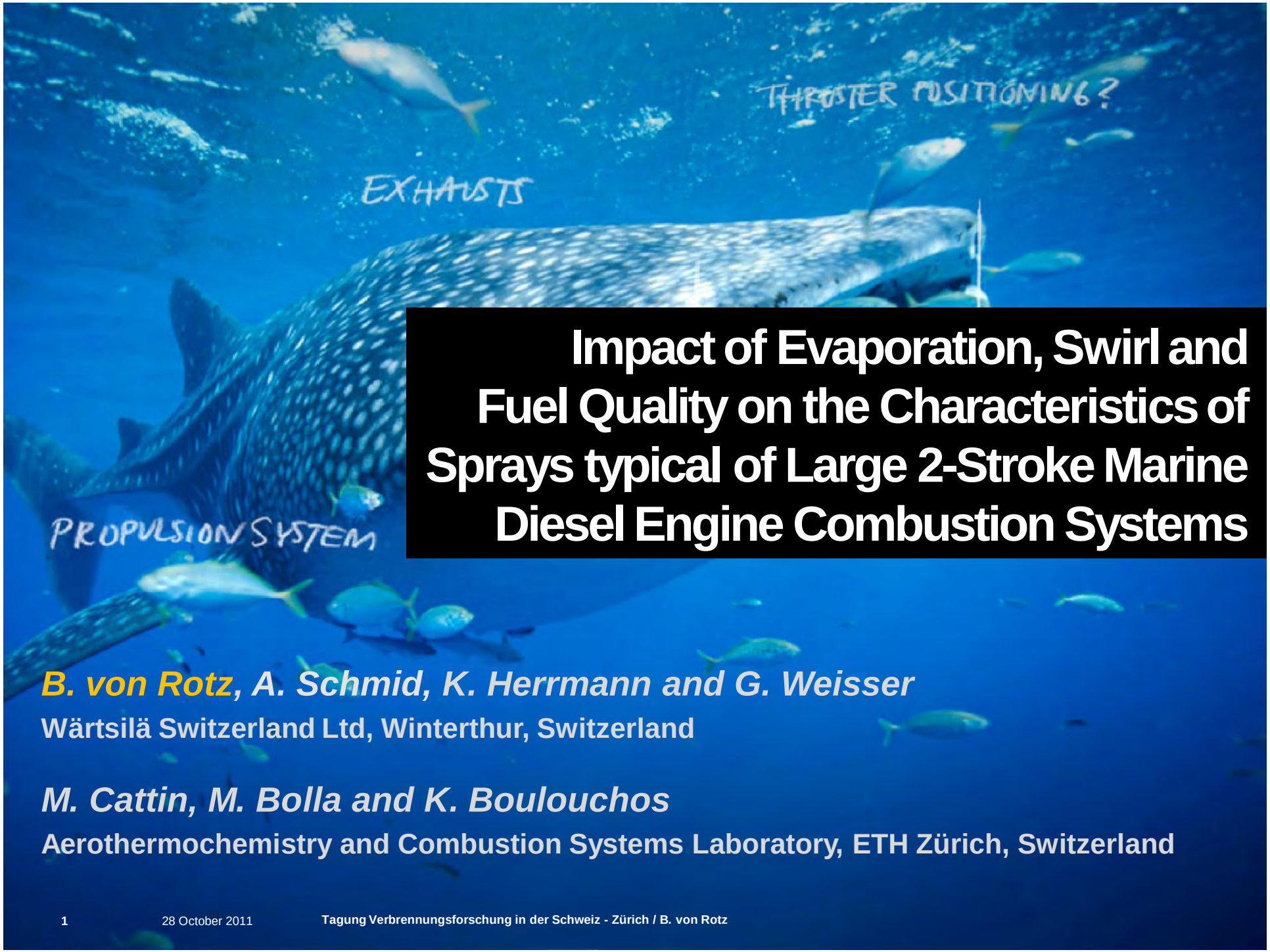
Correlation between KL end value and exhaust soot measurement can be found

Kraftstoffkennzahlen für homogene Verbrennung: TP3



Current Status and Future Perspectives

- The Swiss Combustion Community is well established, diverse and strong, both in fundamental and applied research.
- Given the size of the country, the international visibility is certainly good. In addition future scientific challenges are abundant.
- However: There is a widespread opinion among funding agencies (etc.!), that combustion is a mature technology, where no revolutionary developments can be expected.
- Therefore the community must sharpen its profile and concentrate on few areas of strategic importance for the future energy system.



Impact of Evaporation, Swirl and Fuel Quality on the Characteristics of Sprays typical of Large 2-Stroke Marine Diesel Engine Combustion Systems

B. von Rotz, A. Schmid, K. Herrmann and G. Weisser

Wärtsilä Switzerland Ltd, Winterthur, Switzerland

M. Cattin, M. Bolla and K. Boulouchos

Aerothermochemistry and Combustion Systems Laboratory, ETH Zürich, Switzerland

Introduction

Container Ship „ESTELLE MAERSK“

- **Length:** 397 m (1,302 ft)
- **Speed:** 25.5 knots (47.2 km/h)
- **Capacity:** 156,907 DWT ; 14,770+ TEU

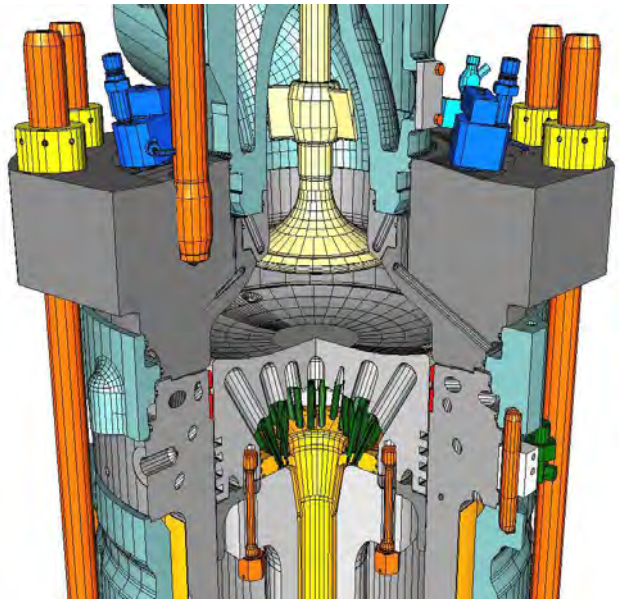
Introduction

2-Stroke Marine Diesel Engine

- **Cylinder bore:** 350 - 960 mm
- **Piston stroke:** 1550 - 3150 mm
- **Speed:** 61 - 167 rpm
- **Power Output:** 5'560 - 80'080 kW

Introduction

Combustion Chamber



- **Dimensions**
- **Injection (peripherical, multiple orifice)**
- **Swirl (uniflow-scavenged)**
- **Large p-, T-levels (13 MPa / 900 K)**
- **Range of fuel qualities (HFO, MDO, LFO)**

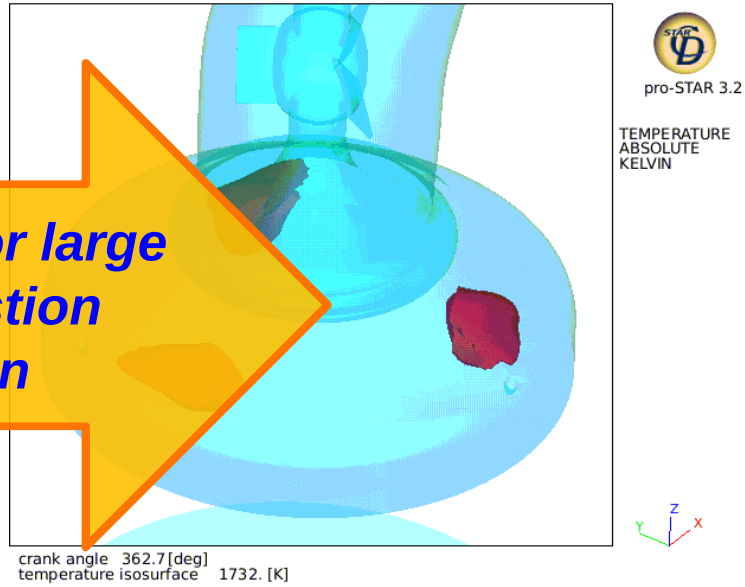
LAV WÄRTSILÄ

Introduction

Development and Optimization of the Combustion System

Test Engine (RTX-4)

Reference experiment for large diesel engine combustion system optimization



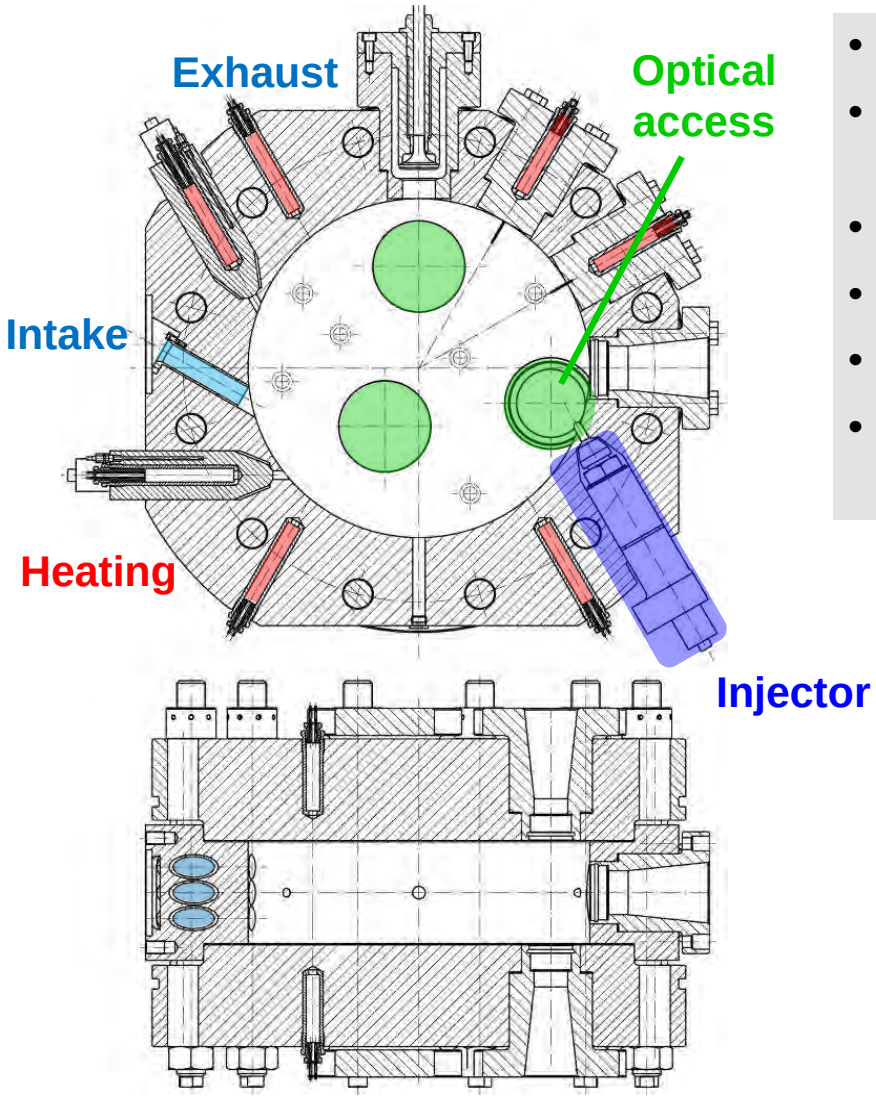
Spray / Combustion Simulation

Spray Combustion Chamber

LAV WÄRTSILÄ

Experimental Setup

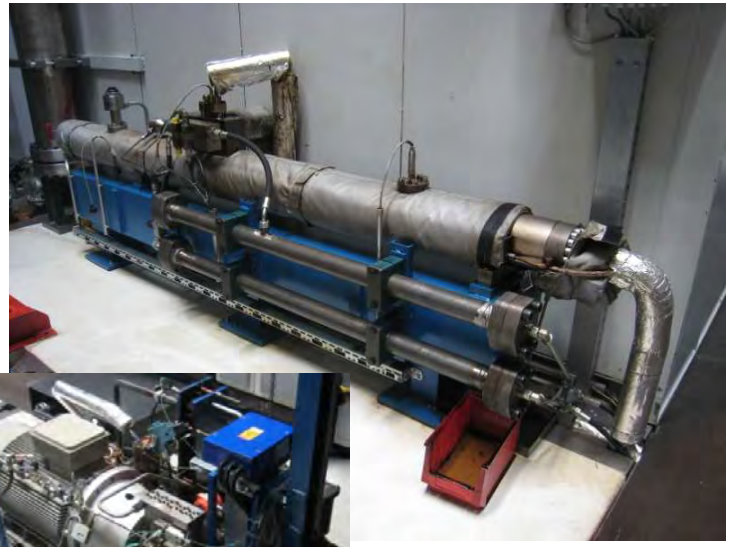
Test Facility „Spray Combustion Chamber“ (SCC)



- **Dimension:** Ø 500 x 150 mm
- **Optical Access:** Ø 100 / 65 mm sapphire windows
- **Specifications:** $p_{SCC} \approx 12$ MPa; T > 900 K
- **Swirl:** 15 - 25 m/s
- **Process gas:** Air / N_2
- **Injector:** RT-flex50 Injector 1-hole (Ø 0.875 mm)

Experimental Setup

Test Facility „Spray Combustion Chamber“ (SCC)



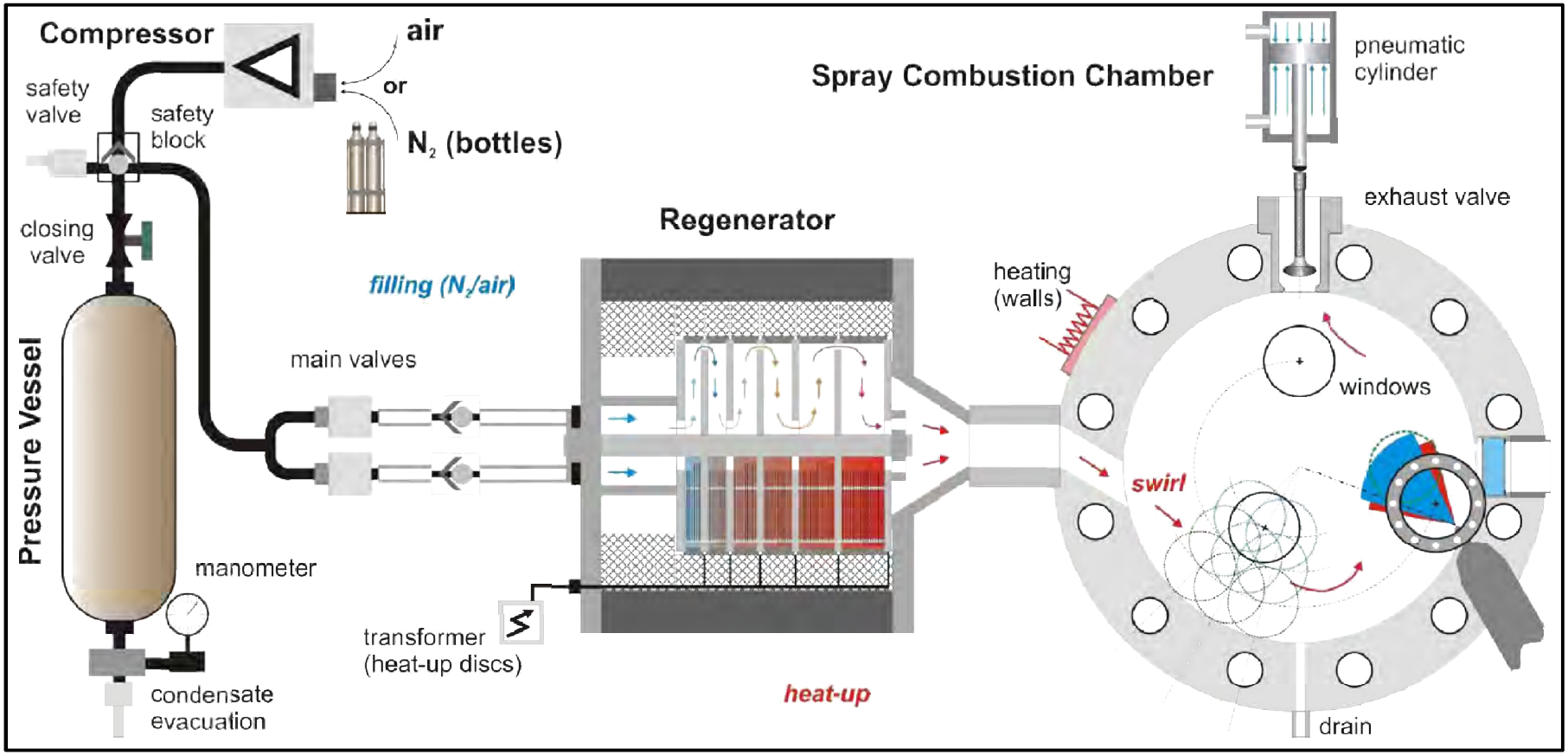
HFO Injection System

- **Dimension:** Ø 500 x 150 mm
- **Optical Access:** Ø 100 / 65 mm sapphire windows
- **Specifications:** $p_{SCC} \approx 12$ MPa; T > 900 K
- **Swirl:** 15 - 25 m/s
- **Process gas:** Air / N_2
- **Injector:** RT-flex50 Injector 1-hole (Ø 0.875 mm)
- **Injection system:** LFO / HFO 2 separate systems $p_{max} = 120$ MPa

Properties	Unit	LFO	HFO	Method
Density at 15°C	kg/m³	**851.4**	**1001.1**	ISO 12185
Viscosity at 40°C	mm²/s	**2.928**	**-**	ISO 3104
Viscosity at 50°C	mm²/s	**-**	**1255**	ISO 3104
Gross Heat of Combustion	MJ/kg	**45.02**	**42.74**	ASTM D240/D4809

Experimental Setup

Spray Combustion Chamber Concept

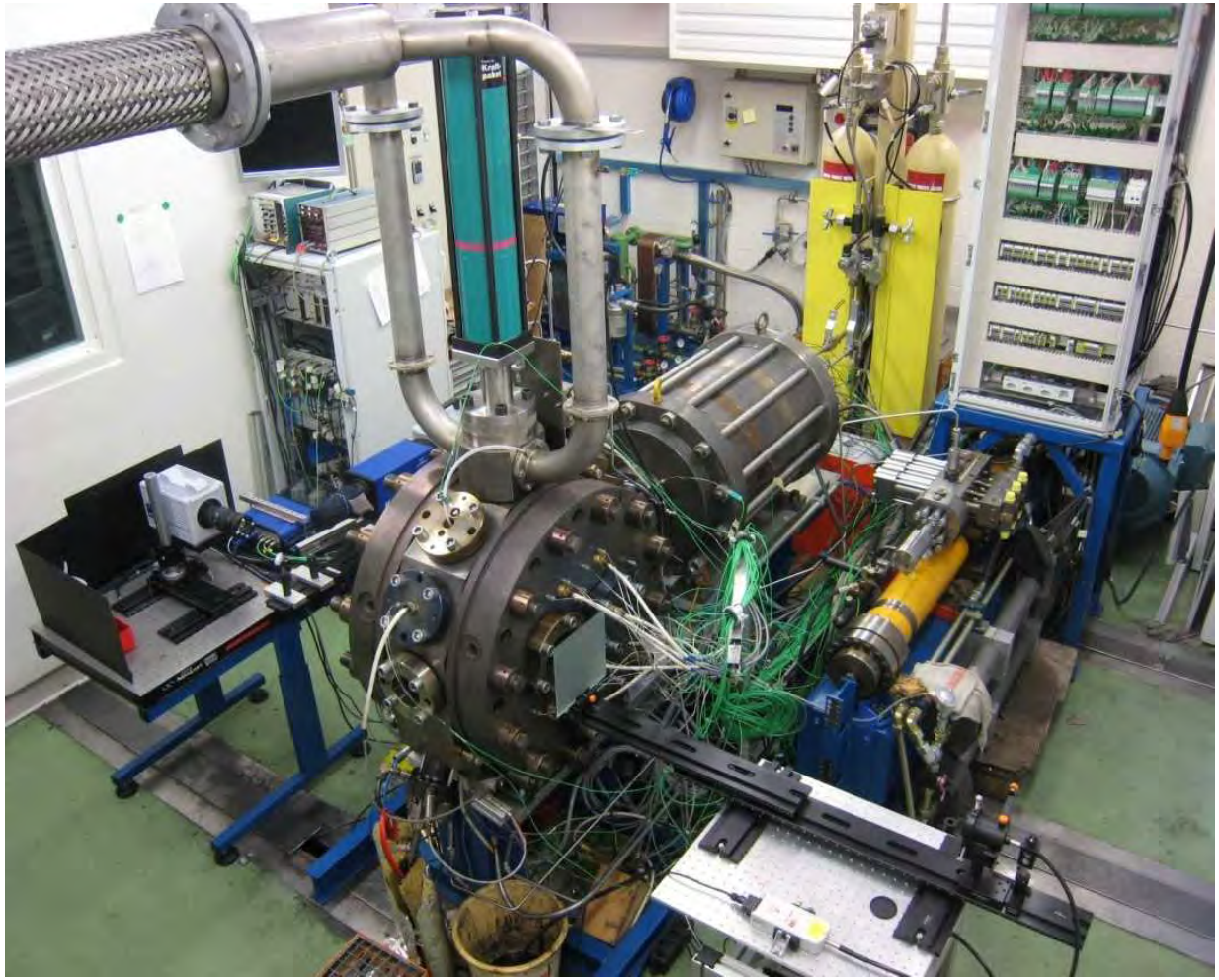


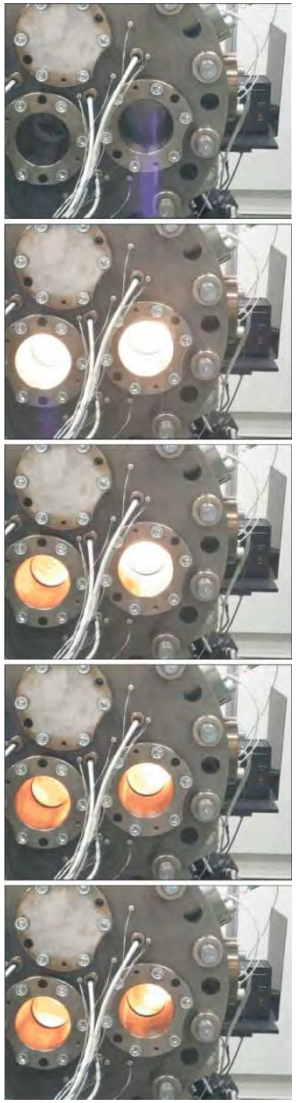
SCC conditions (p_{SCC}, T_{SCC}) ⇨ adjusted by p_{bottle}, t_{fill}, T_{REG}

typical: p_{bottle}=100...340bar, t_{fill}=0.25...0.75s, T_{REG}=900...950°C ⇨ swirl level: ↑ p_{bottle} , ↓ t_{fill}

Experimental Setup

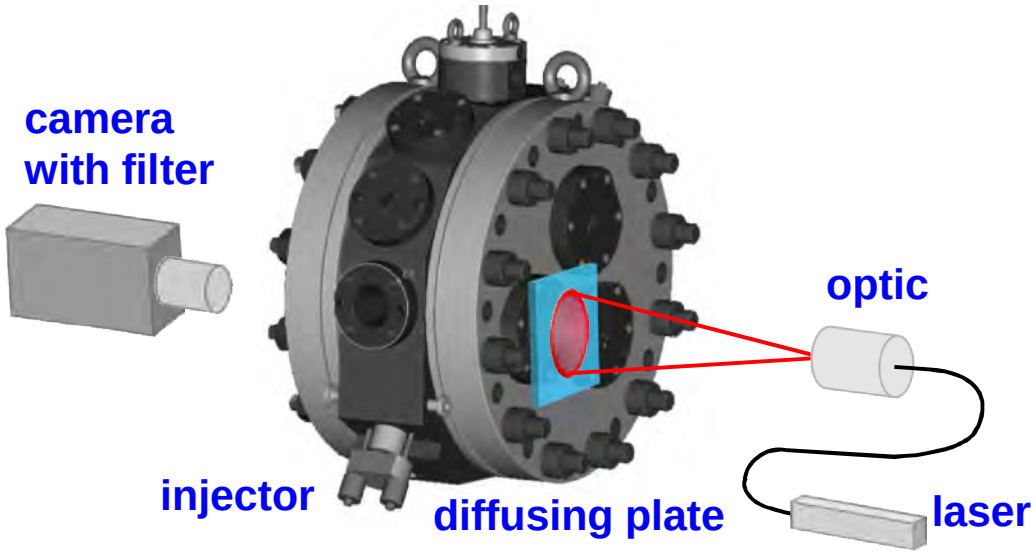
Test Facility „Spray Combustion Chamber“ (SCC)





Measurement Method & Analysis

“Improved” Shadow-Imaging Setup



- **Light Source:** pulsed laser diode 690 nm
- **Filter:** CWL 689.1 nm, T 60%
- **Recording rate:** 20 kHz (512 x 512 pixel)
- **Exposure time:** 1 µs
- **Laser pulse:** 50 ns

common light source (e.g. Arc, QTH)

9 MPa / 930 K *2-hole nozzle tip*

pulsed diode laser

Measurement Method & Analysis

Spray Analysis and Measurement

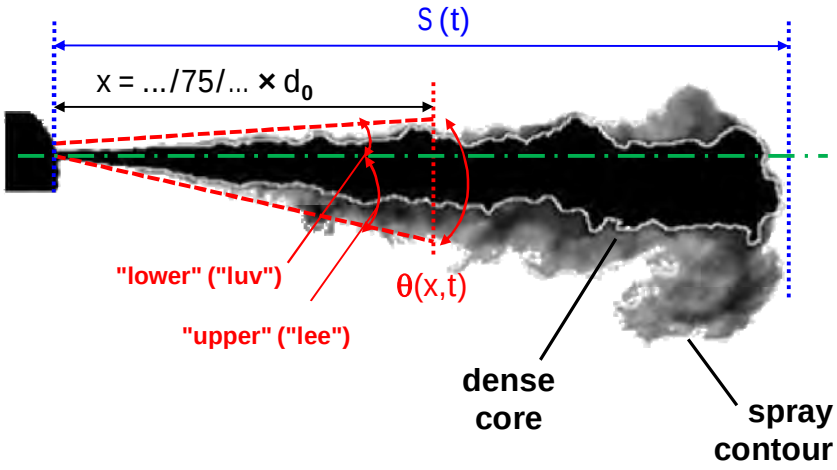
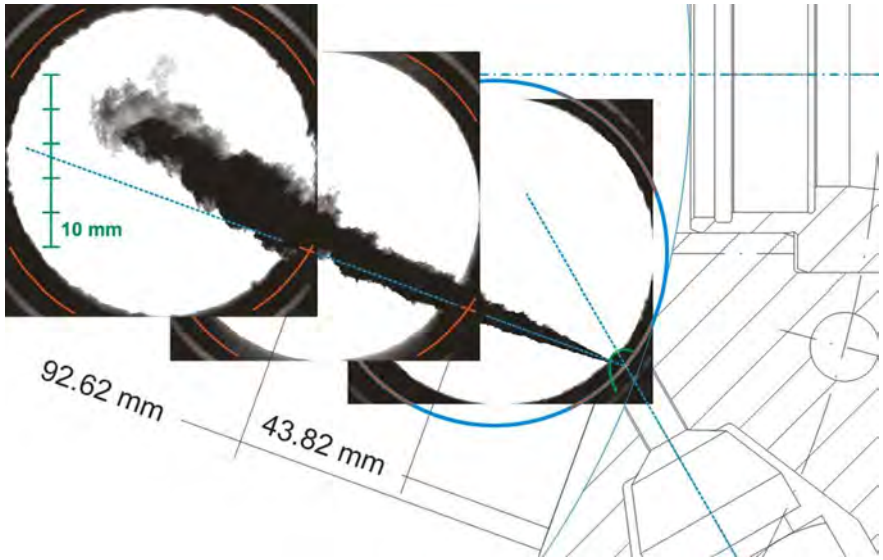


Image post-processing:

- Intensity distribution correction
- Correction absolute image intensity
- Threshold setting:
  - Dense core = 300 counts (10%)
  - Spray contour = 2700 counts (90 %)

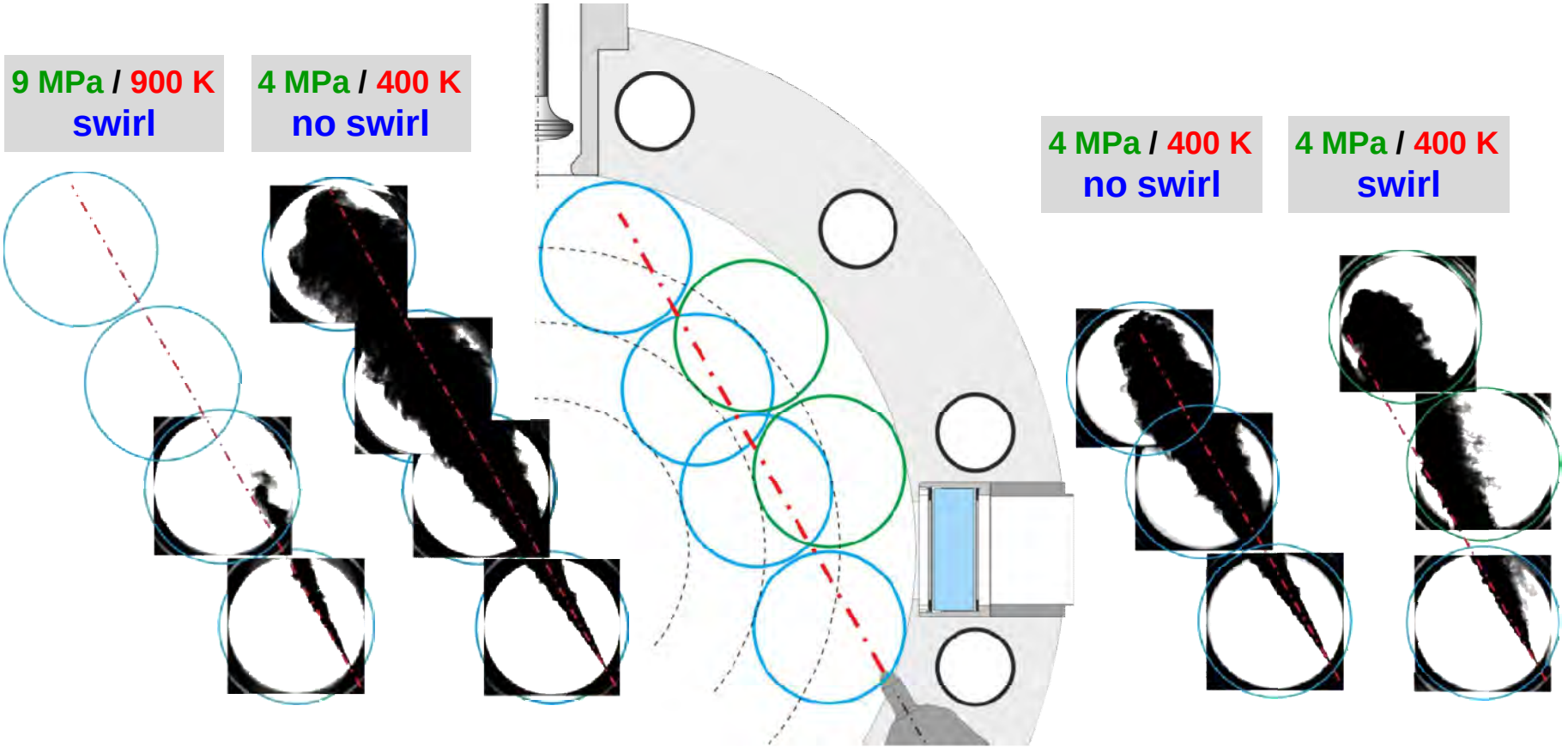


Origin & Scaling:

- Focus middle plane
- Adjust scale image Ø100 mm
- Magnification factor [mm/px]
- Define origin nozzle exit

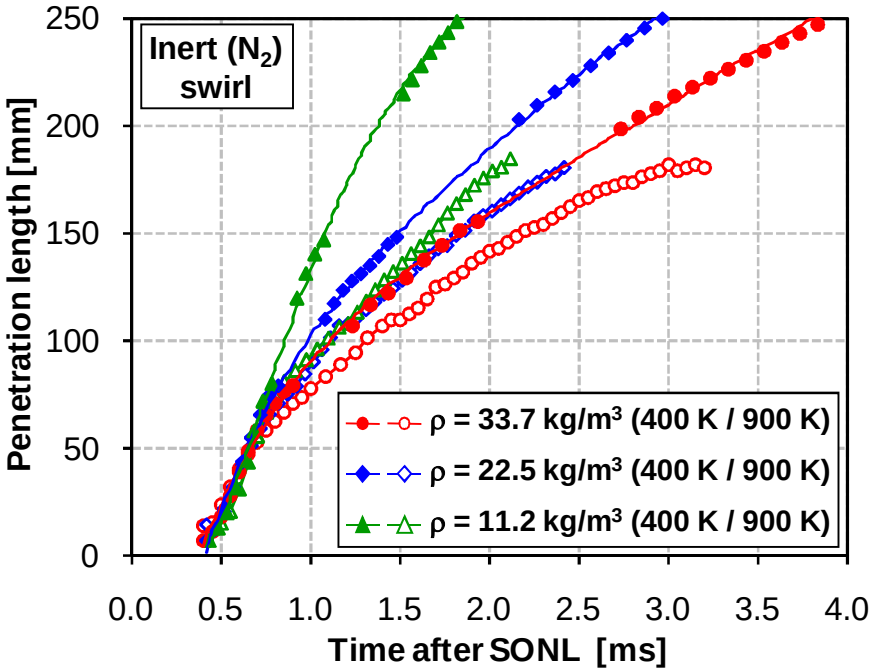
Measurement Method & Analysis

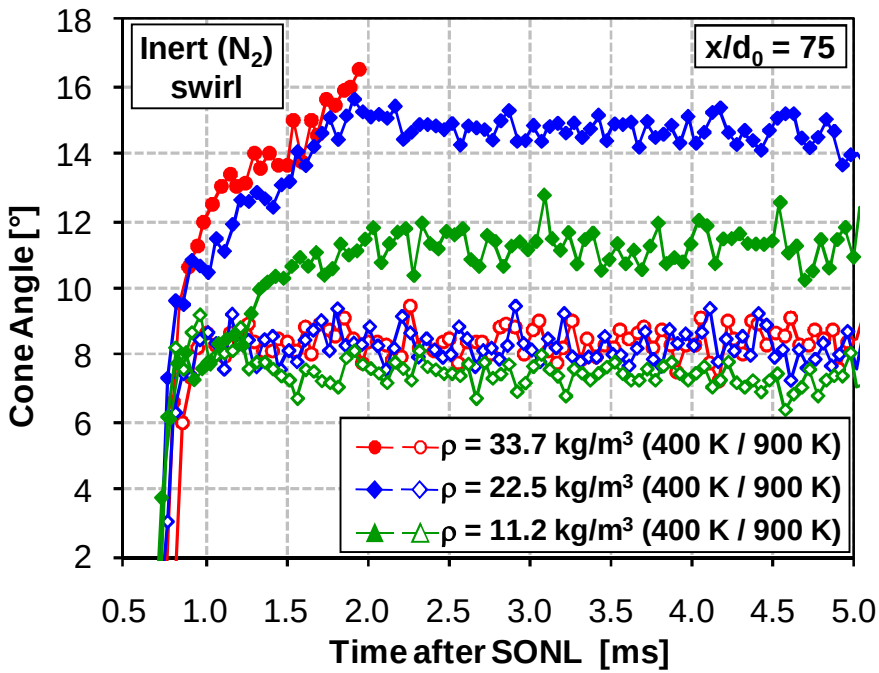
Spray Evolution (Assembling)



Results and Discussion

Impact of Evaporation





Penetration length (spray contour):

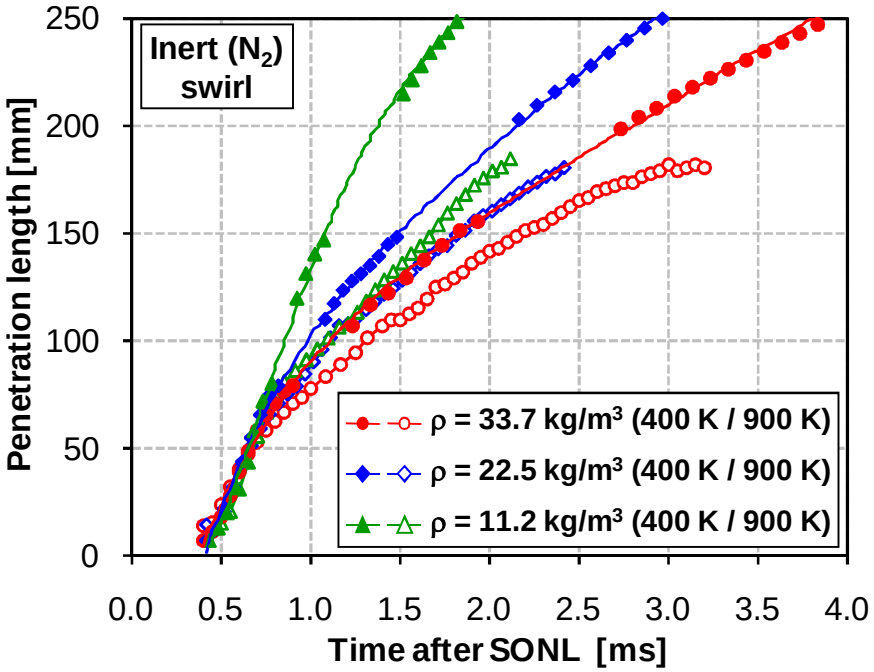
- linearly (first stage)
- Increased at non-evaporating conditions
- More distinct towards lower gas densities

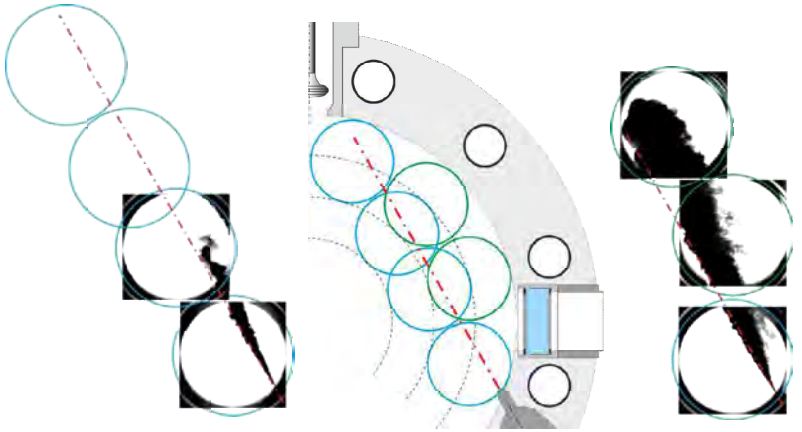
Cone angle (dense core):

- Wider at non-evaporating conditions
- Additional swirl influence!
- Not completely measurable (out of range)

Results and Discussion

Impact of Evaporation





9 MPa / 900 K swirl

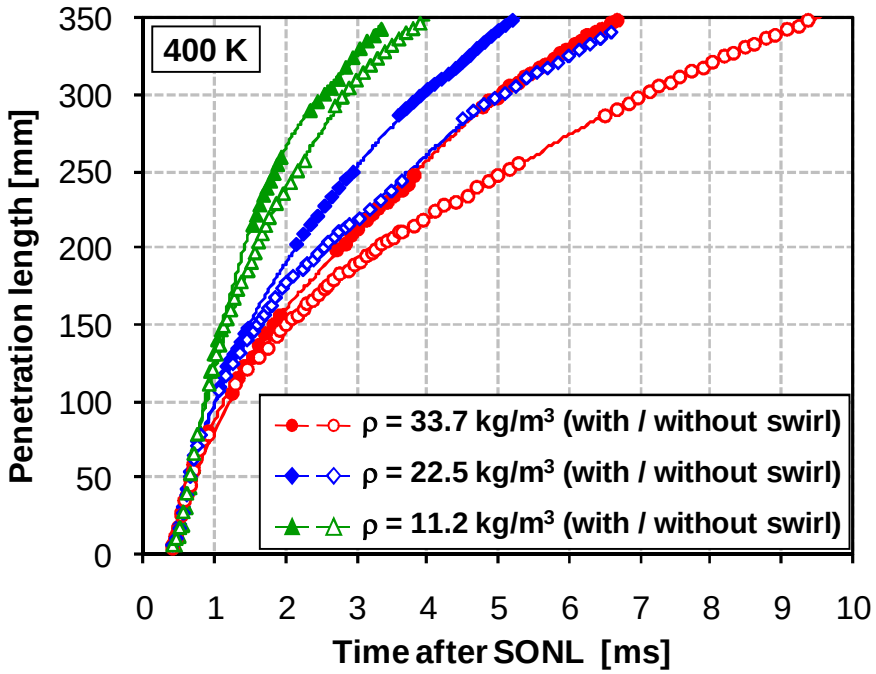
4 MPa / 400 K swirl

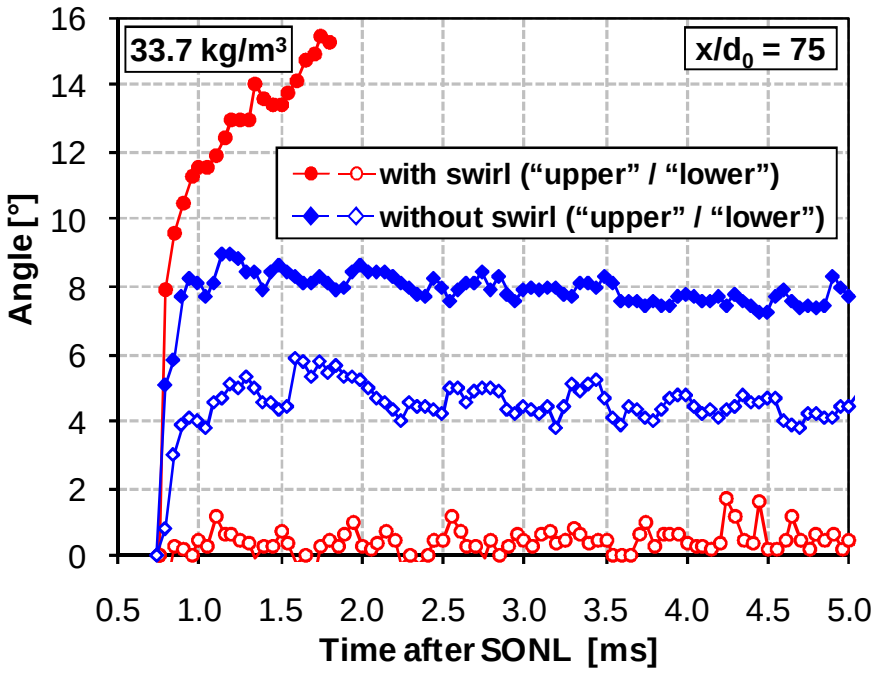
Penetration length (spray contour):

- linearly (first stage)
- Increased at non-evaporating conditions
- More distinct towards lower gas densities

Results and Discussion

Swirl Influence





Penetration length (spray contour):

- No affection in the first stage
- Reduction in absence of swirl
- More pronounced at higher gas densities

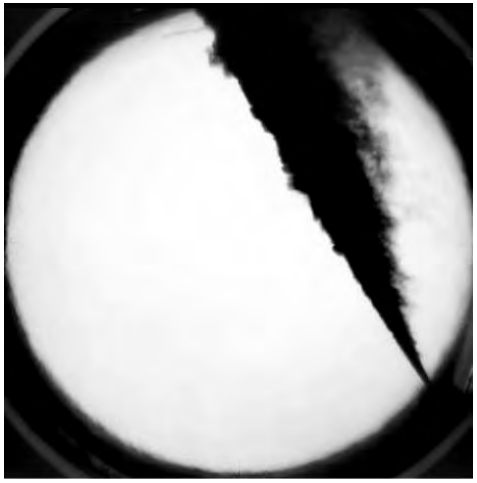
"upper" / "lower" angle (dense core):

- Strong effect of swirl on both angles
- Clear deflection to the „upper" side
- Almost uniform distributed without swirl
- Not completely measurable (out of range)

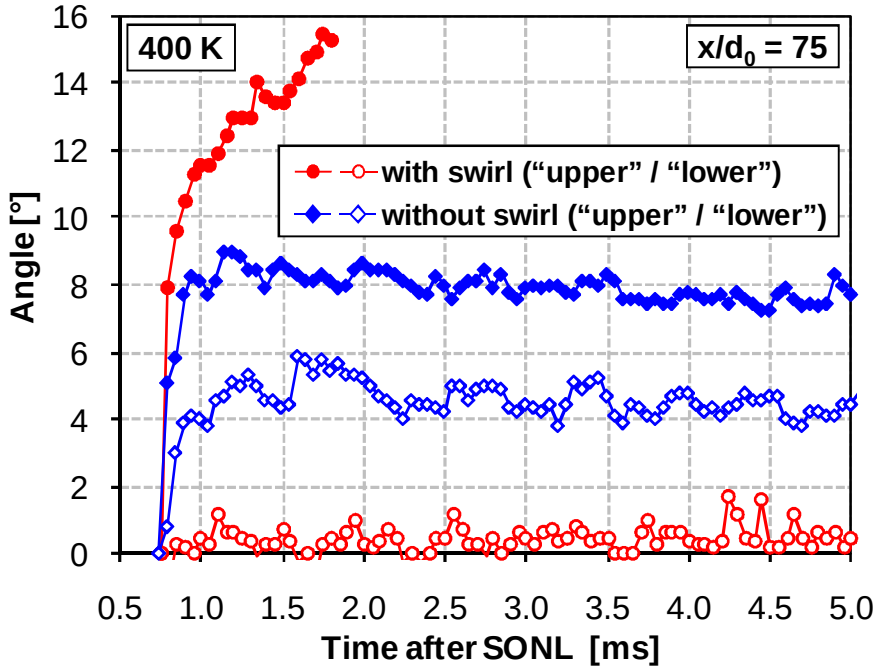
Results and Discussion

Swirl Influence

4 MPa / 400 K
swirl



4 MPa / 400 K
no swirl

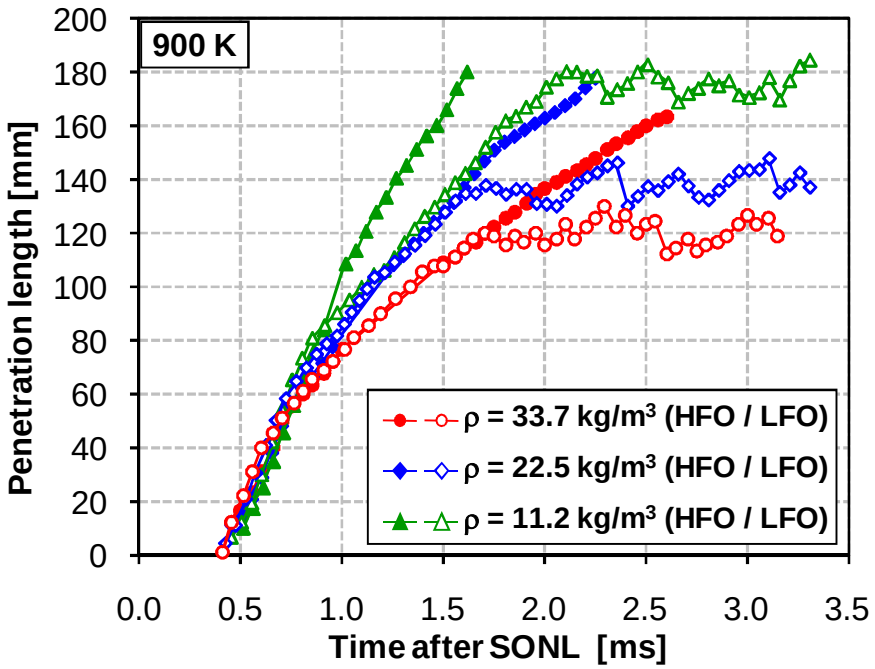


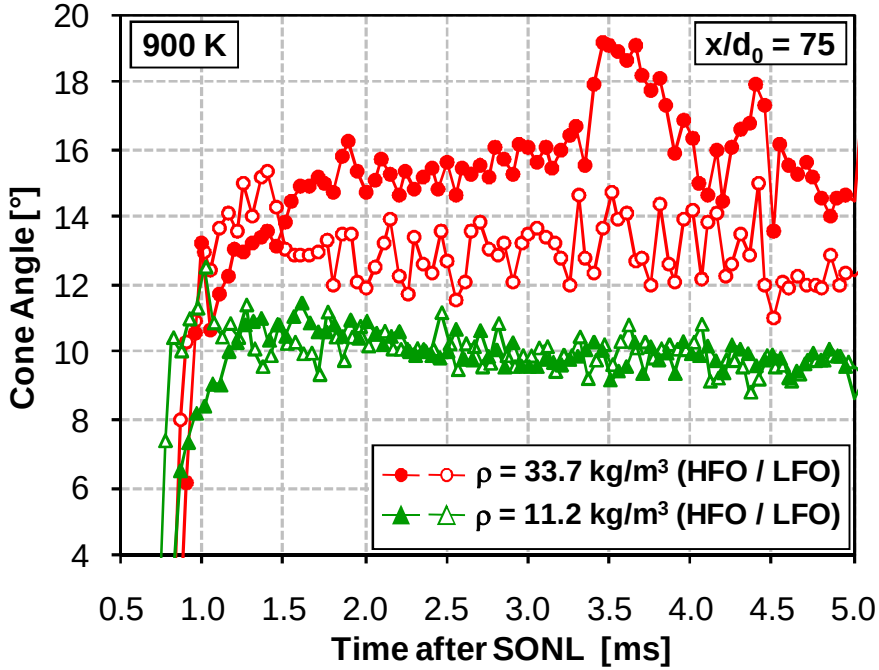
“upper” / “lower” angle (dense core):

- **Strong effect on both angles**
- **Clear deflection to the „upper“ side**
- **Almost uniform distributed without swirl**
- **Not completely measurable (out of range)**

Results and Discussion

Fuel Quality Effect





Penetration length (dense core):

- In line at first stage
- Stabilization of LFO spray dependent on gas density
- Further propagation of HFO spray

Cone angle (dense core):

- Similar at lower gas density
- At higher gas density more pronounced influence
- Cone angle of HFO spray wider

Conclusion

Summary

- Investigation at evaporating and non-evaporating conditions
- Swirl influence study at non-evaporating conditions
- First measurement campaigns with HFO
- Initial study on the effect of fuel quality *(HFO vs LFO)*
- Analysis of spray evolution: penetration and angles *(cone, "upper" / "lower")*

Outlook

- Development spray model *(penetration, angles ⇨ comparison literature)*
- Advanced optical measurement techniques *(e.g. PDA, chemiluminescence)*

Financial Support

- Swiss Federal Office of Energy SFOE
- EC's 6th & 7th Framework Programme
- Wärtsilä Switzerland Ltd
- LAV - ETH Zürich

Acknowledgments

- T. Hartmann (WCH)
- M. Cattin (LAV - ETH Zurich)

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

LAV

WÄRTSILÄ

Thank you for your interest!

Beat von Rotz
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Swiss Federal Institute of Technology Zurich

LAV

Miller Cycle for Low NOx Emissions and High Efficiency in Medium-Speed Diesel Engines: Potential and Limitations

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

PAUL SCHERRER INSTITUT
PSI

Panagiotis Kyrtatos,
Laboraboratorium für Aerothermochemie und Verbrennungssysteme,
ETH Zürich

Presentation Overview

- Introduction
  - Objective
  - In-Cylinder NO_x Formation and Reduction
  - Miller Valve timing
- The Large Engine Research Facility (LERF) at PSI
- Engine Measurements – Combustion analysis at high Miller degrees
  - Observations
    - NO_x trends with increasing Miller degree
    - NO_x trends with increasing ignition delay
    - Pressure Fluctuations - Cycle-to-Cycle Variations
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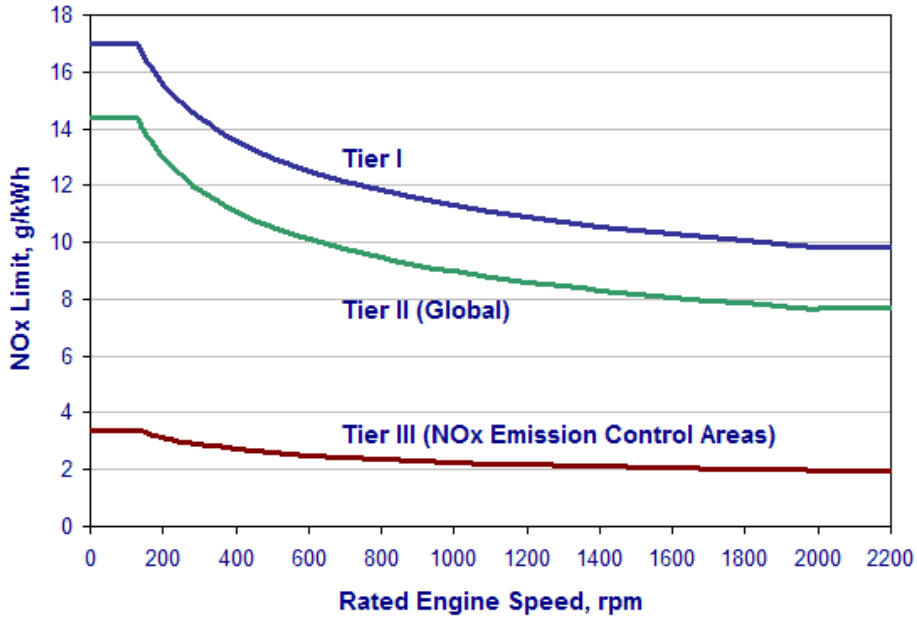
Objective

- Aim is to reduce NO_x emissions from diesel engines, to achieve compliance with current and future emission legislations
  - Marine sector: IMO Tier III:
    - ~80% reduction from Tier I in ECAs
- Current options for NO_x reduction:
  - In-cylinder NO_x reduction
  - Exhaust gas aftertreatment
- Main question:
  - **How much NO_x reduction will individual technologies allow/achieve?**



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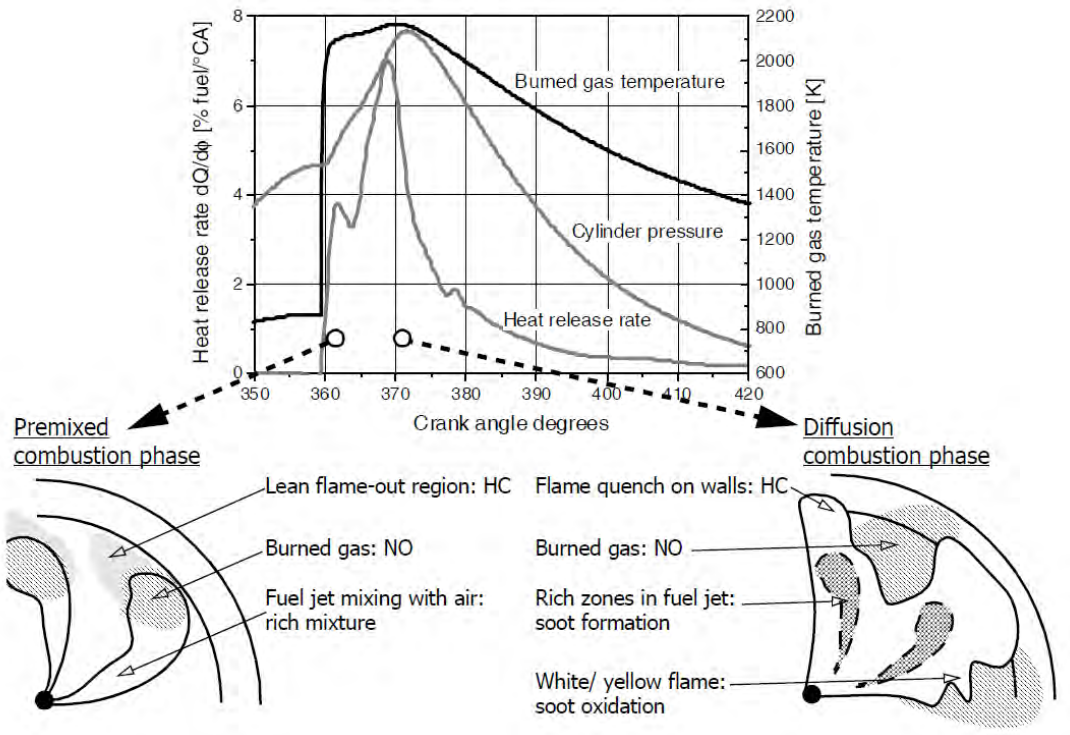
In-Cylinder NO_x Formation

- NO_x formation mechanisms:
  - Thermal NO (Zeldovich mechanism)
    - Formed in high temperature burned gas regions
    - Exponential temperature dependency
    - Significant amounts above 2000K
    - Accounts for ~90% of NO in typical diesel engines
  - Prompt NO
    - Formed in the reaction zone
    - Lower temperature dependency
    - More significant than thermal at low temp
  - Fuel NO
    - Not significant for low-NO fuels



In-Cylinder NO_x Reduction

- Ever increasing requirement for NO_x reduction while maintaining efficiency

- In-cylinder NO_x reduction technologies:
  - Reduction of adiabatic flame temperature to reduce Thermal NO
    - Change in composition (increase in heat capacity, oxygen reduction):
      - EGR
      - Nitrogen enrichment
      - Air humidification
    - Flame cooling:
      - Direct water injection
      - Water-fuel emulsions
    - Reduction of charge temperature:
      - Miller timing
      - Charge air cooling
      - Reduced compression ratio

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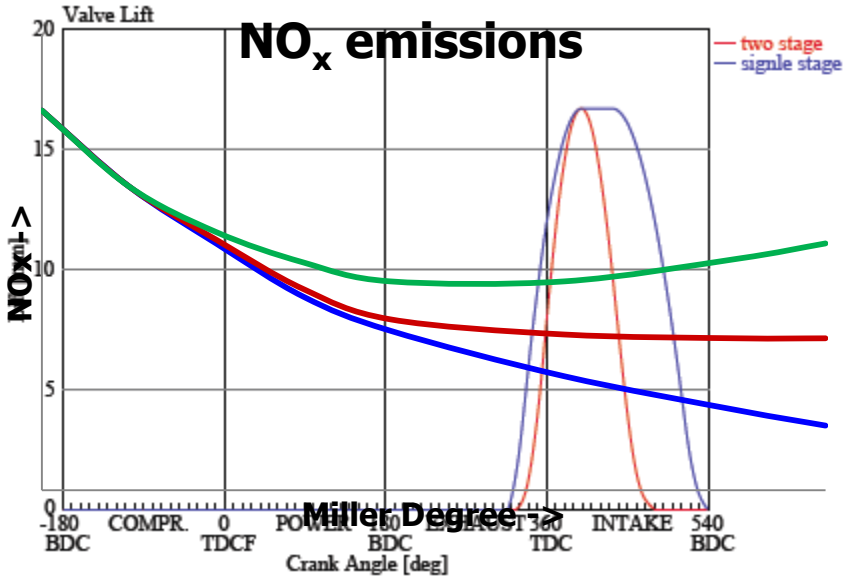
Miller Valve Timing

- Miller concept: Advanced IVC in order to reduce cycle temperatures through expansion

- Benefits:
  - Reduction in NO_x production through lower adiabatic flame temperature
  - Increase in cycle efficiency due to lower heat losses
  - Lower exhaust/component temperatures

- Drawbacks:
  - Need for higher inlet pressures to achieve the same power output
  - Deteriorated part-load operation
  - Higher ignition delay, causing higher pressure rise rates



- **Question: How much NO_x reduction can be achieved through Miller (and why)?**

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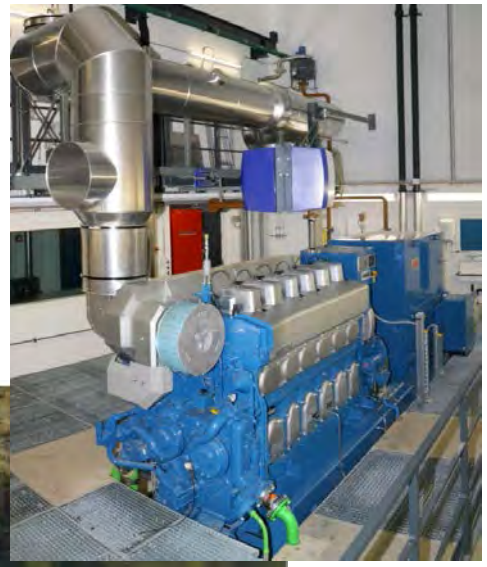
LERF – Test Facility

- Realized within the Competence Centre for Energy and Mobility (CCEM) at the Paul Scherrer Institut (PSI) in Villingen, CH
- Purpose-built building, with engine/brake base frame resting on spring-damper elements on a large concrete foundation
- Engine cooling through heat exchanger, with water from the Aare river
- Variable speed electric brake system (ABB AMA 450L6L) allows variable speed operation
- Urea SCR system integrated to comply with Swiss regulations for the conservation of air quality



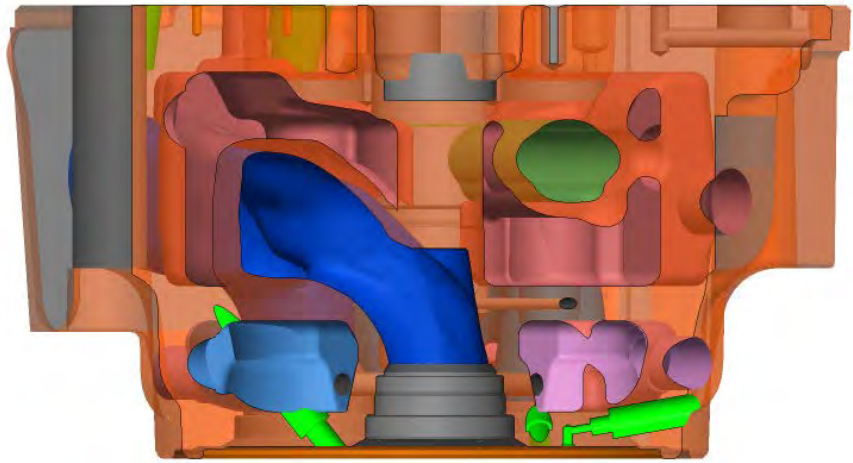
Wärtsilä 6L20 and Measurement Equipment

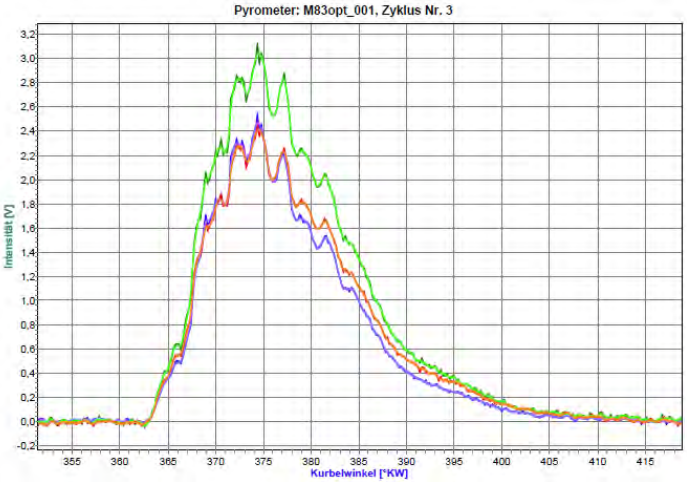
- Medium-speed 4-stroke Wärtsilä 6L20 Diesel engine equipped with Common-Rail fuel injection system
- Prototype 2-stage turbocharging system developed by ABB Turbo Systems
- FTIR for broad spectrum exhaust gas analysis.

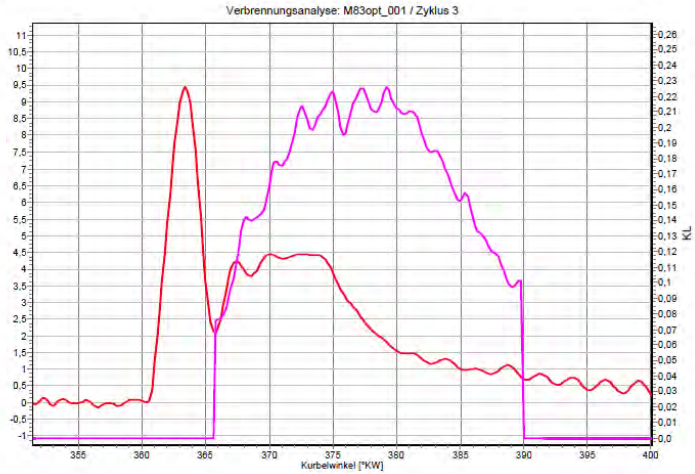
Bore	mm	200
Stroke	mm	280
Number of Cylinders		6
Compression Ratio		16
Nominal Speed	rpm	1000
Rated Power	kW	1080

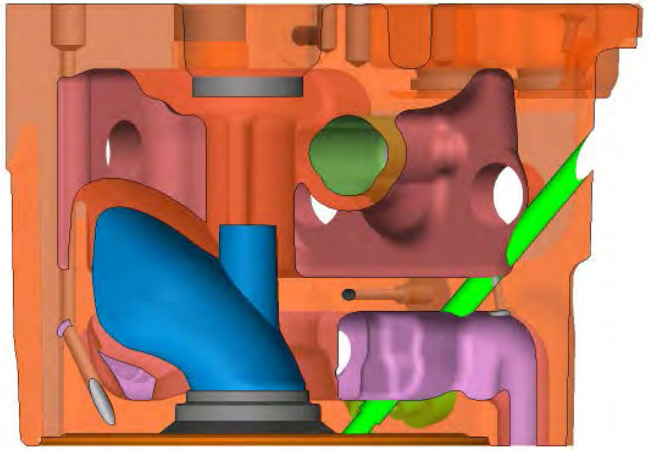
In-Cylinder Measurements

- Cylinder head with multiple sensor accesses
- Cylinder access suitable for pyrometry soot measurements using Kistler optical sensor
- Possibility of using pressure and optical sensors simultaneously









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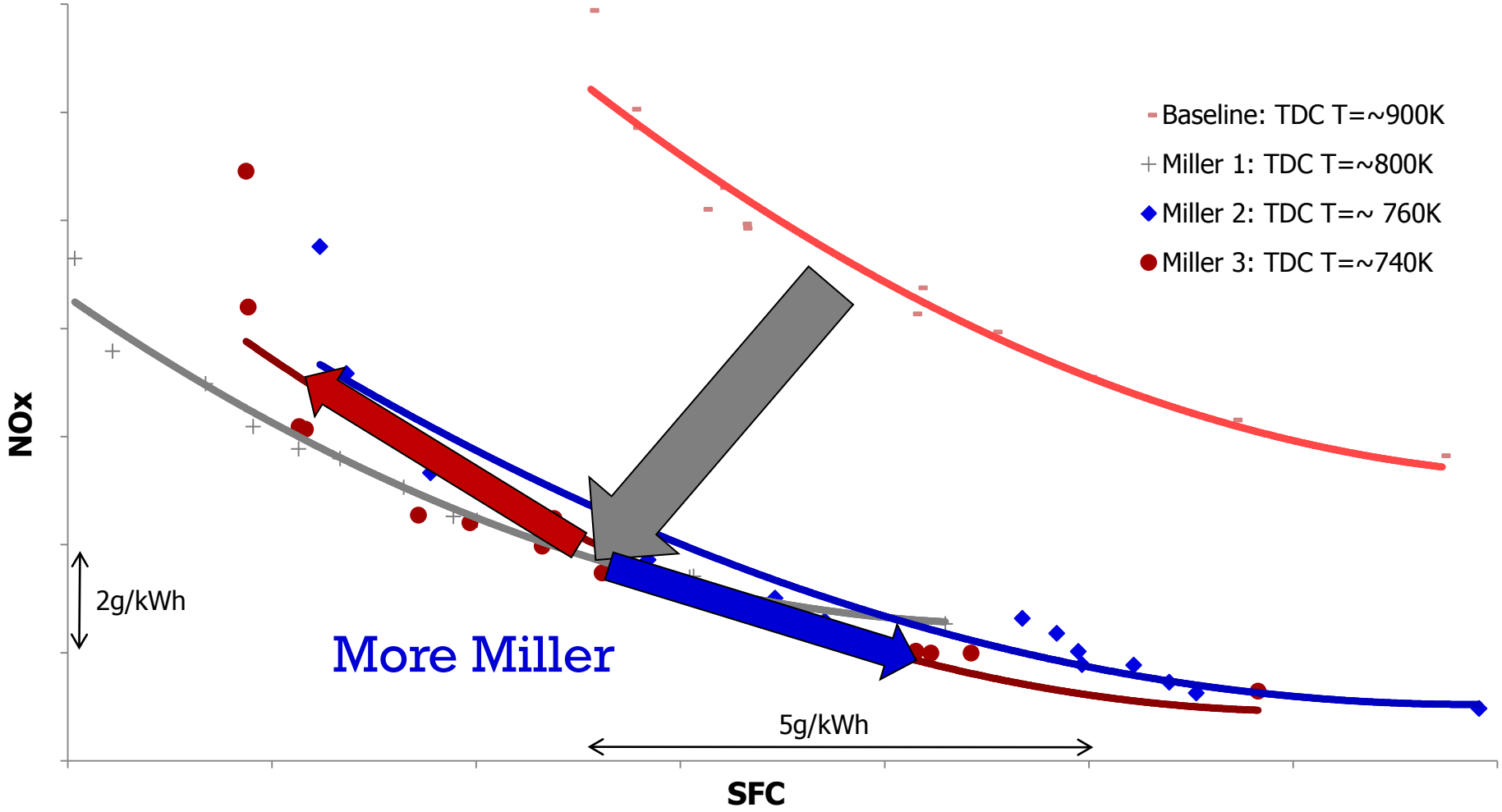
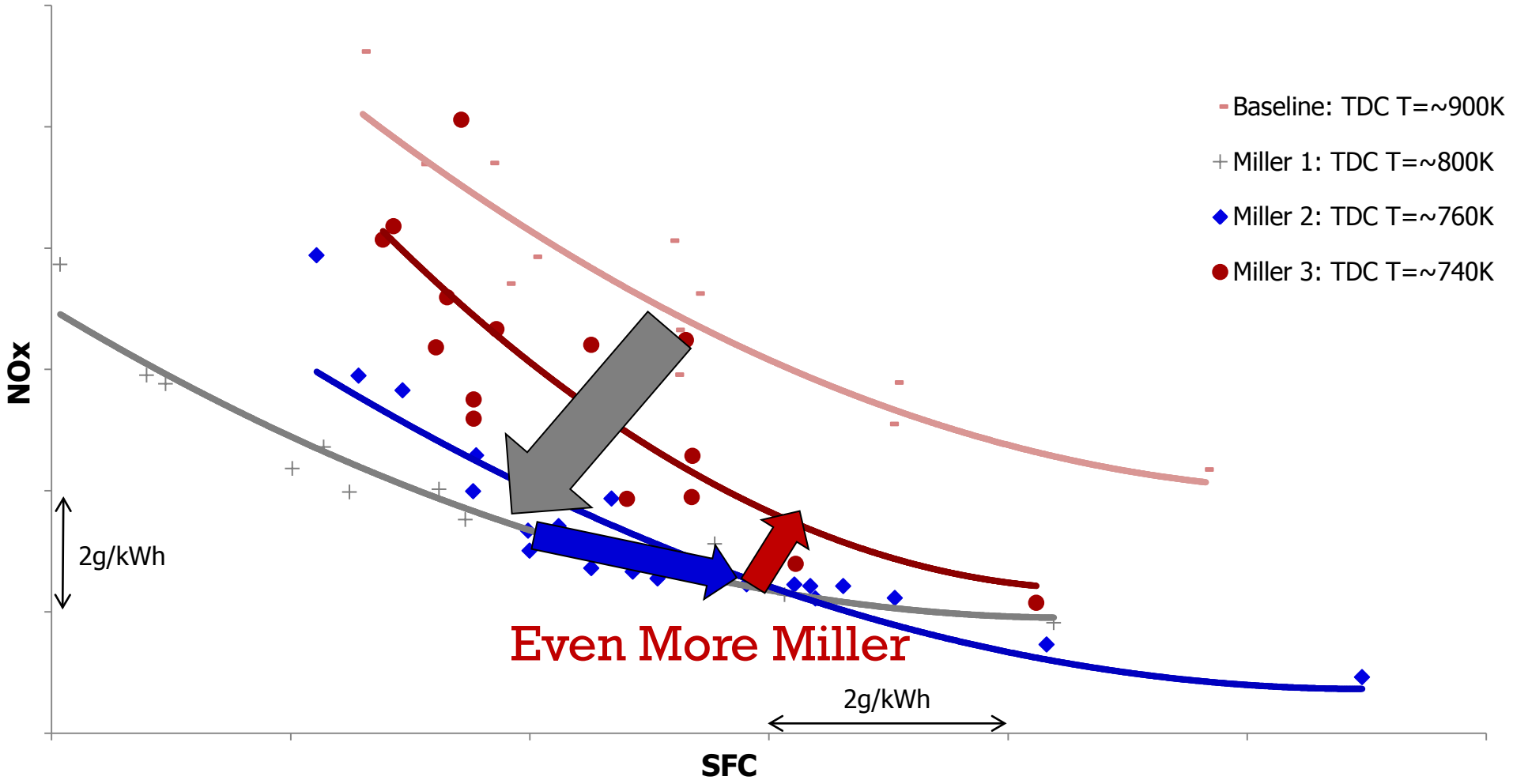
NO_x-BSFC Tradeoff – High load



NO_x-BSFC Tradeoff – Medium load



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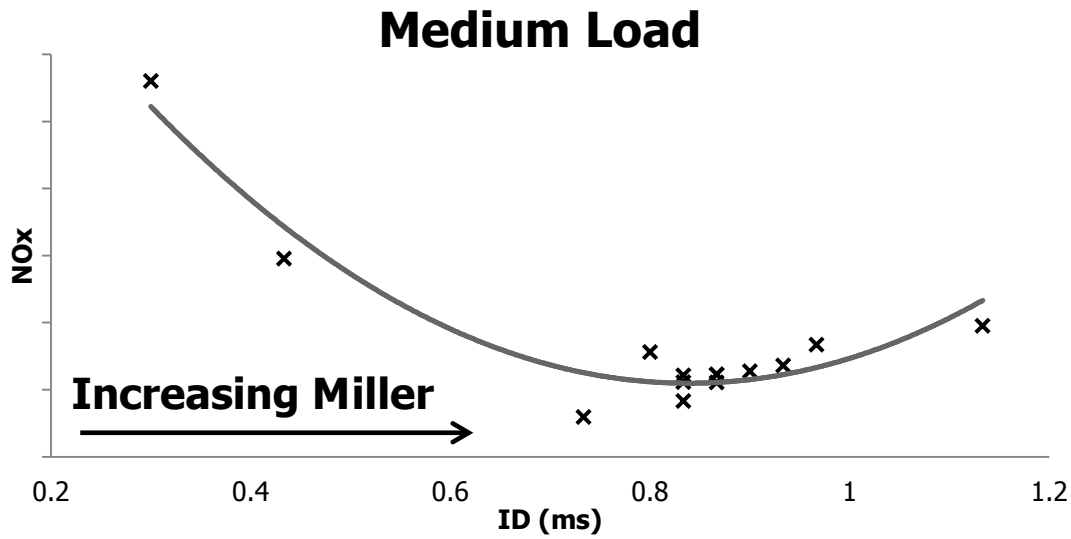
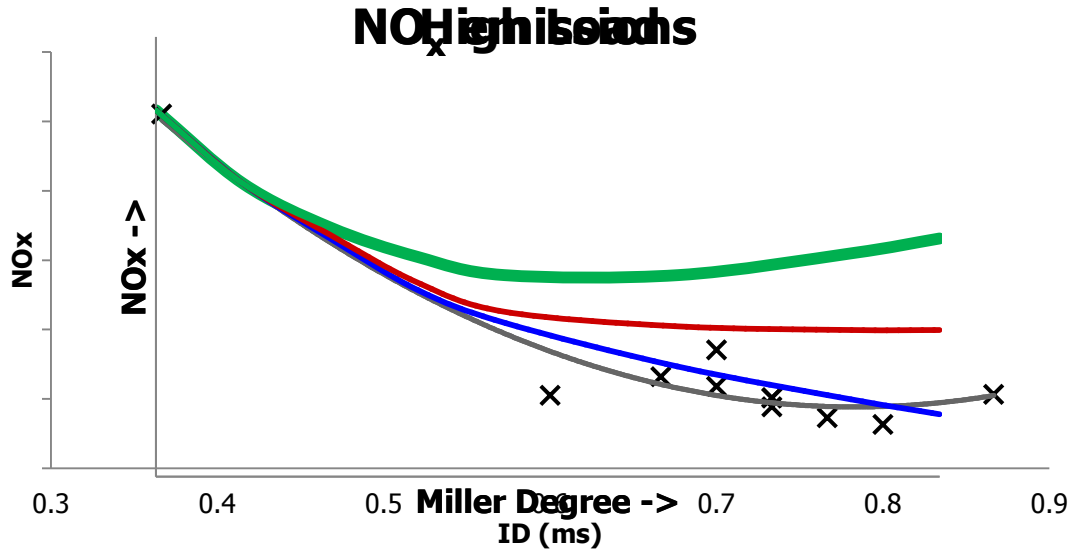
NO_x vs Ignition Delay

- Irrespective of load, higher Miller degree (lower temperature – increasing ID) reduces NO_x produced for constant injection conditions, up to a point
- At very long ID (low pressure and temperature), NO_x increases for increasing ID
- Increase in NO_x emissions at high Miller degrees, especially at low loads (low charge pressure – high ID)





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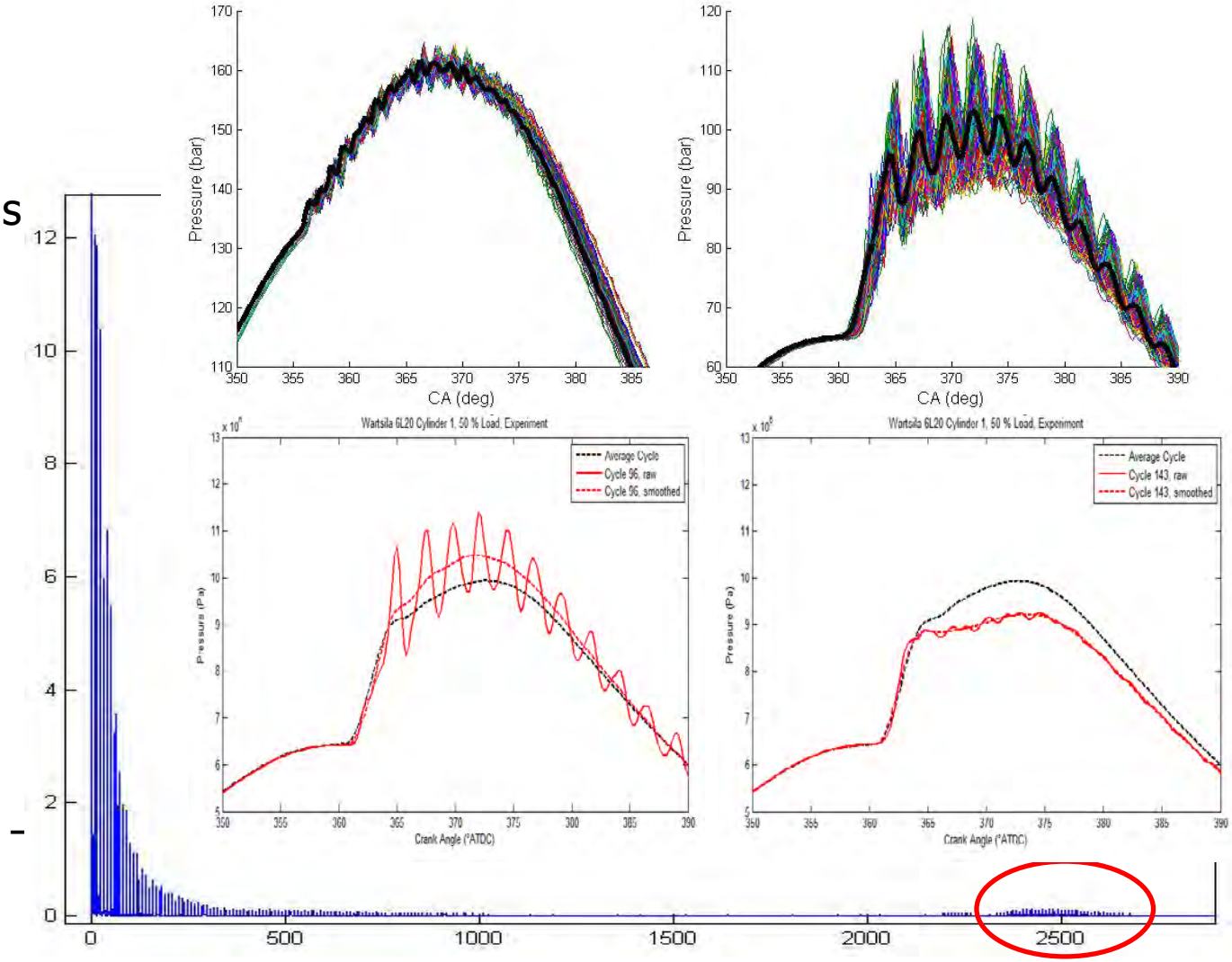
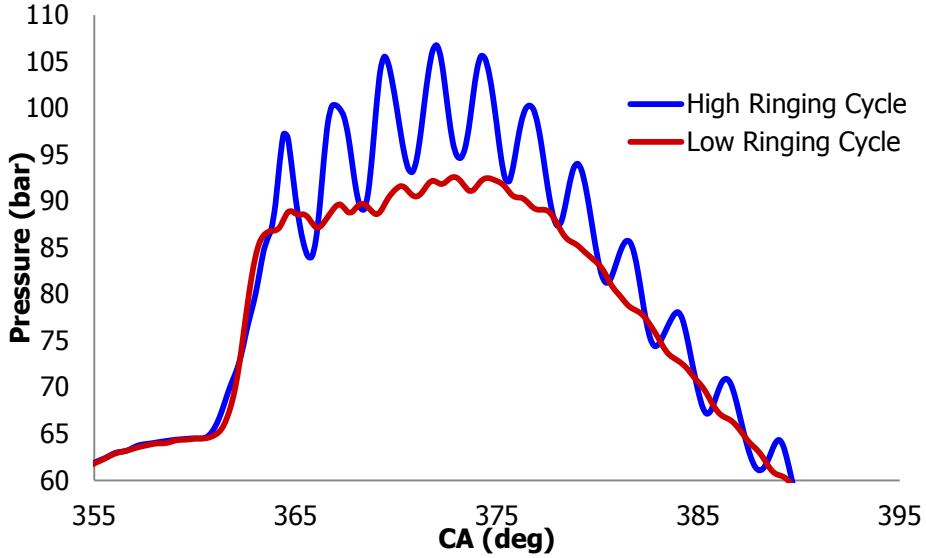
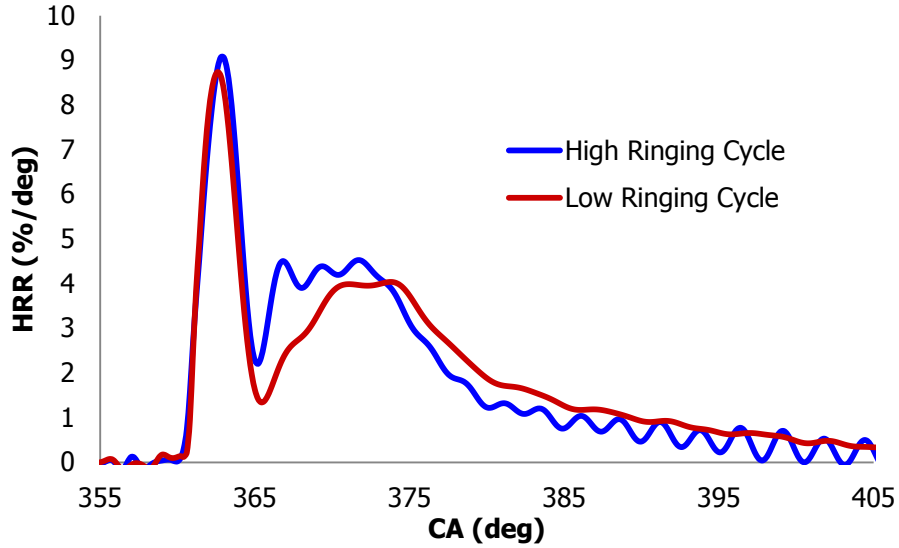
Pressure Fluctuations – Cycle-to-Cycle Variations

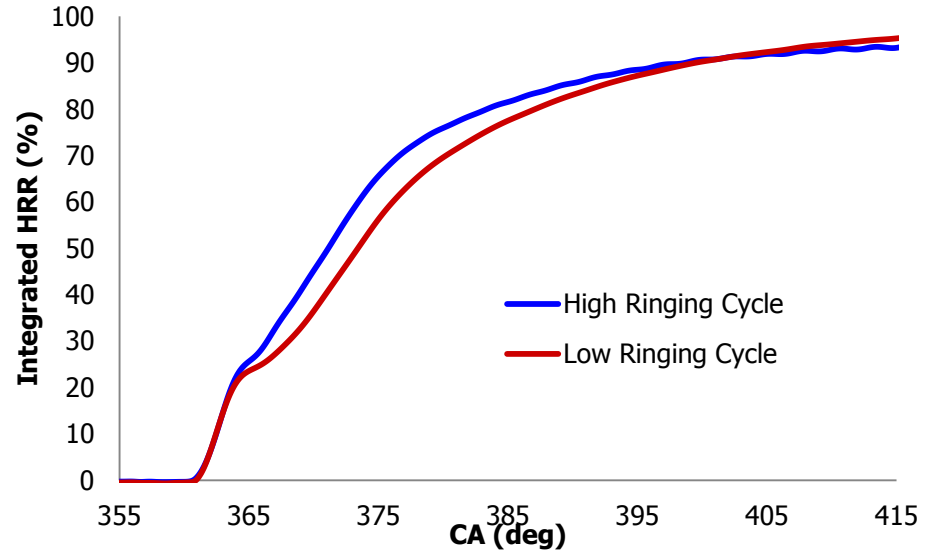
- At cycles with long ID/High Miller:
  - high pressure fluctuations
  - high cycle-to-cycle variations
- FFT shows frequency of fluctuation ~2.5kHz, corresponding to the first mode of oscillation of the cylinder
- Highly fluctuating cycles reach higher peak pressures - seem to burn faster during diffusion combustion

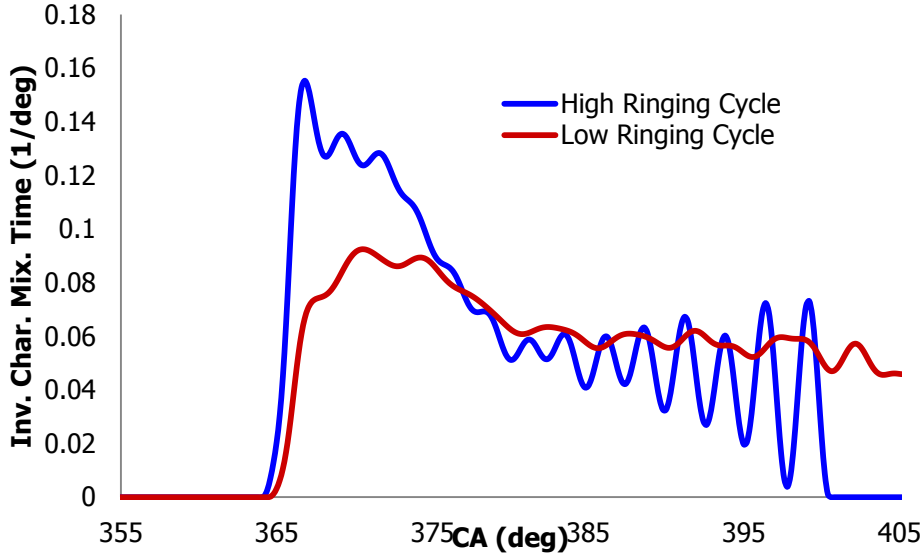


High vs Low Ringing Cycles









Presentation Overview

- Introduction
  - Objective
  - In-Cylinder NO_x Formation and Reduction
  - Miller Valve timing
- The Large Engine Research Facility (LERF) at PSI
- Engine Measurements – Combustion analysis at high Miller degrees
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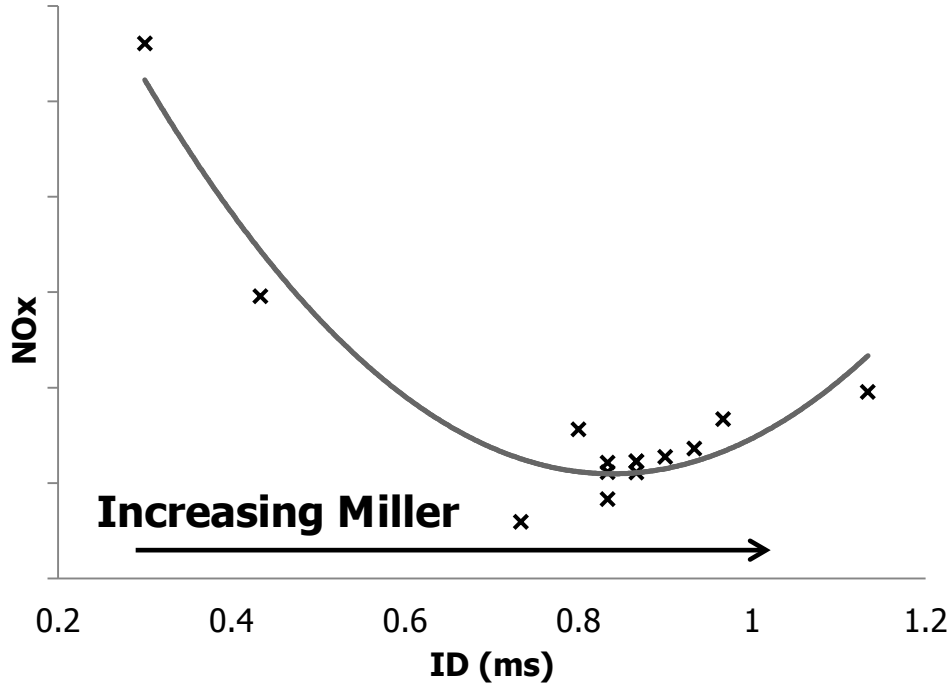
    - NO_x trends with increasing ignition delay
    - Pressure Fluctuations - Cycle-to-Cycle Variations
  - Understanding of trends – implications
- Conclusions

Possible Causes for NO_x Trend Reversal

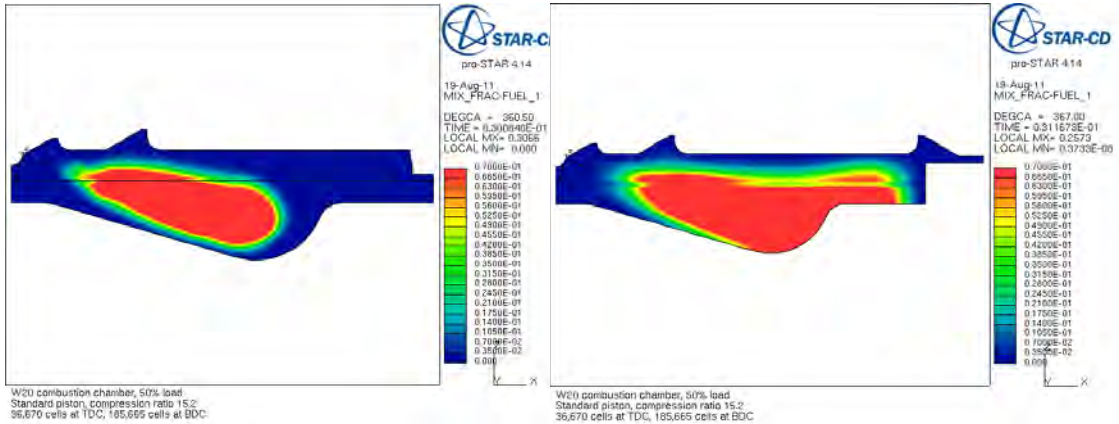
- **Longer Ignition Delay**
  - Larger proportion of premixed combustion
  - Longer spray penetration before combustion
- **Observed Mixing Effects**
  - Increased flame temperature
  - Increased oxygen availability for NOx formation
- **Mixing effects on soot and radiation heat losses**
  - Reduced soot present due to mixing reduces radiation heat losses resulting in higher flame temperature
- **Pressure Fluctuations**
- **Prompt NO**



Possible Causes for NO_x Trend Reversal (1)

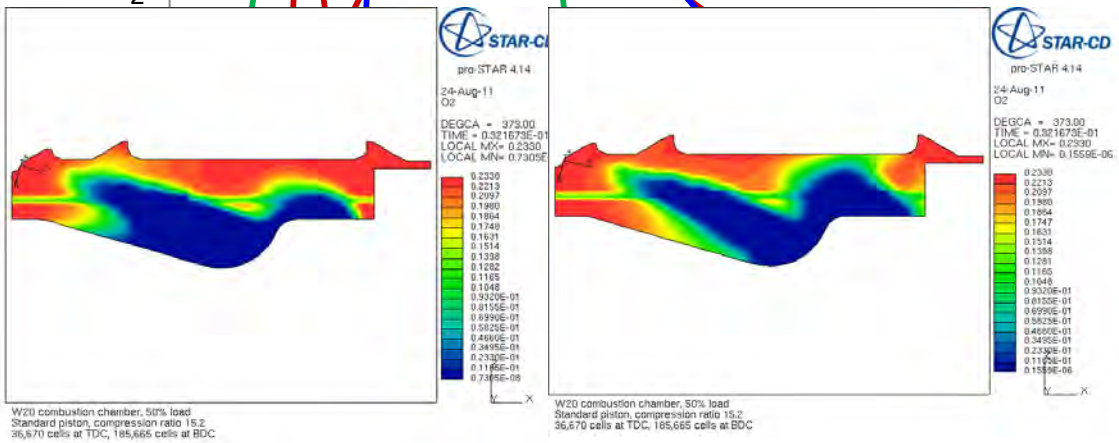
- **Longer Ignition Delay:**
  - Larger proportion of premixed combustion + leaner premixed zone -> higher NO_x during premixed combustion
  - Longer spray penetration
    - Better utilization of available O_2
      - Faster combustion -> higher temperature -> higher thermal NO_x formation
      - More thermal NO_x formed due to leaner high temperature burned gas zones

Mix. Fraction at Ignition



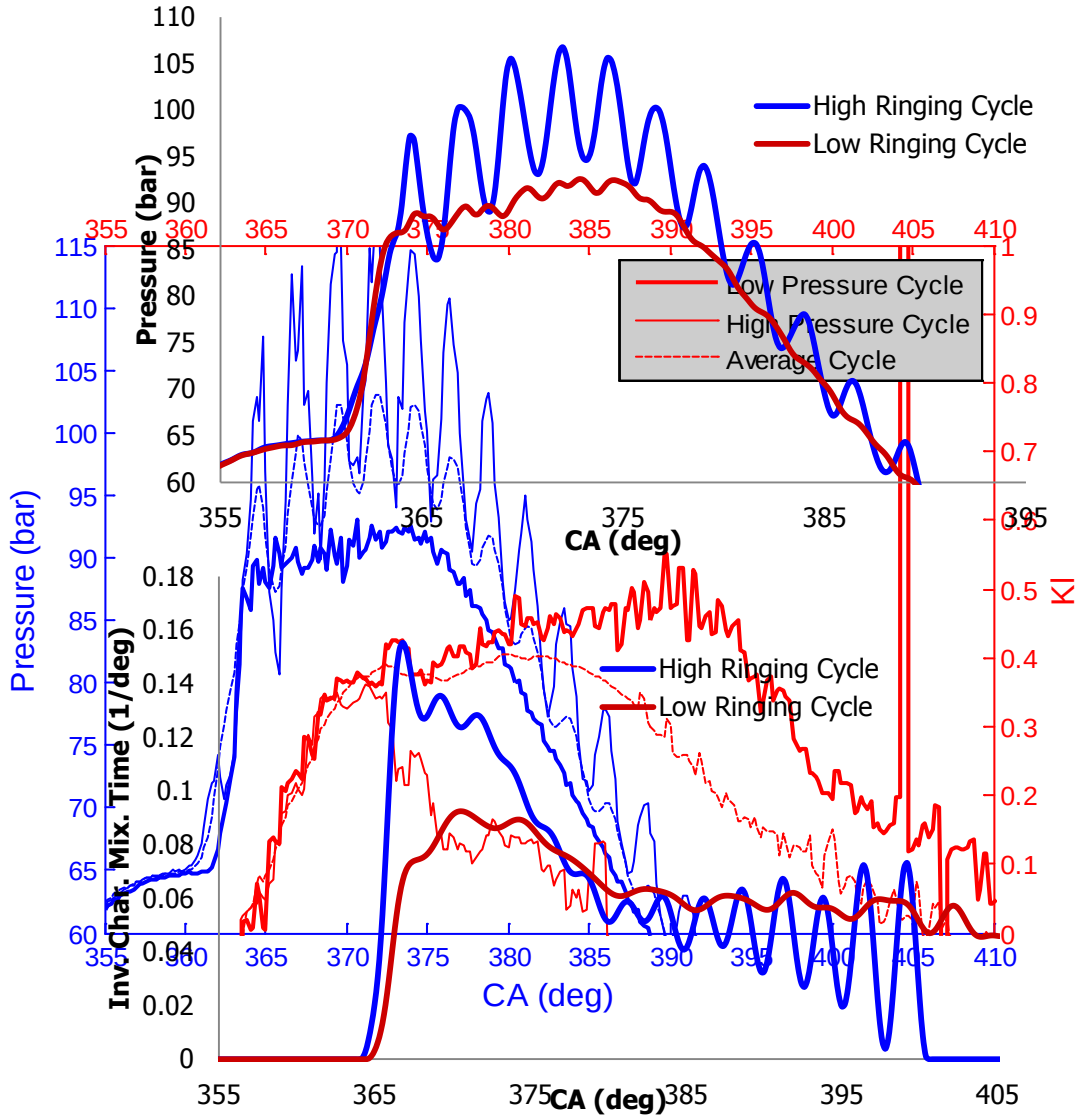
HHR/Inj 3 2

Oxygen Content at 373CA



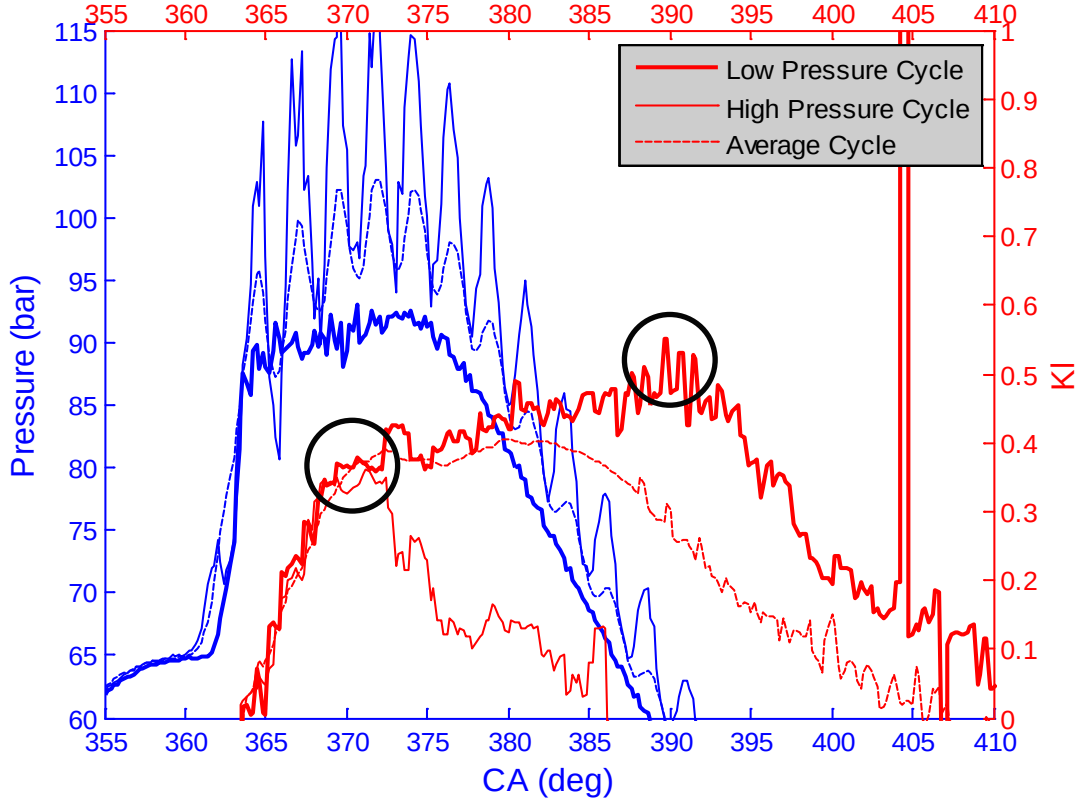
Possible Causes for NO_x Trend Reversal (2)

- **Observed Mixing Effects:**
  - Increased mixing – cycles with pressure fluctuations have been shown to have increased mixing rates
    - Faster combustion -> higher temperature -> higher thermal NO_x formation
    - Faster mixing of burned gases with O_2 at high temperature -> higher thermal NO_x formation in burned zones
  - Observation also supported by KI measurements
    - Similar formation rates for all cycles
    - Higher oxidation rates pointing to increased mixing



Possible Causes for NO_x Trend Reversal (3)

- **Mixing/Premixed Combustion influence on soot radiation**
  - Both increased mixing and increased proportion of premixed combustion have been shown to suppress soot
    - Reduced soot reduces radiation heat losses of the flame
    - Results show ~30% lower peak/ reduced level of soot (KI) at high ringing cycles
    - Literature[1] indicates up to 50K increased flame temperature, resulting in **~10% more NO_x**



[1]Musculus, 2005, SAE 2005-01-0925

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- Conclusions

Conclusions

- Miller valve timing coupled to two-stage turbocharging allows significant in-cylinder NOx reduction (up to ~60%) without BSFC penalty, by improving NOx-BSFC tradeoff
- With increasing Miller degree and increasing ID, beneficial trend in NOx-BSFC tradeoff reverses, thus limiting effect of extreme Miller degrees
- This trend reversal is an insufficiently understood subject, with significant implications on in-cylinder NOx reduction potential for marine diesels without EGR
  - Several possible contributing causes presented here should be studied further and – if possible – individually
  - Solutions to the issue could be pre-injections, slower injection ramps
- Understanding and controlling the causes of the reversal could prove critical for future applications of marine diesels, following introduction of very strict NOx emission legislation

PAUL SCHERRER INSTITUT
PSI

Wir schaffen Wissen – heute für morgen

H2IGCC
Energy without CO2

carma

Combustion Properties of Hydrogen-Rich Fuel Gases at Gas Turbine Relevant Conditions

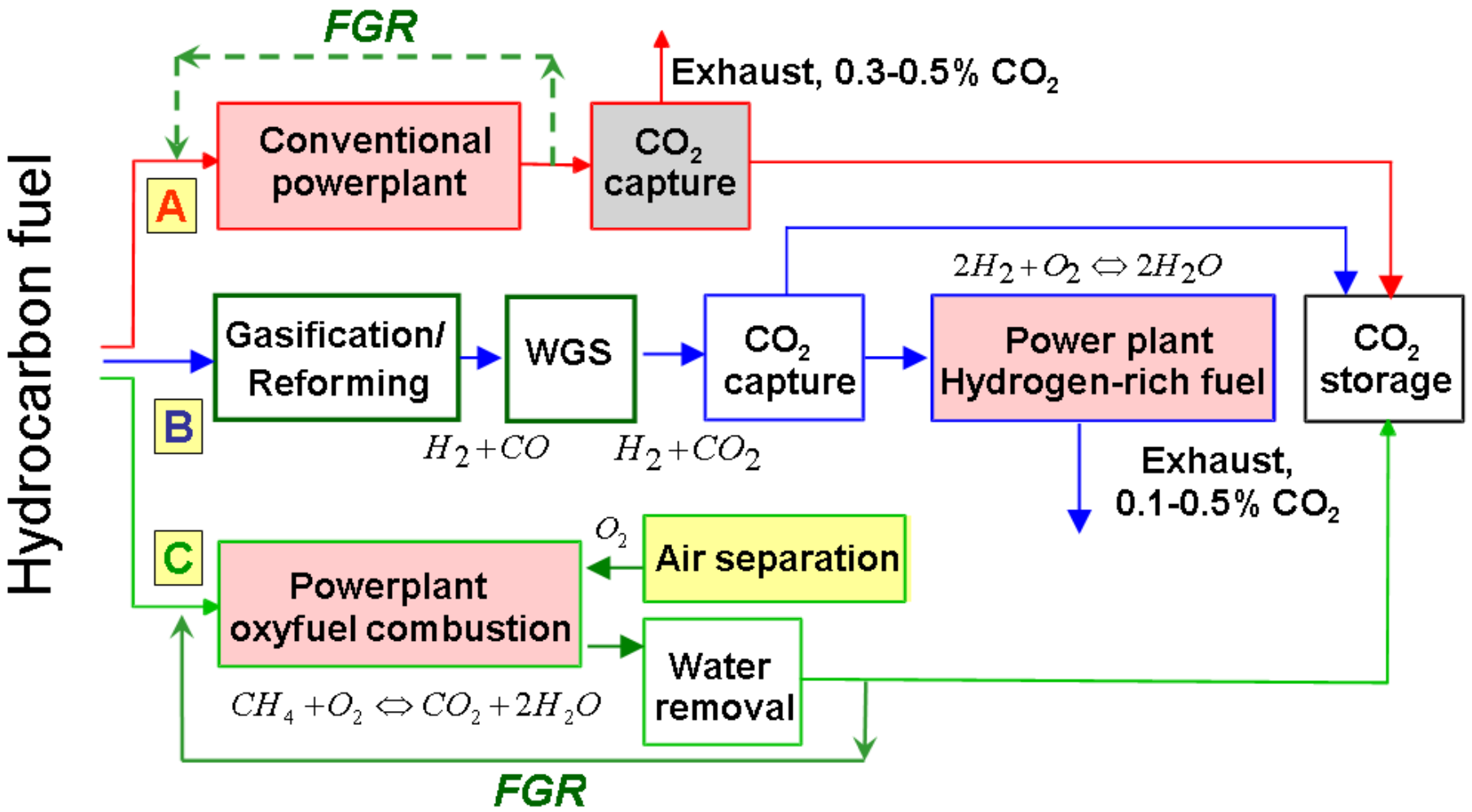
Yu-Chun Lin

Combustion Research Laboratory, Paul Scherrer Institute

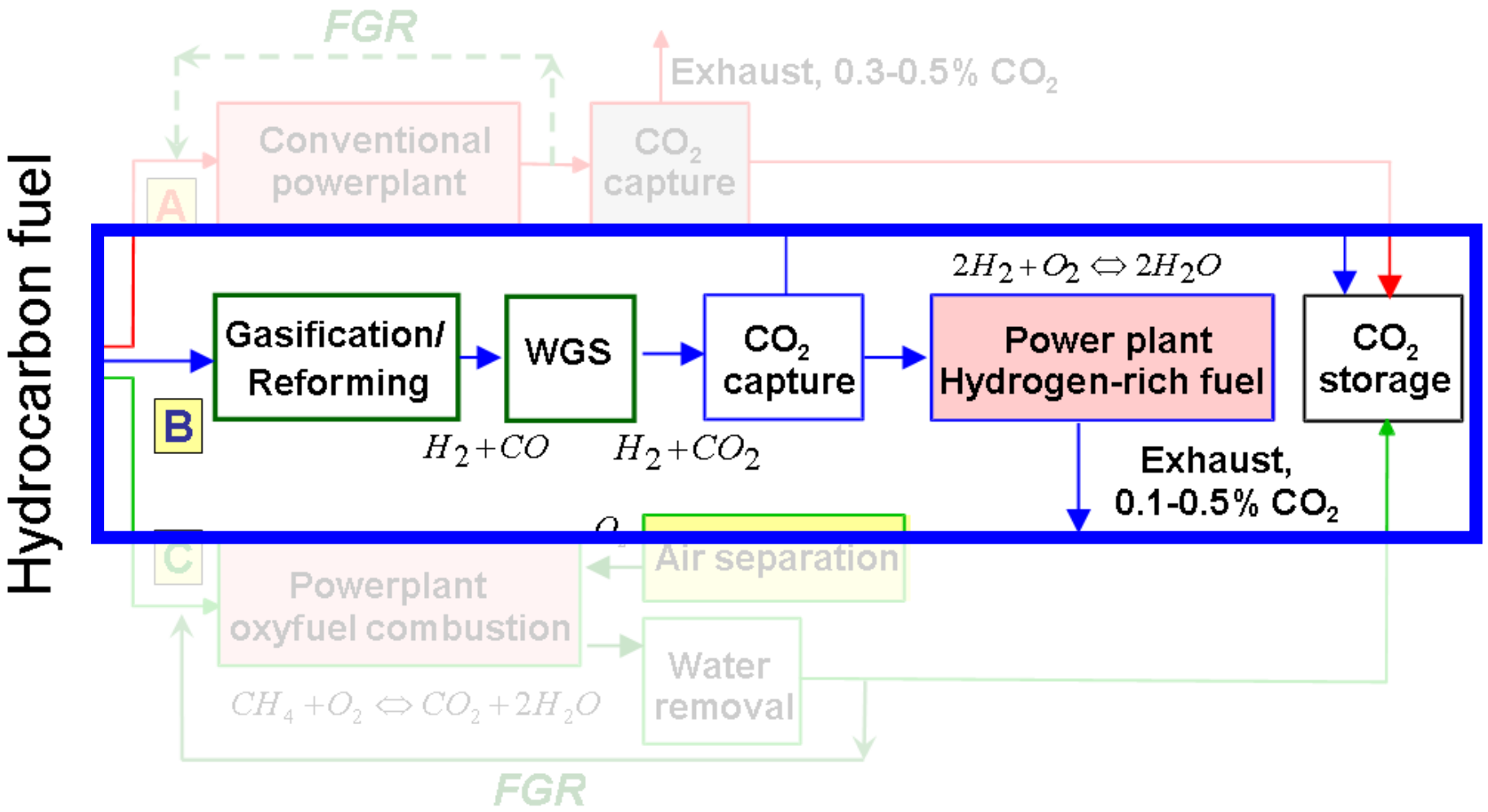
Presentation Outline

- Background
- Approach
- Preliminary Results
  - ✓ S_{L0}
  - ✓ S_T
  - ✓ NO_x
- Summary

Background


FGR
Exhaust, 0.3-0.5% CO_2
Hydrocarbon fuel
A
Conventional powerplant
CO_2 capture
$2H_2 + O_2 \Leftrightarrow 2H_2O$
B
Gasification/ Reforming
WGS
CO_2 capture
Power plant Hydrogen-rich fuel
CO_2 storage
$H_2 + CO$
$H_2 + CO_2$
Exhaust, 0.1-0.5% CO_2
C
O_2
Air separation
Powerplant oxyfuel combustion
Water removal
$CH_4 + O_2 \Leftrightarrow CO_2 + 2H_2O$
FGR

Background


FGR
Exhaust, 0.3-0.5% CO_2
Conventional powerplant
CO_2 capture
A
Hydrocarbon fuel
$2H_2 + O_2 \Leftrightarrow 2H_2O$
Gasification/ Reforming
WGS
CO_2 capture
Power plant Hydrogen-rich fuel
CO_2 storage
B
$H_2 + CO$
$H_2 + CO_2$
Exhaust, 0.1-0.5% CO_2
C
Air separation
Powerplant oxyfuel combustion
Water removal
$CH_4 + O_2 \Leftrightarrow CO_2 + 2H_2O$
FGR

Background

- Supporting projects: H2-IGCC (EU-FP7) & CARMA (CCEM/CCES)

carbon management in power generation

- Feasibility study of hydrogen-rich combustion for gas turbine applications in power generation

- Investigating the physical/chemical effects and intricate flame-vortex interactions with the presence of high hydrogen content in fuel gases

Background

- Supporting projects: H2-IGCC (EU-FP7) & CARMA (CCEM/CCES)

Pre-combustion carbon sequestration

H_2-rich fuel mixtures

- Feasibility study of hydrogen-rich combustion for gas turbine applications in power generation

- Investigating the physical/chemical effects and intricate flame-vortex interactions with the presence of high hydrogen content in fuel gases

Background (cont'd)

Mixtures of interest

Mixtures corresponds to various degree of decarbonization or catalytic conversion (>80% H_2 in the fuel component; with CH_4, CO, CO_2, H_2O, N_2)

Approaches

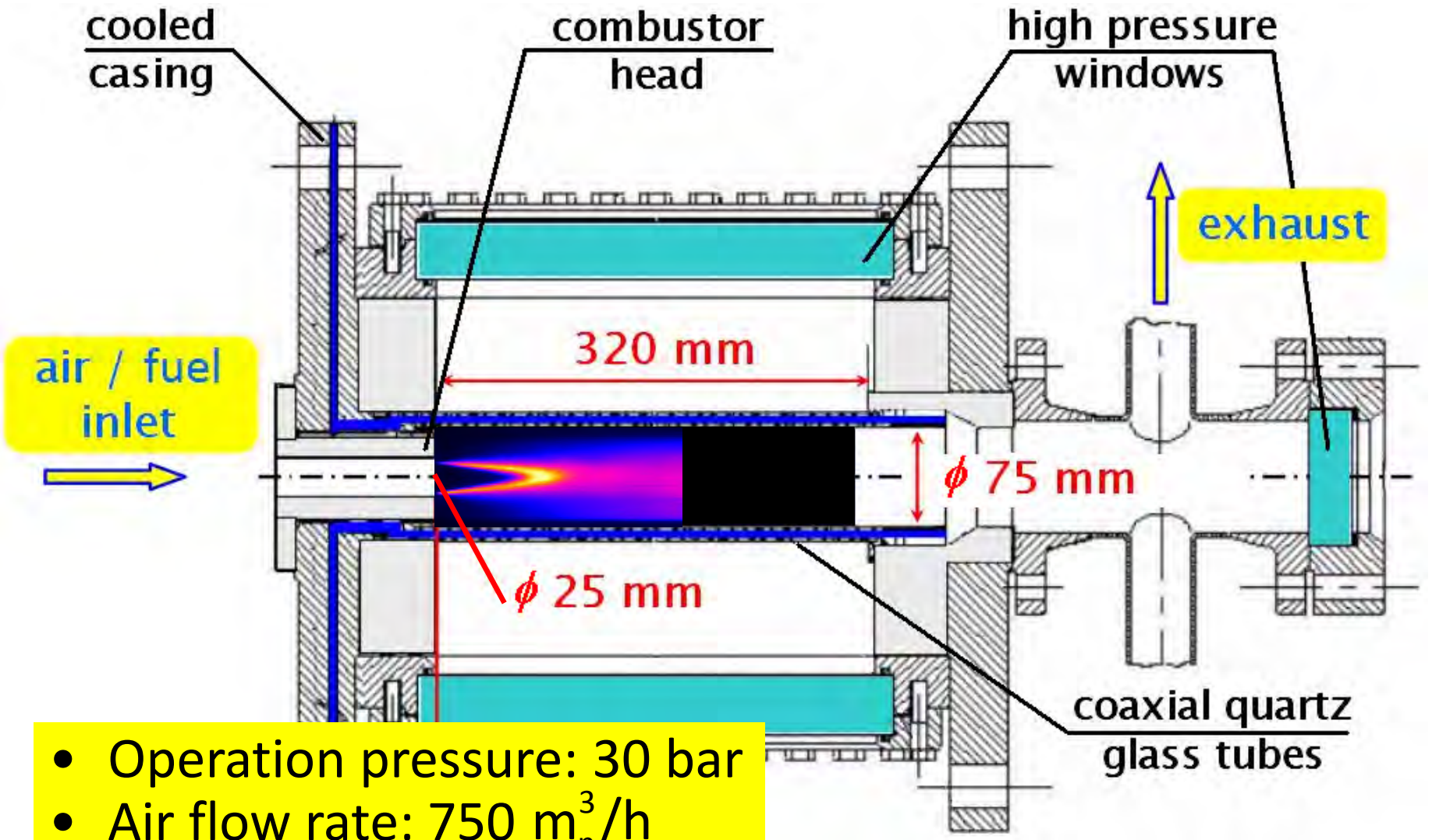
- High-pressure combustion test rig
- OH-PLIF diagnostics
- Chemical-kinetic calculations (CANTERA)
- Exhaust gas analysis (NO_x, CO, CO_2)

Objectives

- Stability limits (LBO/flashback)
- Flame front characteristics
- Emission characteristics

Prescribed conditions ("gas turbine-relevant condition"):
$u_{bulk} \geq 40$ m/s, $1.6 < \lambda < 4.0$; $P \leq 20$ bar; $T_{ph} \leq 773$ K)

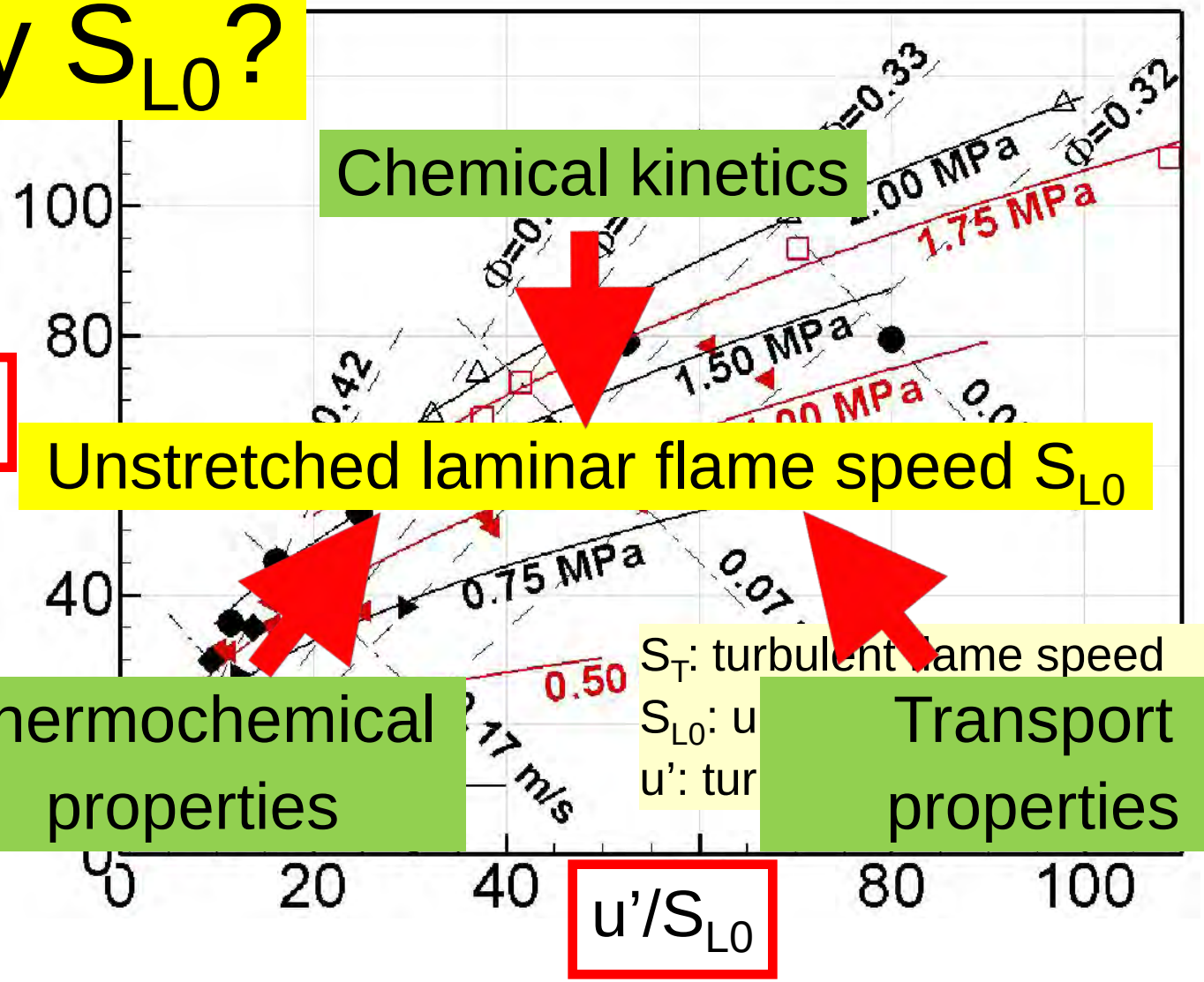
Approach: Experiments



- Operation pressure: 30 bar
- Air flow rate: 750 m_n^3/h
- Max. Preheat: 823 K

Approach: Chemical-Kinetic Calculations

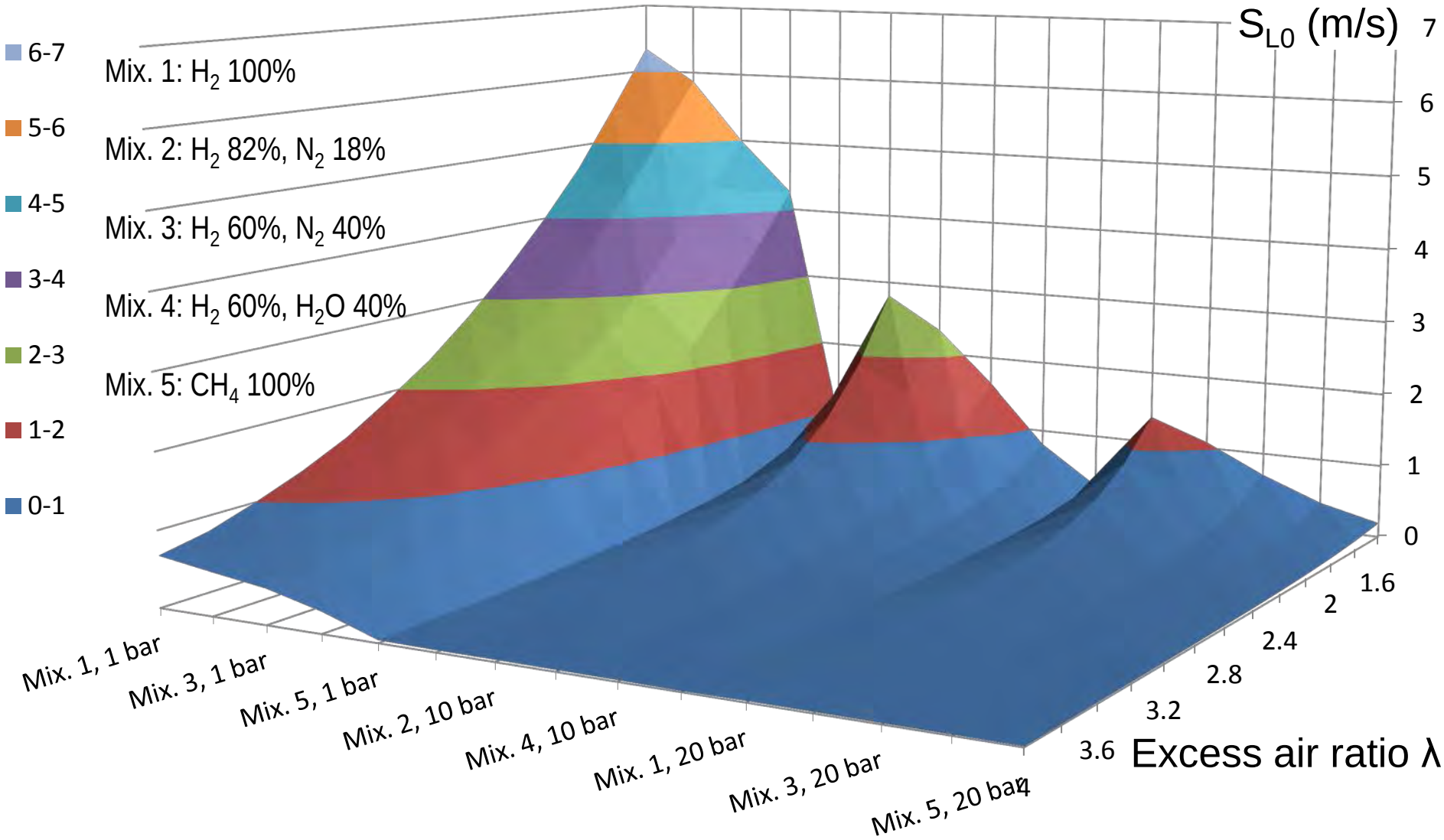
Why S_{L0}?



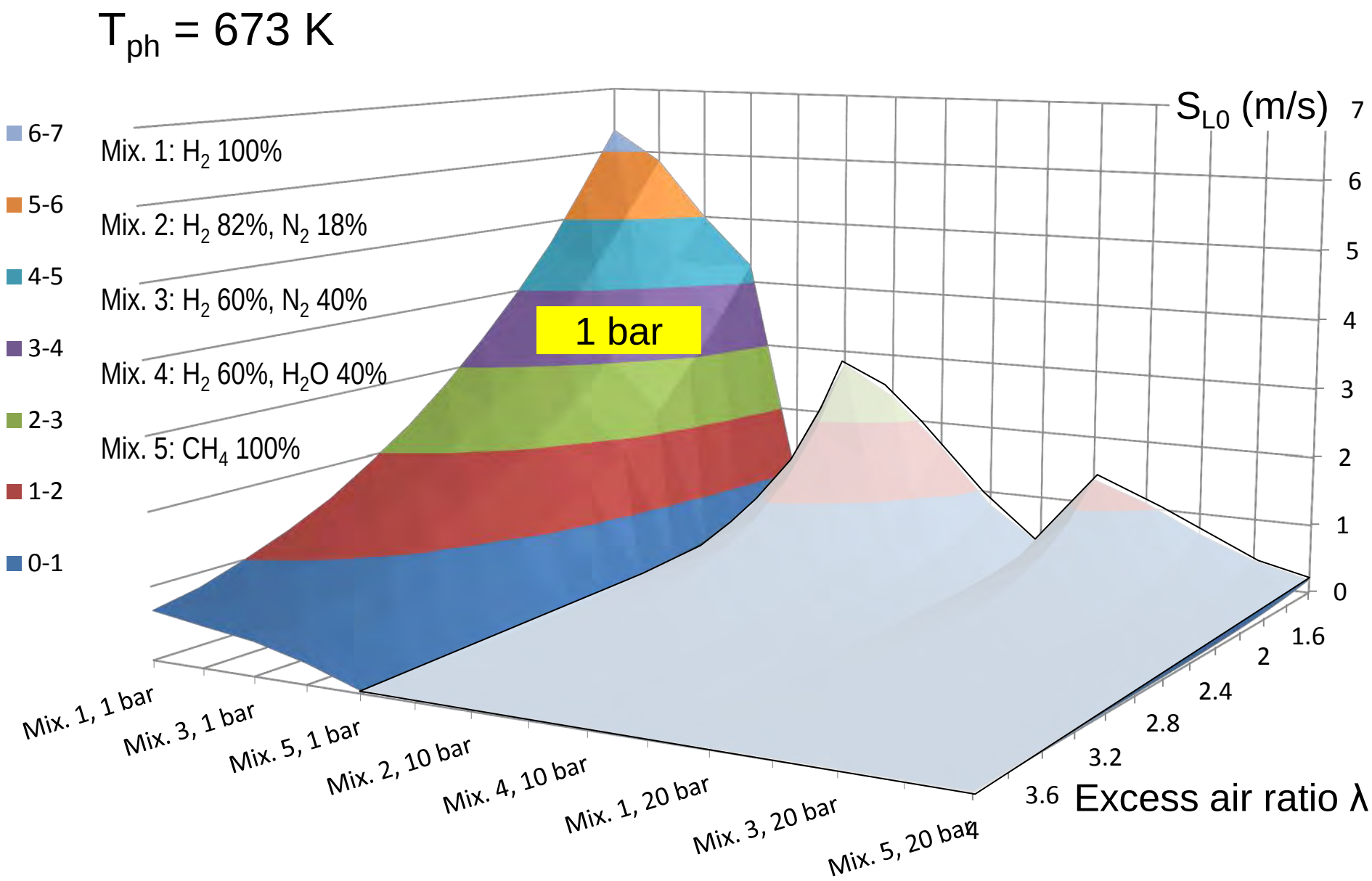
Graph origin: Salvatore Daniele, "Lean Premixed Syngas Combustion for Gas Turbines Applications," Ph.D. dissertation, Swiss Federal Institute of Technology Zurich, 2011.

Preliminary Results: S_{L0} Overview

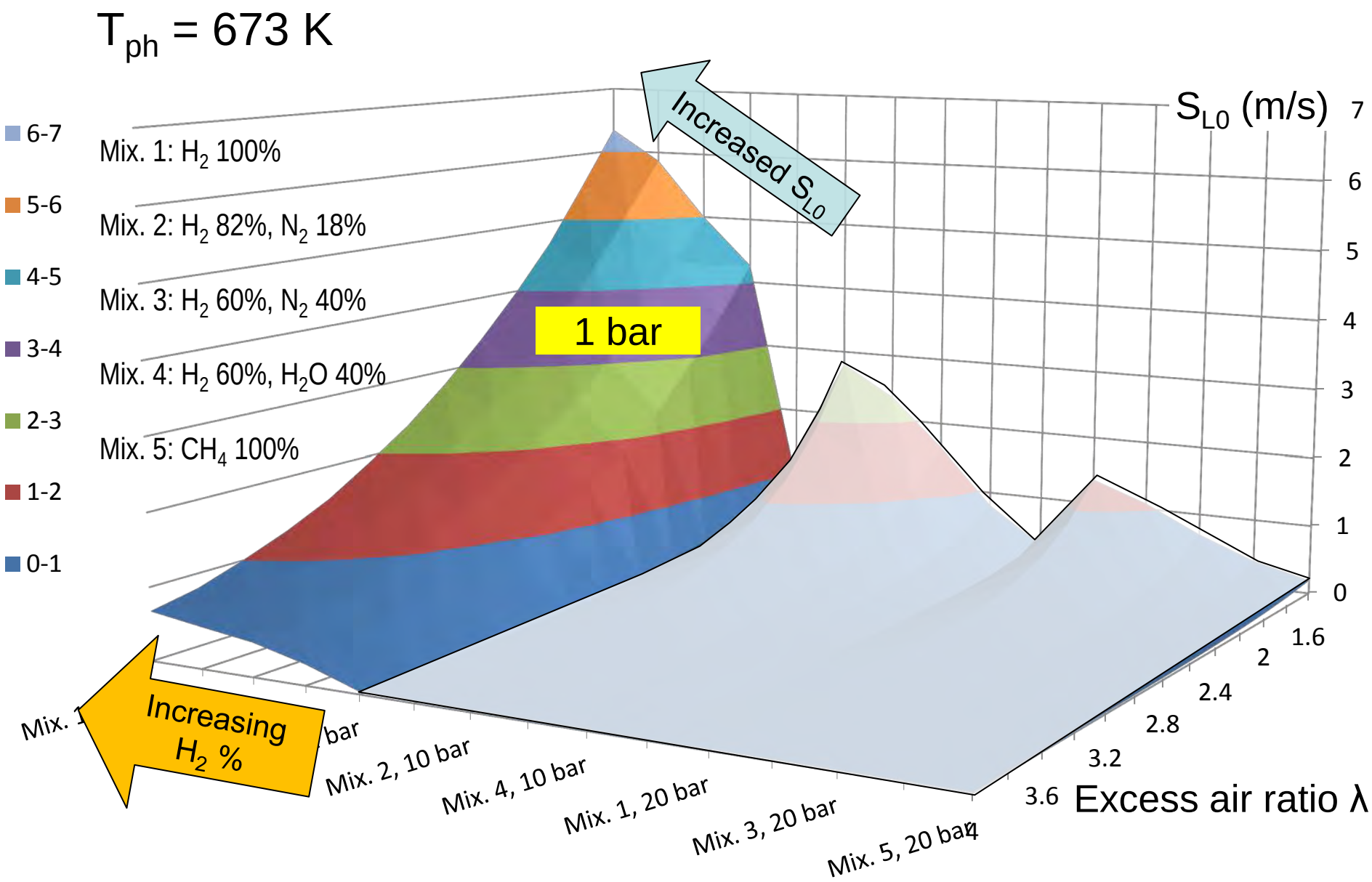
T_{ph} = 673 K



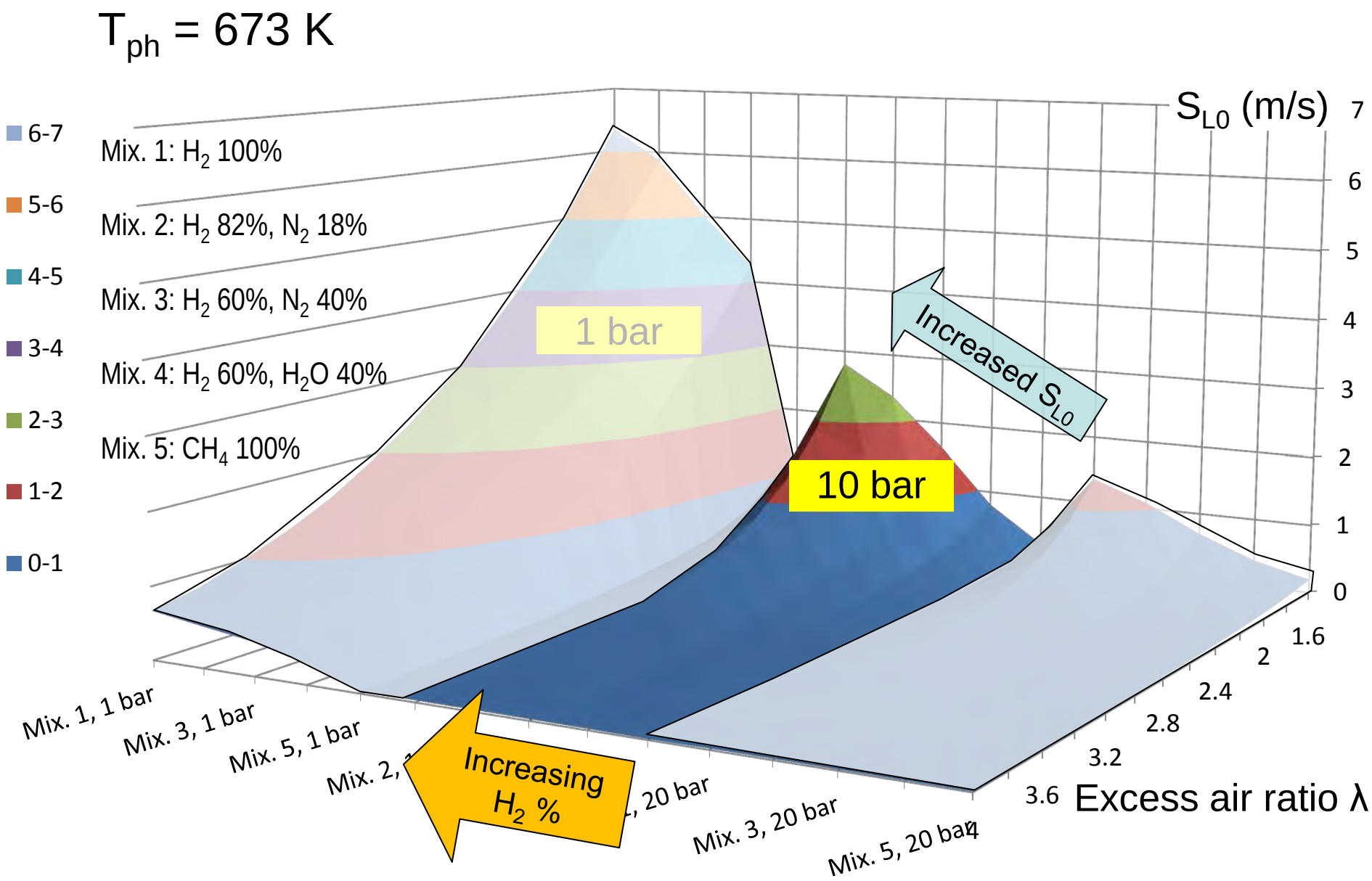
Preliminary Results: S_{L0} Overview



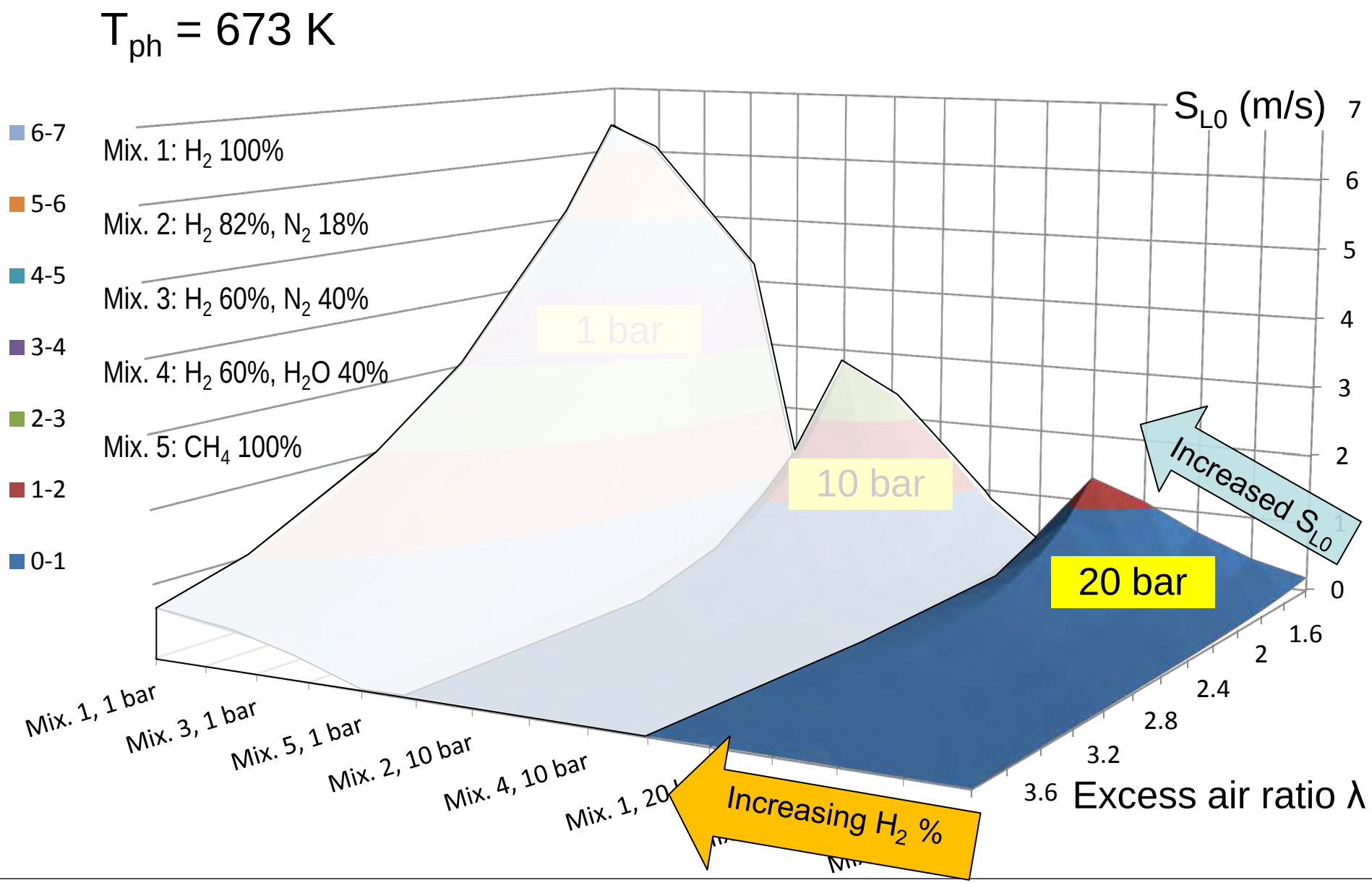
Preliminary Results: S_{L0} Overview



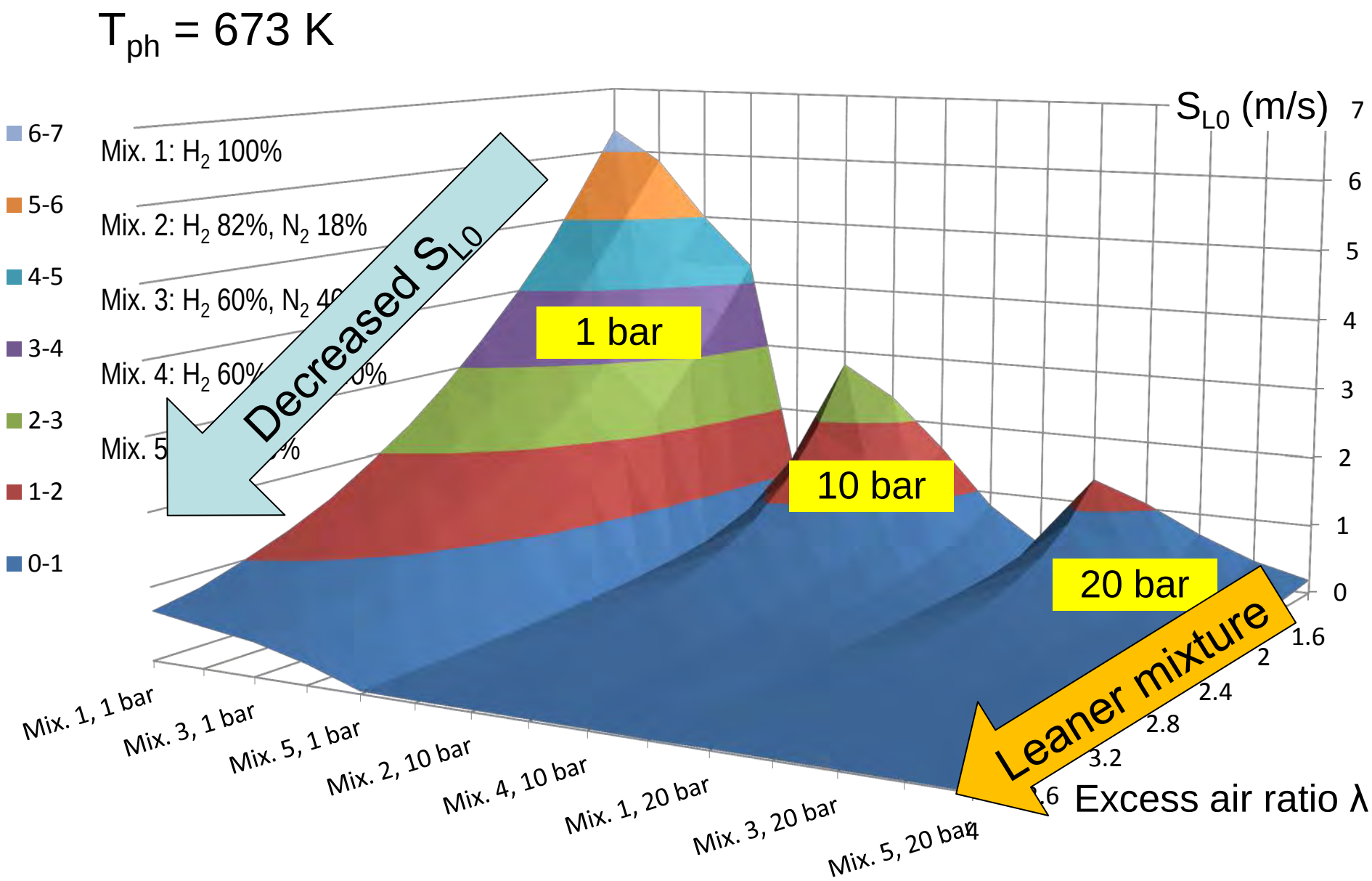
Preliminary Results: S_{L0} Overview



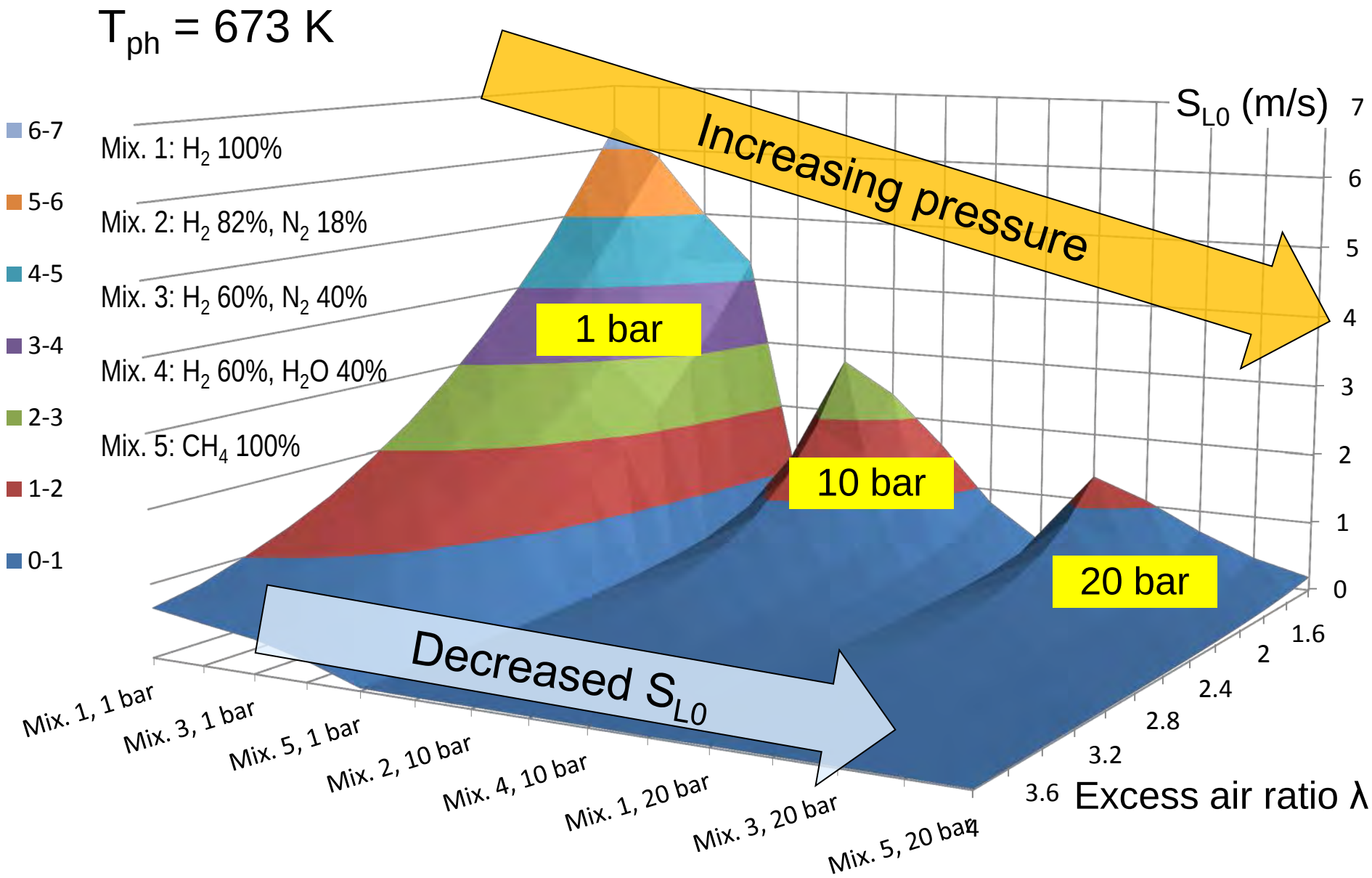
Preliminary Results: S_{L0} Overview



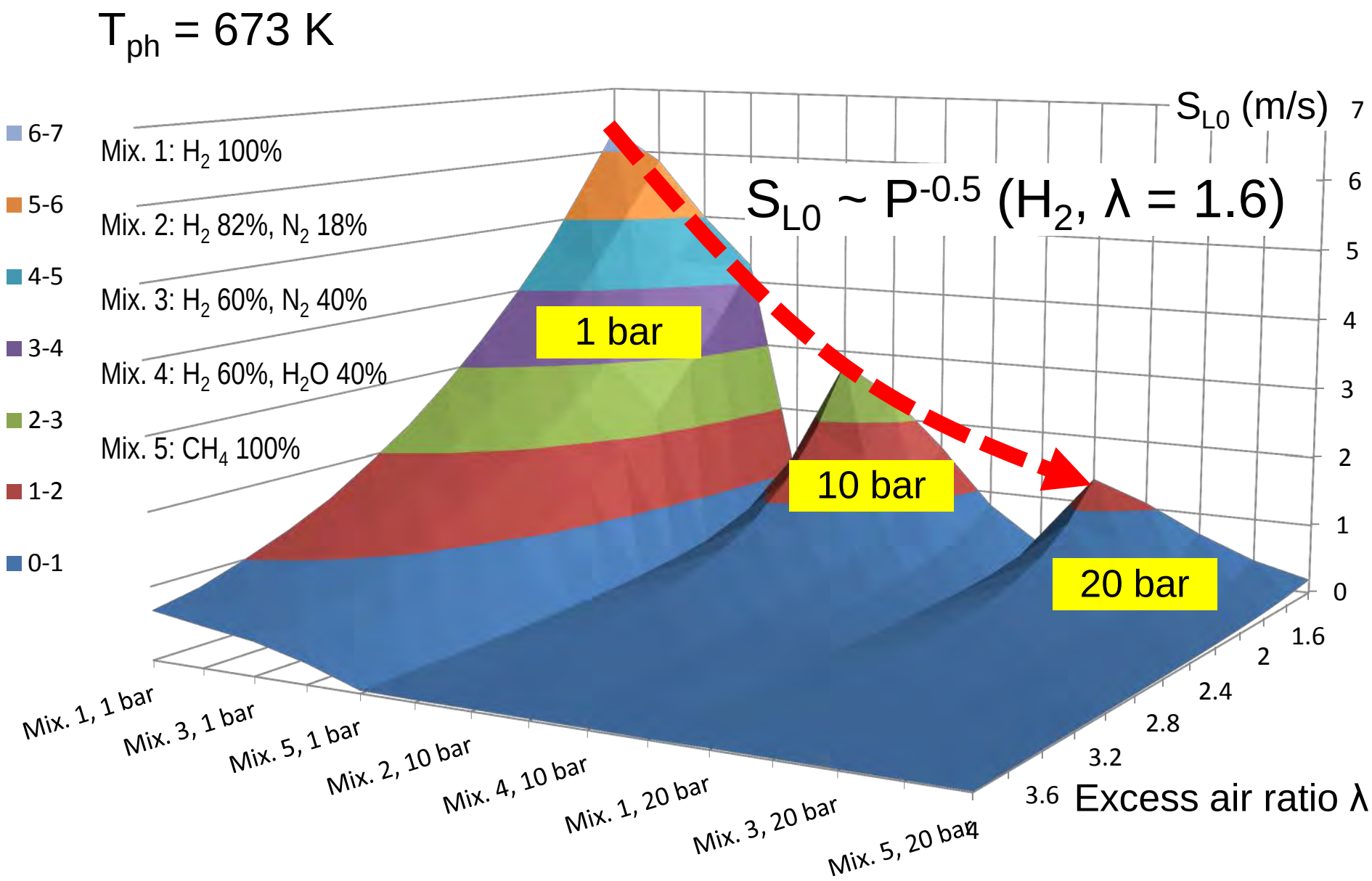
Preliminary Results: S_{L0} Overview



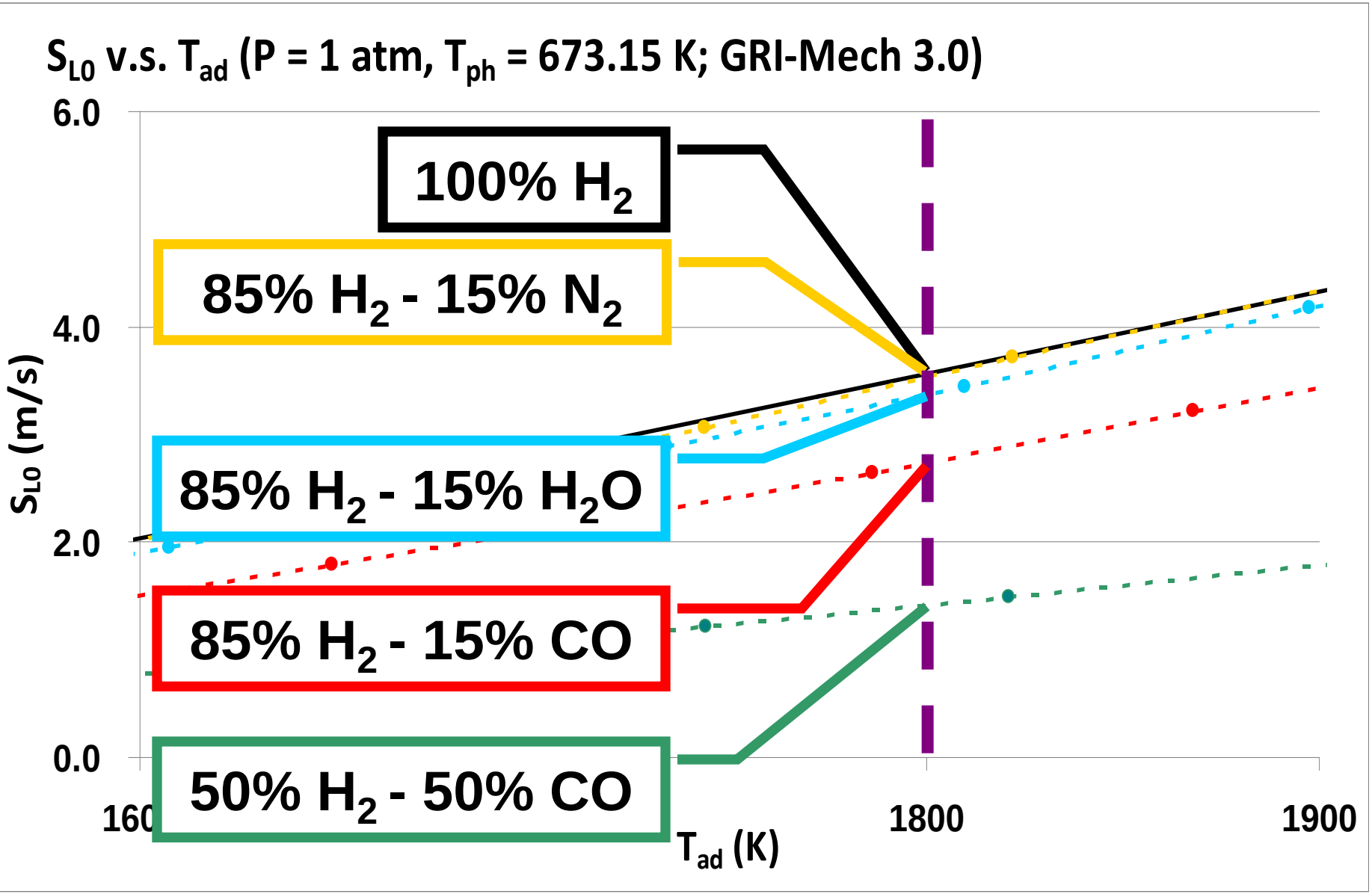
Preliminary Results: S_{L0} Overview



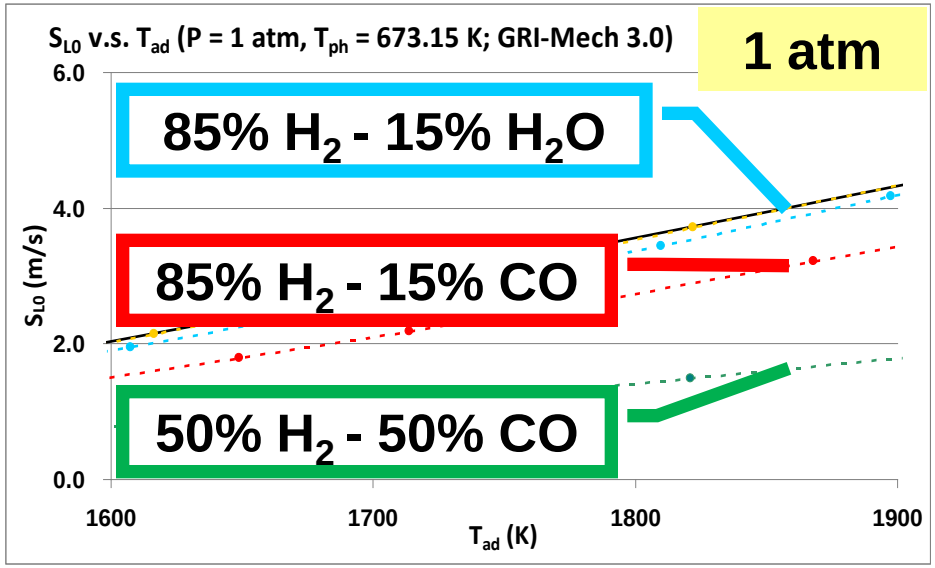
Preliminary Results: S_{L0} Overview

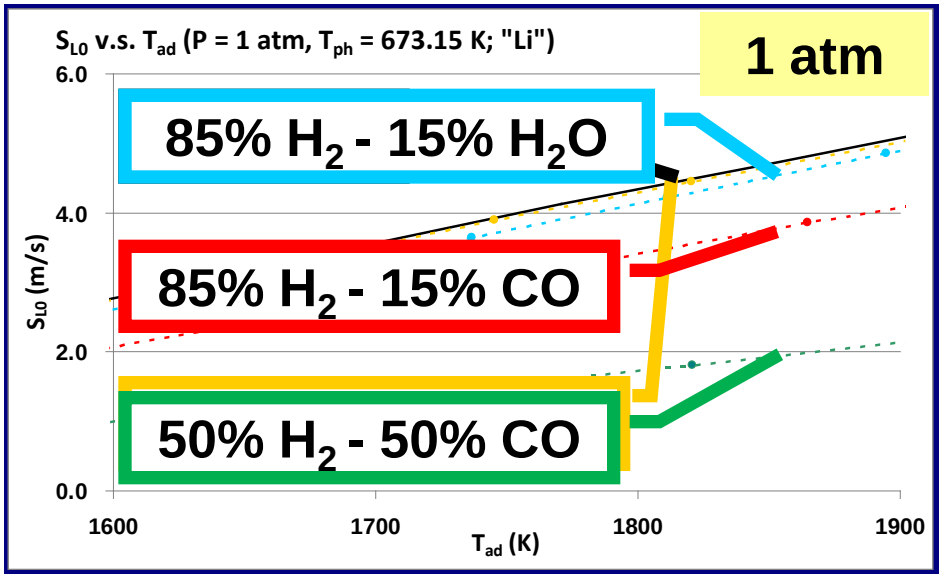


S_{L0}: Alternative Mechanisms



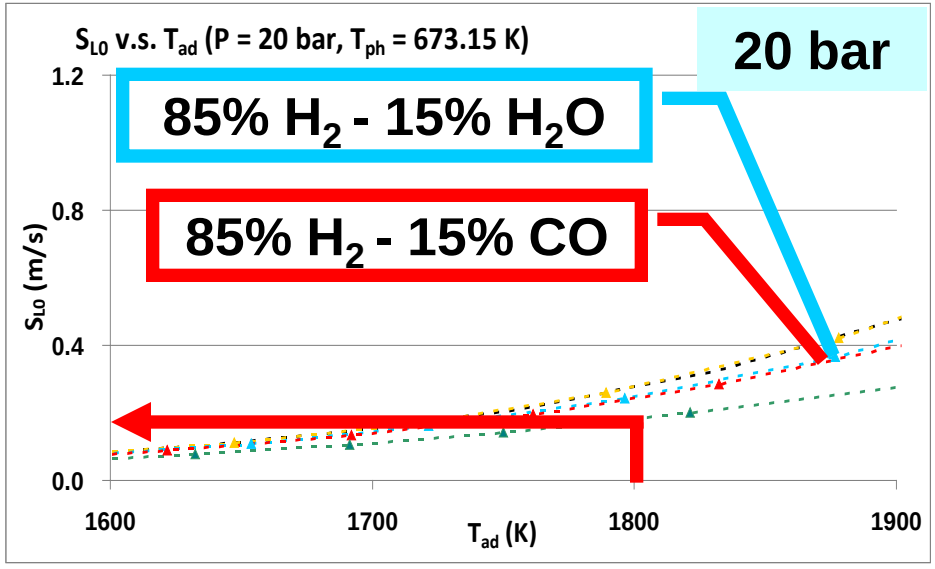
S_{L0}: Alternative Mechanisms (cont'd)

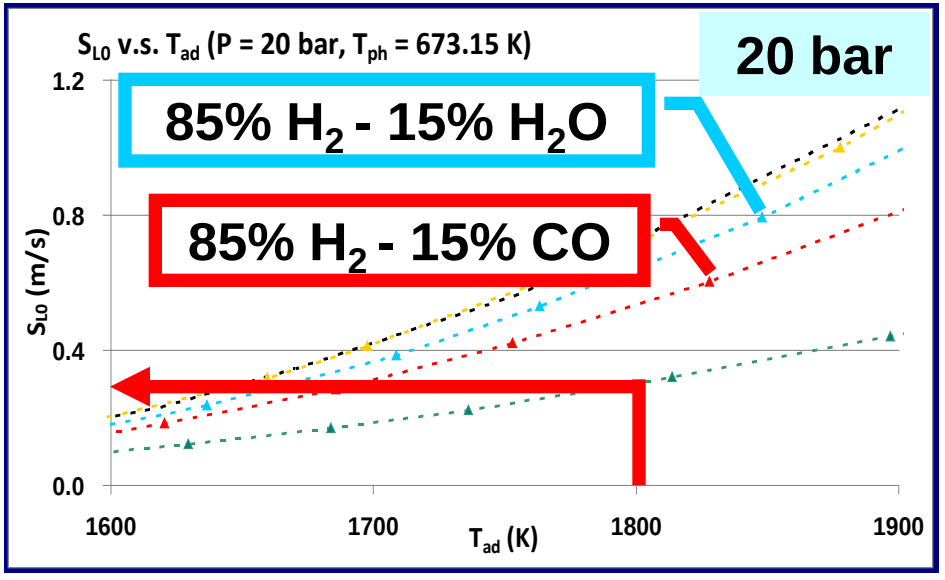




GRI-Mech 3.0

Li

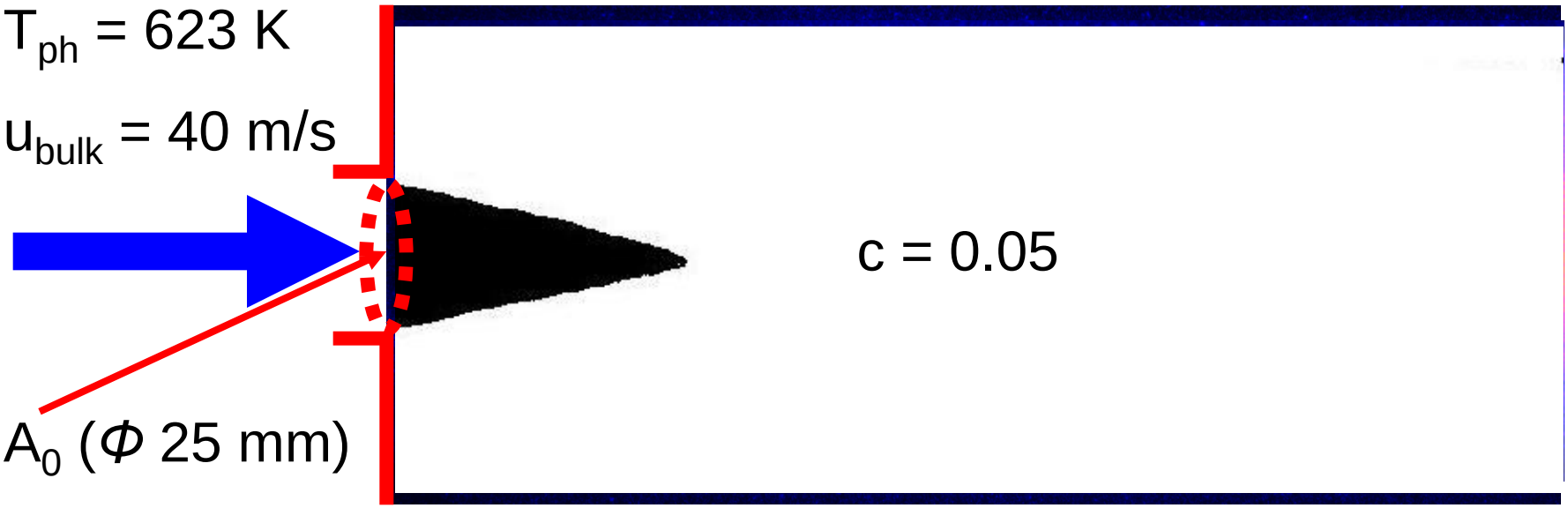




"Li": J. Li *et al.*, "A comprehensive kinetic mechanism for CO, CH2O, and CH3OH combustion," Int. J. Chem. Kinet. 39 (2007) 109-136.

Preliminary Results: S_T

Continuity: $\rho_0 \cdot A_0 \cdot u_{bulk} = \rho_0 \cdot A_{f,\,averaged} \cdot S_T$



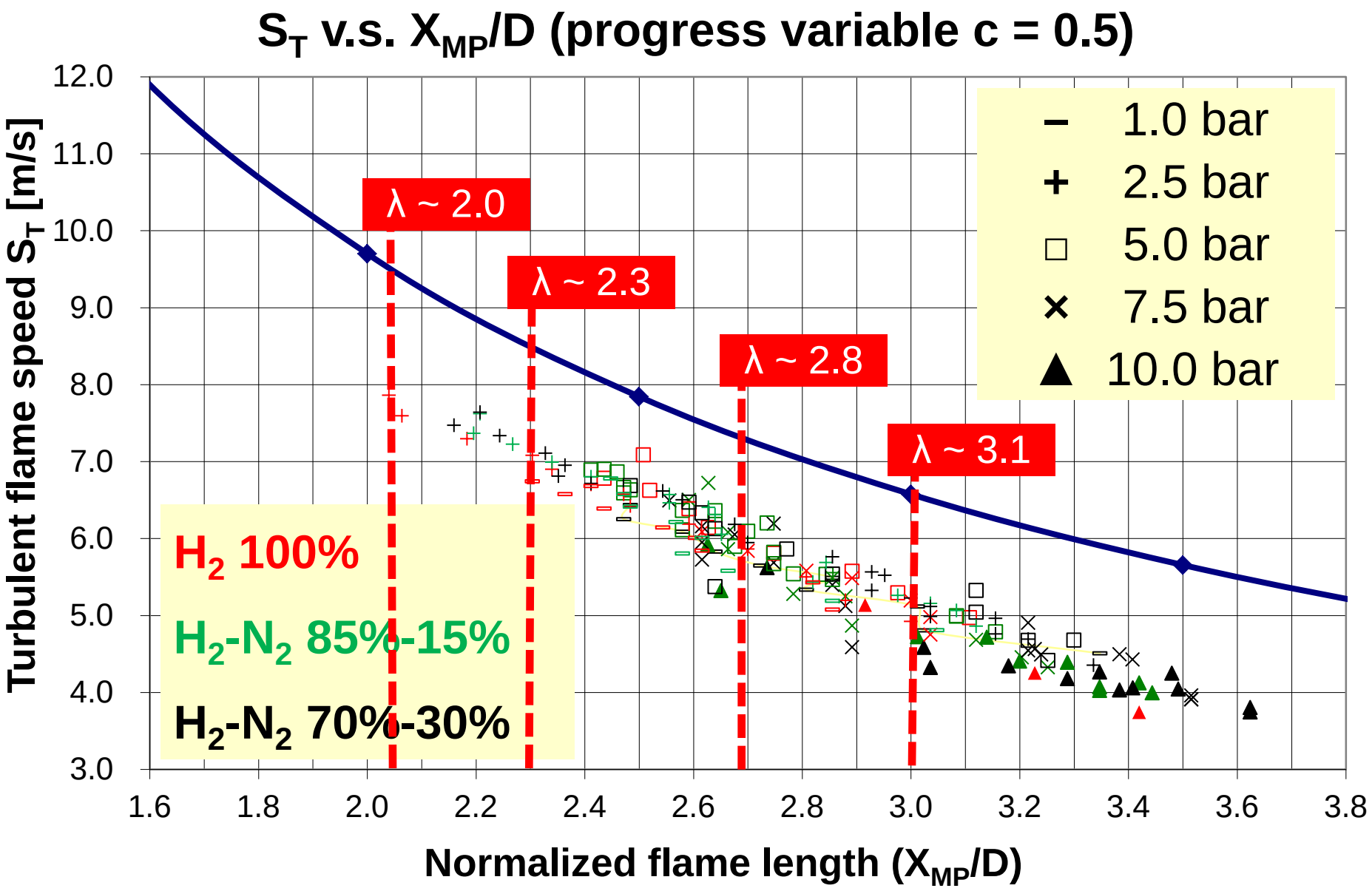
"Progress variable (c)" approach:

c = 0 → fresh mixture

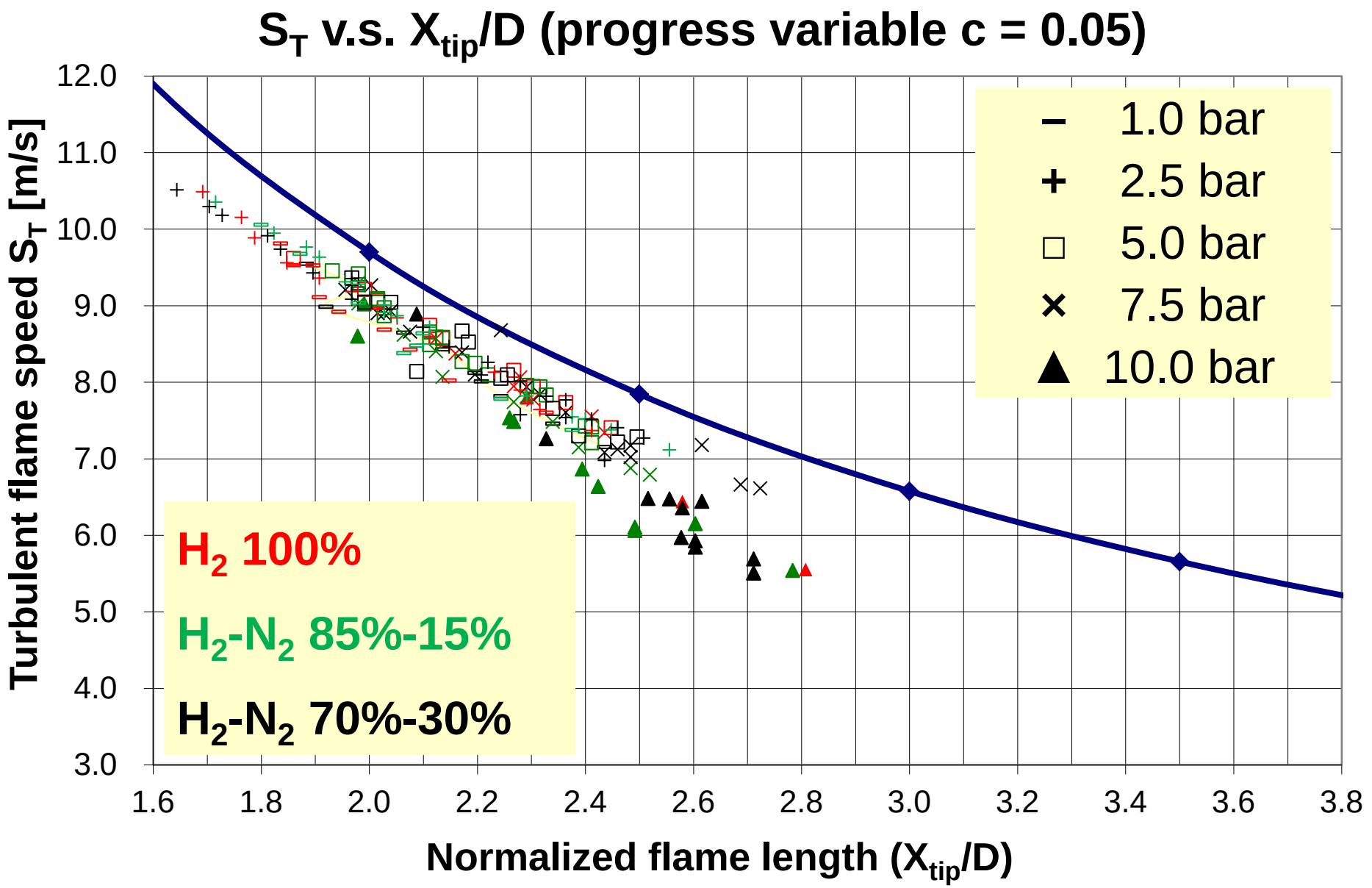
c = 0.5 → "most probable" flame front location

c = 1 → completely burnt gas

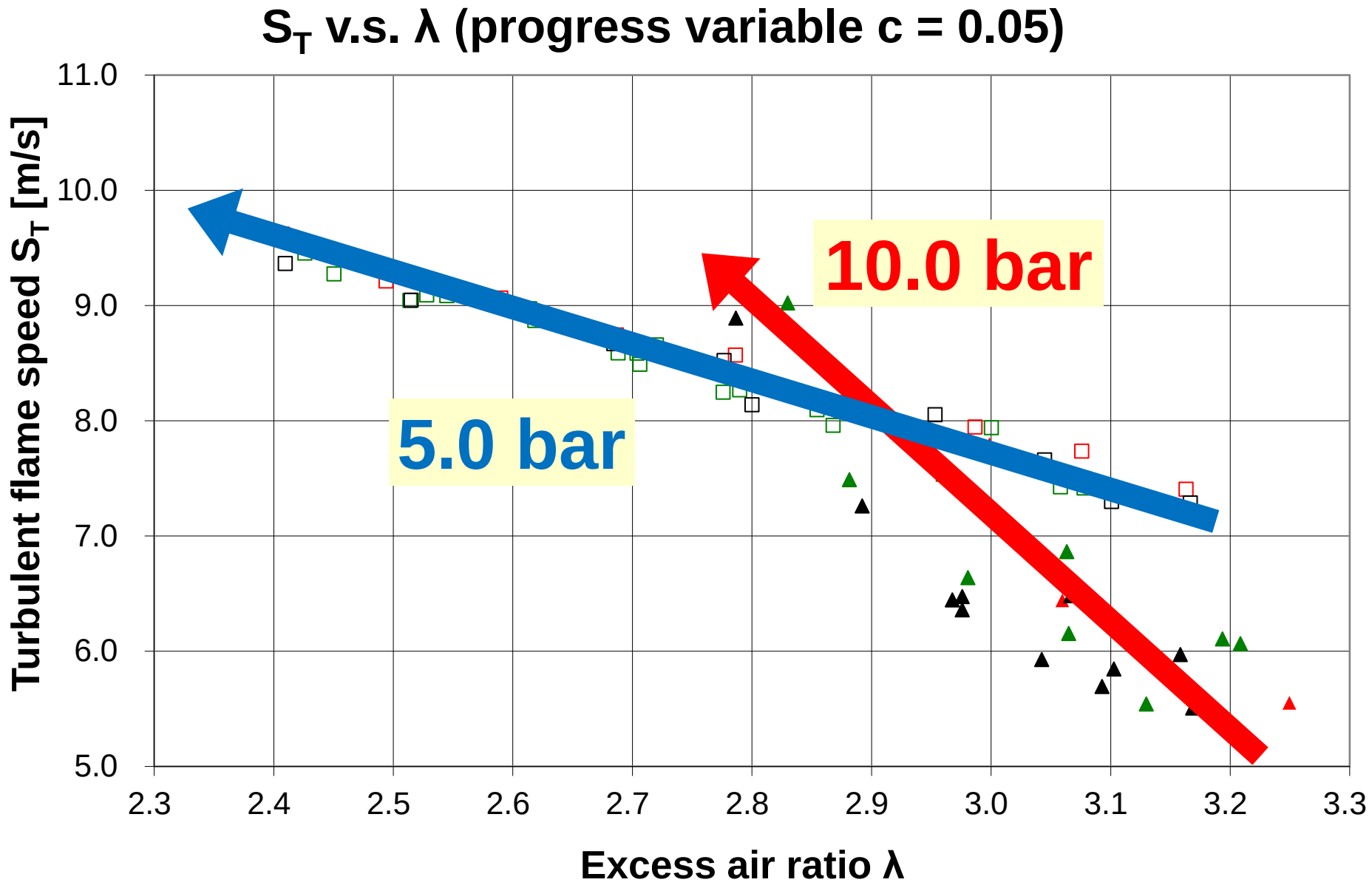
S_T Overview: “Conic” Behavior



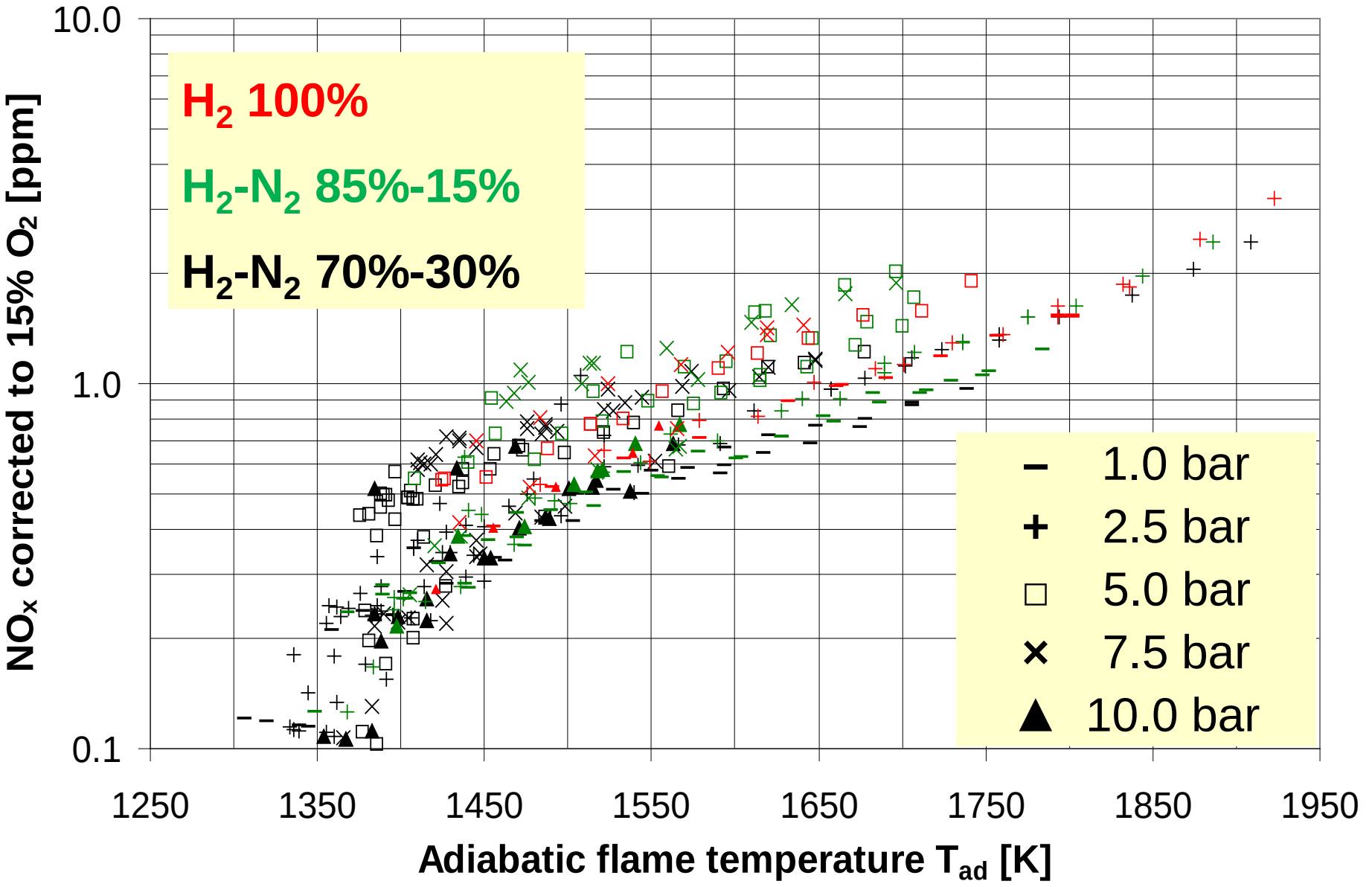
S_T Overview: “Conic” Behavior (cont’d)



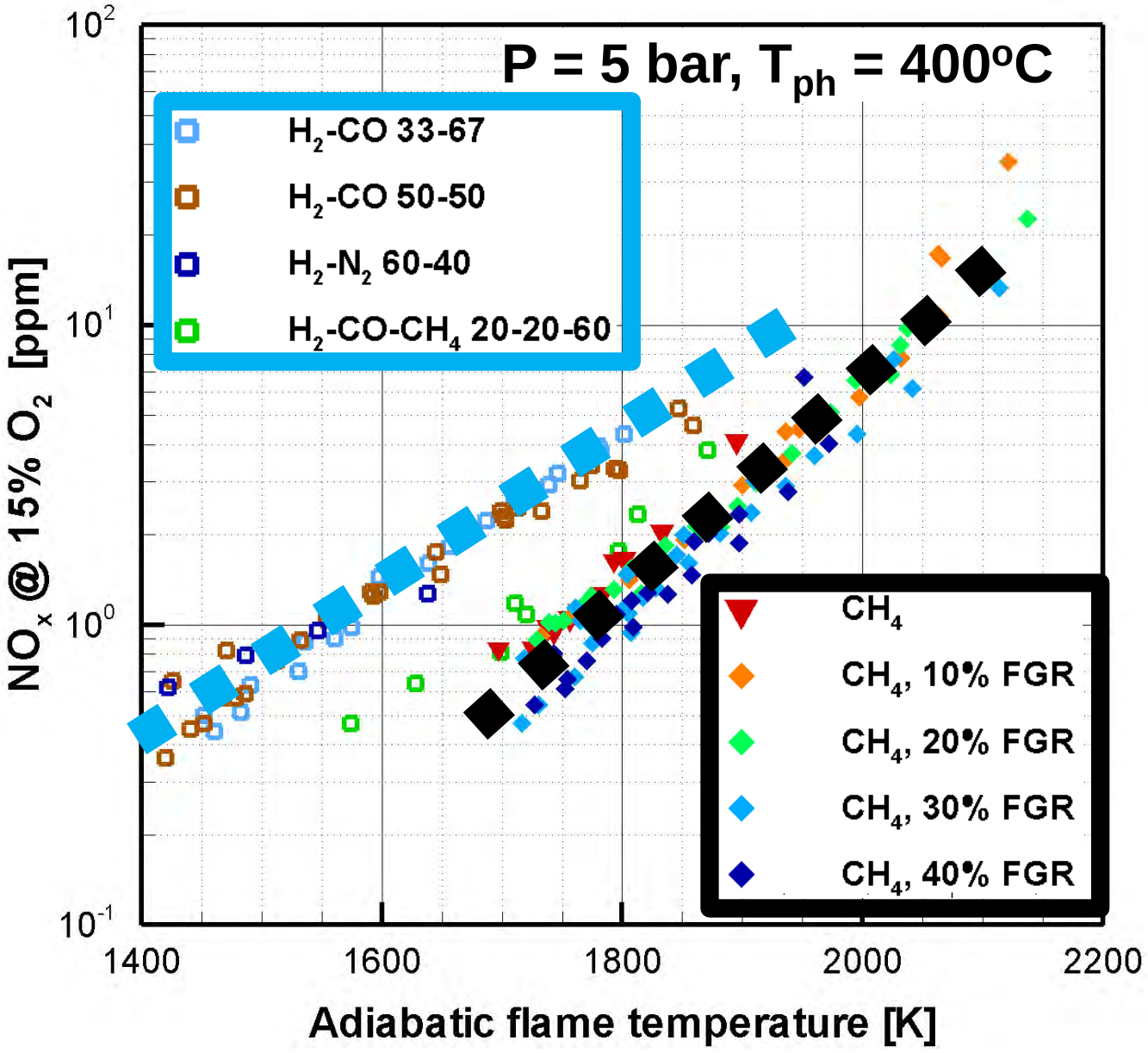
S_T Overview: Pressure Effect



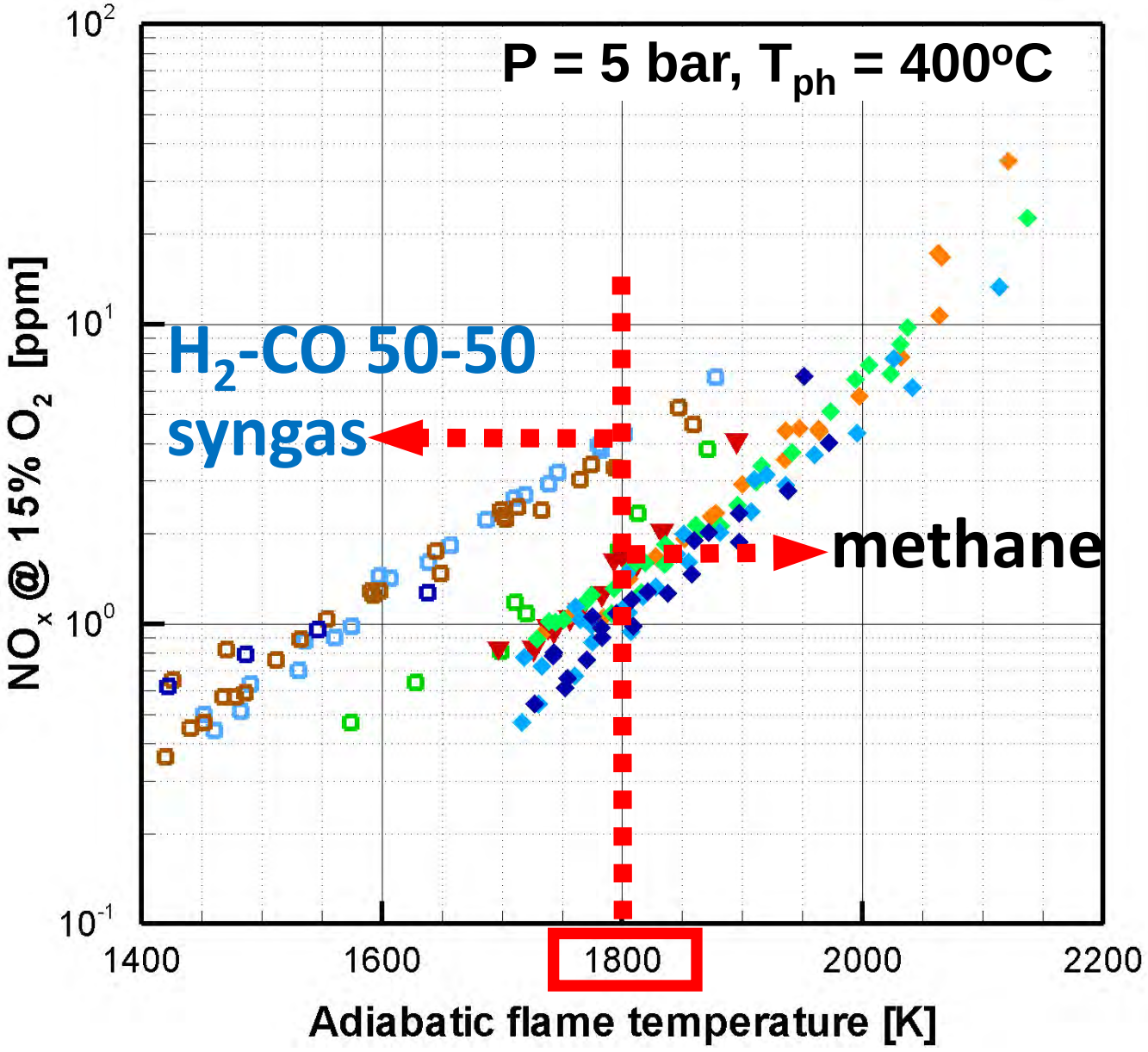
Preliminary Results: NO_x Emission



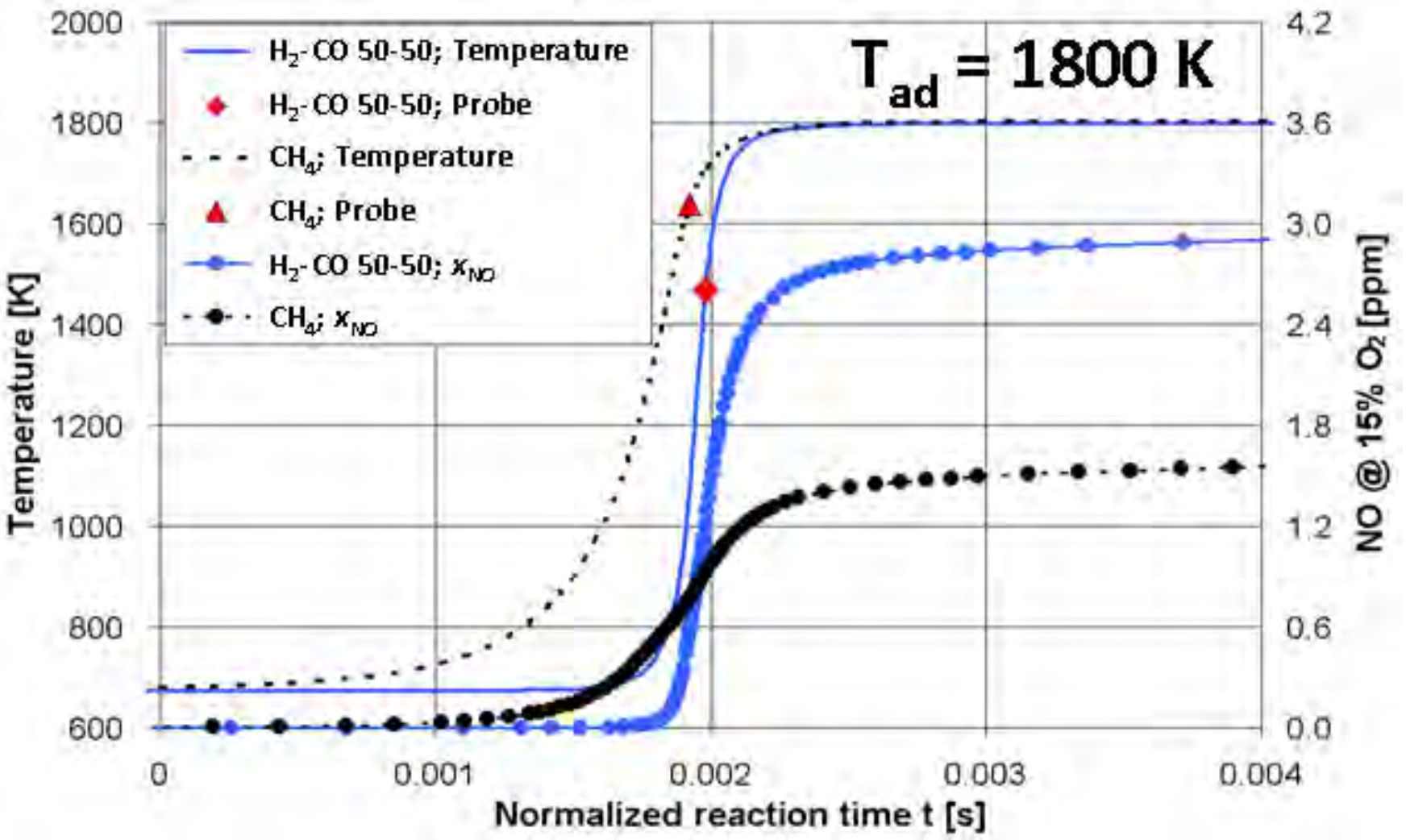
NO_x Emission: Syngas Measurements



NO_x Emission: Syngas Measurements

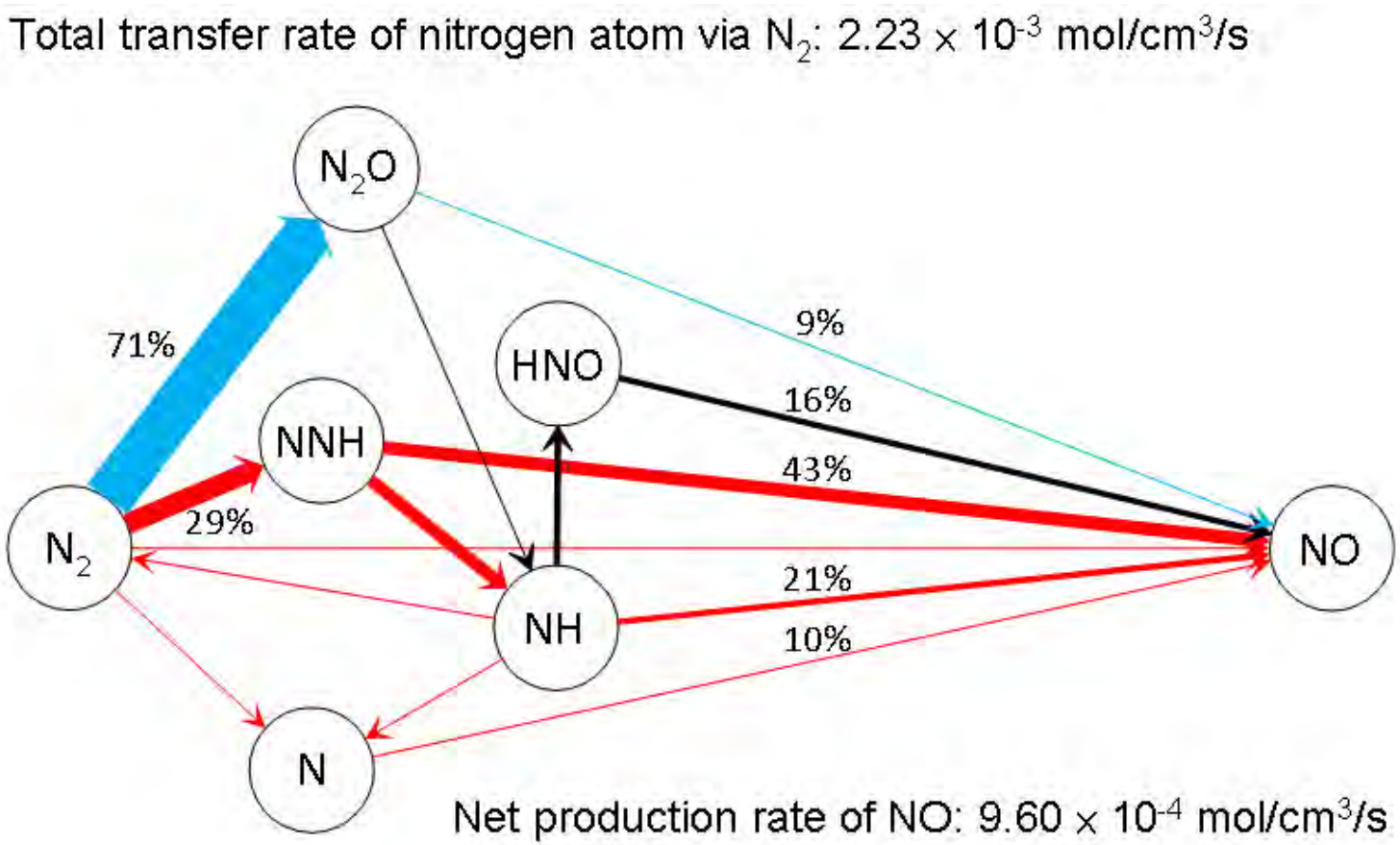


Example: Kinetic Calculations v.s. NO_x



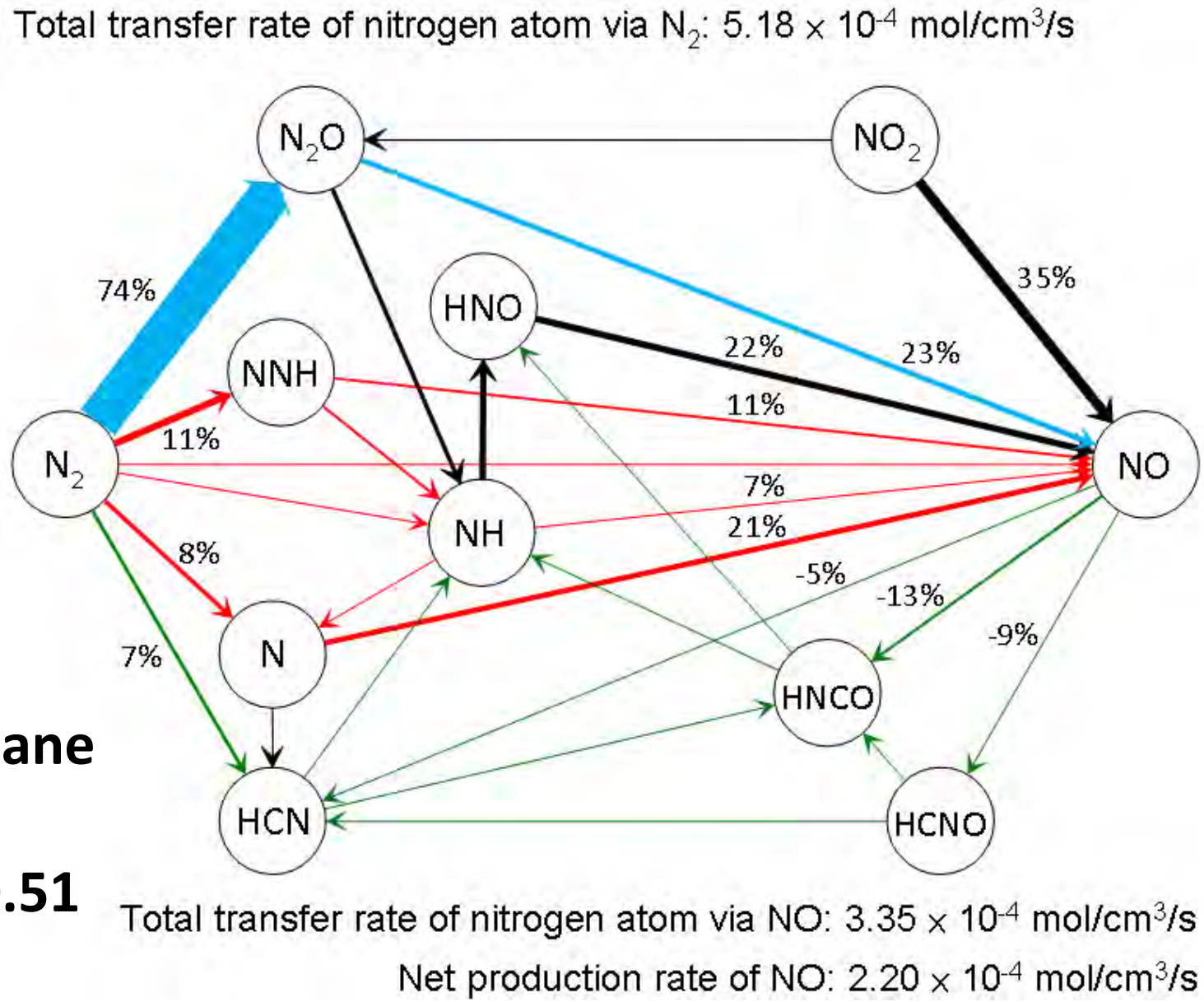
The respective 1-D freely propagating flame is “probed” at the location with the largest X_{NO} gradient for the nitrogen-atom pathway diagrams.

Example: Reaction Path Analysis



Syngas
(H_2-CO 50-50)
$\Phi = 0.41$

Example: Reaction Path Analysis



Methane (CH_4)
Φ = 0.51

Summary

- Compared to the syngas, flashback occurs at even leaner conditions for hydrogen-rich fuel gases. A **significantly reduced operational envelope** is observed at elevated pressure.

- The profile of flame front is generally approaching that of an **ideal cone**. Thus a simplified approach for estimating the S_T only via the location of the flame tip can be applied.

- The **pressure effects on the NO_x emission are weak** for both syngas and hydrogen-rich fuel gases, but a non-monotonic behavior is observed for the latter.

- Results from **reaction path analysis** are expected to complement and provide more insight to the findings from the measurements.

Thank you for your attention.

Many thanks to:

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Mr. Daniel Erne
Dr. Alexey Denisov
Dr. Rolf Bombach
Dr. Salvatore Daniele

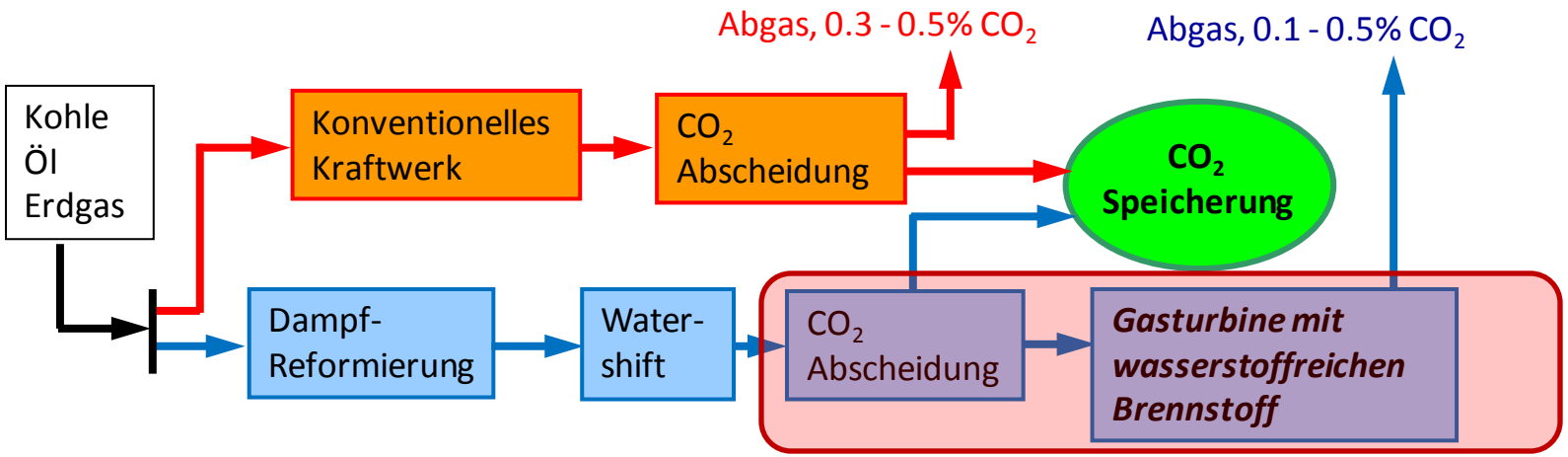
Verbrennungskonzepte für H_2-reiche Brennstoffe unter GT-Bedingungen

Felipe Bolaños, Felipe Piringer, Dieter Winkler, Timothy Griffin

Fachhochschule Nordwestschweiz
Institut für Thermo- und Fluid-Engineering

28. Oktober 2011

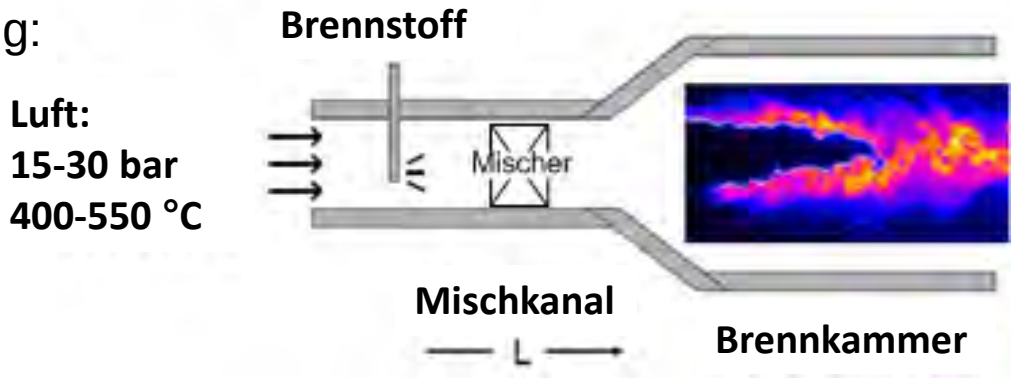
Motivation: *Warum >80% H_2 Brennstoffe?*



- Vorteile:
  - Höherer CO_2 Volumenanteil, höherer Druck → CO_2 Abscheidung effektiver (höherer Partialdruck)
  - Gasturbine kann mit jedem fossilen Brennstoff betrieben werden (Öl, Erdgas, Kohle…)
- Nachteile:
  - Wasserstoffreicher Brennstoff → sehr reaktiv

Motivation: *Wasserstoffnutzung*

- Konventionelle Eindüsung:

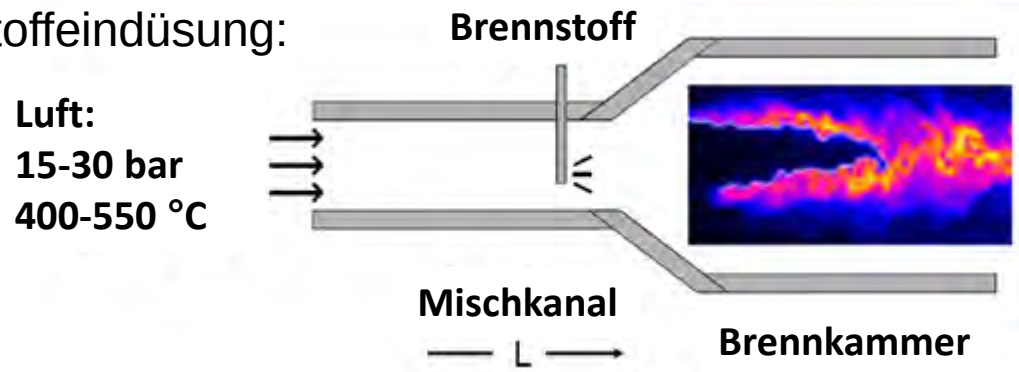


- Heutzutage verwendete GT-Brenner sind für wasserstoffreiche Brennstoffe nicht geeignet. Flashback und Selbstzündung können Brenner beschädigen.

- Hohe **Flashback** (Rückschlag) Gefahr:
  - Turbulente Flammenfront breitet sich gegen die Strömungsrichtung aus (Strömungsgeschwindigkeit kleiner als die Flammengeschwindigkeit)

Motivation: *Wasserstoffnutzung*

- Herkömmliche Wasserstoffeindüsung:



- Schlechte Vormischung → **hohe NOx Emissionen**
- Wasserstoff muss mit Stickstoff oder Wasserdampf verdünnt werden →Wirkungsgradverlust

Inhalt

- **Einstufiges Konzept**
  - Eindüsungsvarianten mit guter Mischung ohne Flashback
  - Ursachen und Vermeidung des Flashbacks
- **Gestuftes Konzept**
  - Fett/Mager Konzept für H_2
  - Auslegung
  - Messergebnisse
- **Ausblick**

Einstufiges Konzept

Ziel: stabile und saubere Verbrennung von Wasserstoff

Stabil = keine/geringe Flashbackgefahr

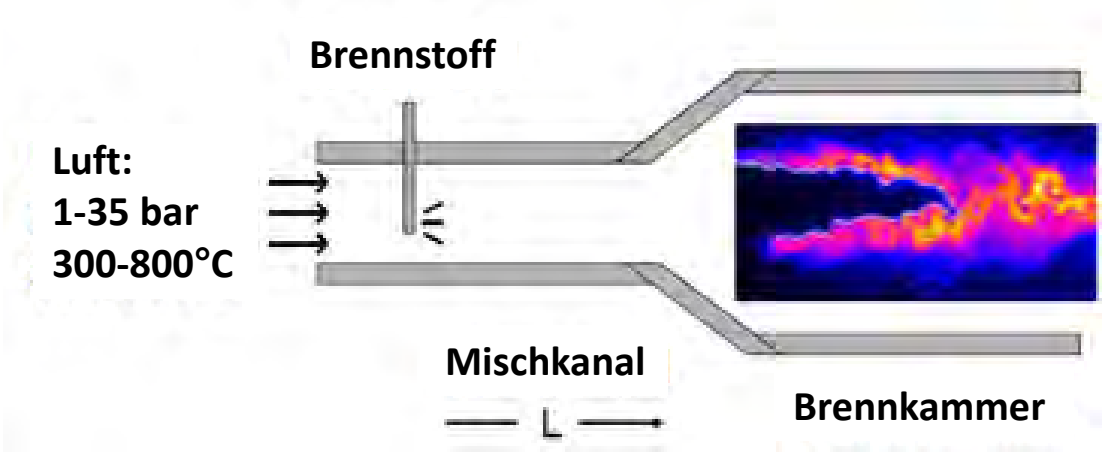
Sauber = tiefe NO_X-Emissionen

Vorgehen?

1. **Gute Vormischung erreichen**

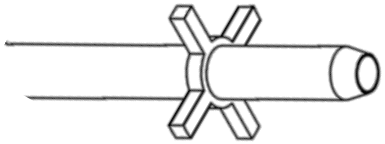
2. **In der Mischstrecke Bereiche mit hoher Turbulenz vermeiden**
   → gegenseitig ausschliessend?

Flashback-Tests: *Eindüsungsvarianten*



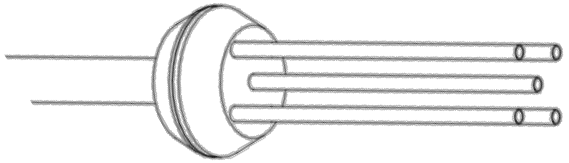
Injector "Lance"

- One injection point
- Injection diam.: variable
- No mixing device



Injector "Cross"

- One injection point
- Injection diam.: 4 mm
- Cross mixing device



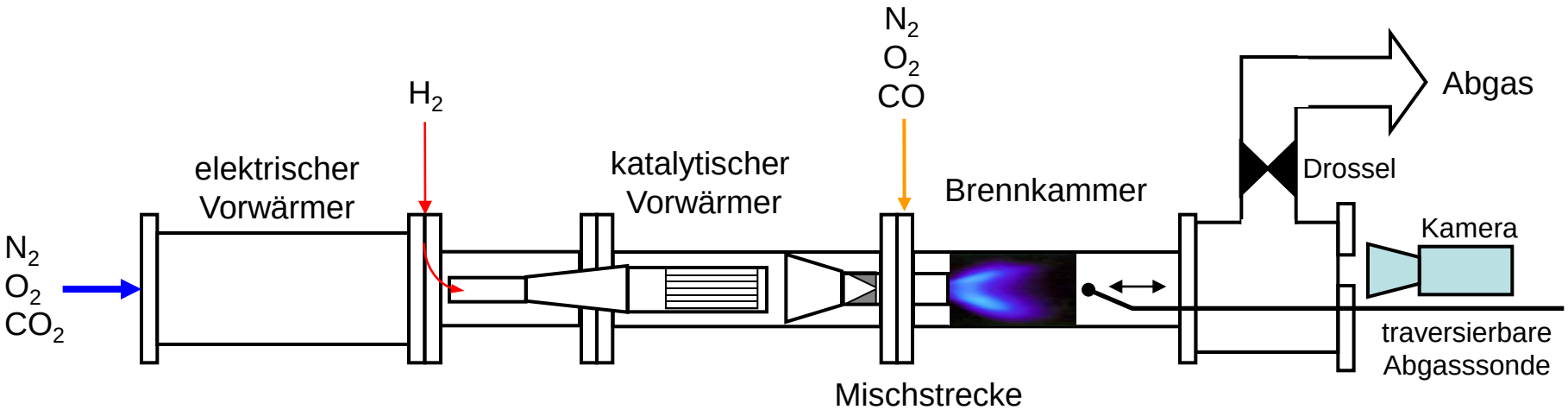
Injector "MA5" (micro axial 5)

- Five injection points
- Injection diam.: 1.65 mm
- No mixing device

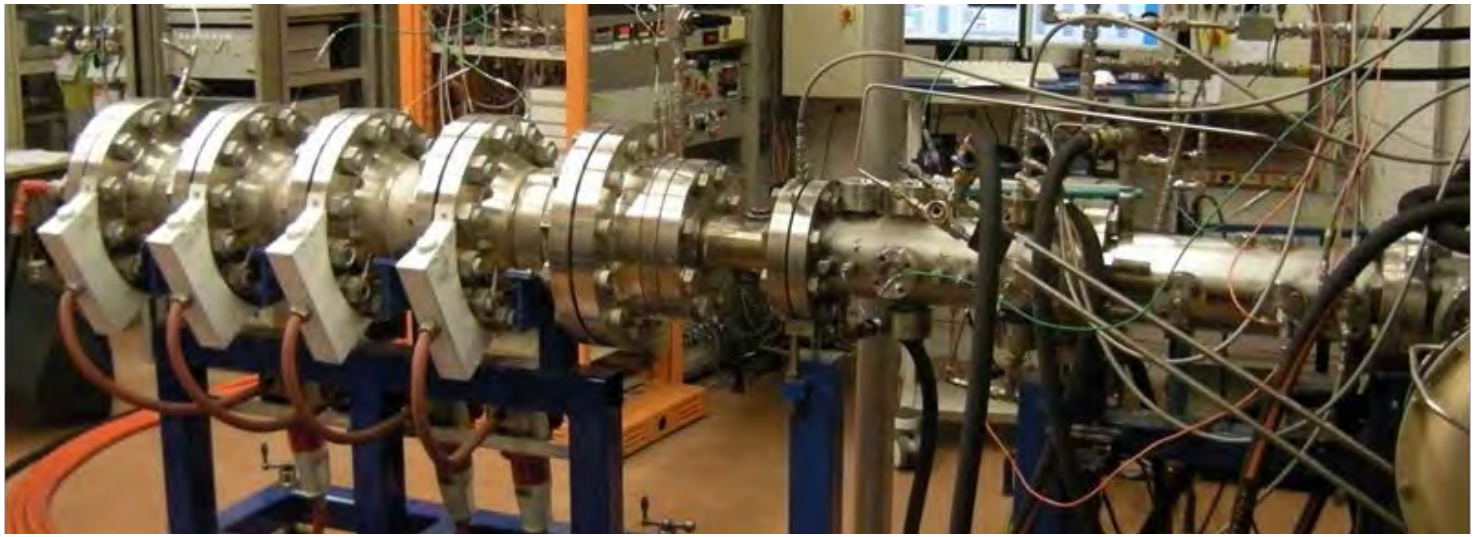
Hochdruck-Prüfstand

Betriebsparameter

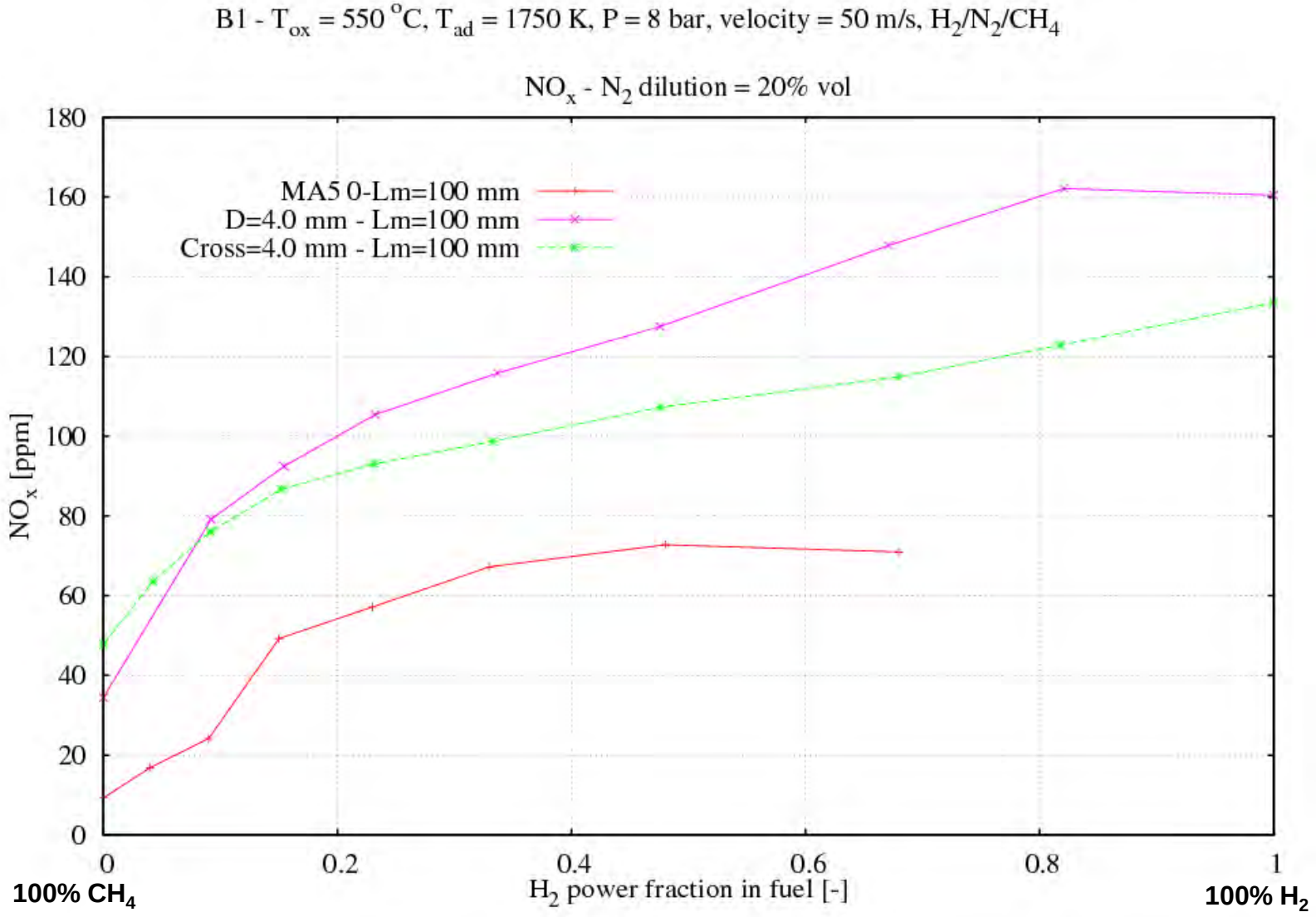
- Maximaler Massenstrom: 180 g/s
- Maximaler Druck: 20 bar
- Maximale thermische Leistung: 200 kW
- Maximale Vorheiztemperatur: 550 °C
- Maximale adiabate Flammentemperatur: 1900 K



Hochdruck-Prüfstand

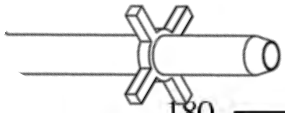


Flashback-Tests: *NOx-Emissionen*



Flashback-Tests: *NOx-Emissionen*

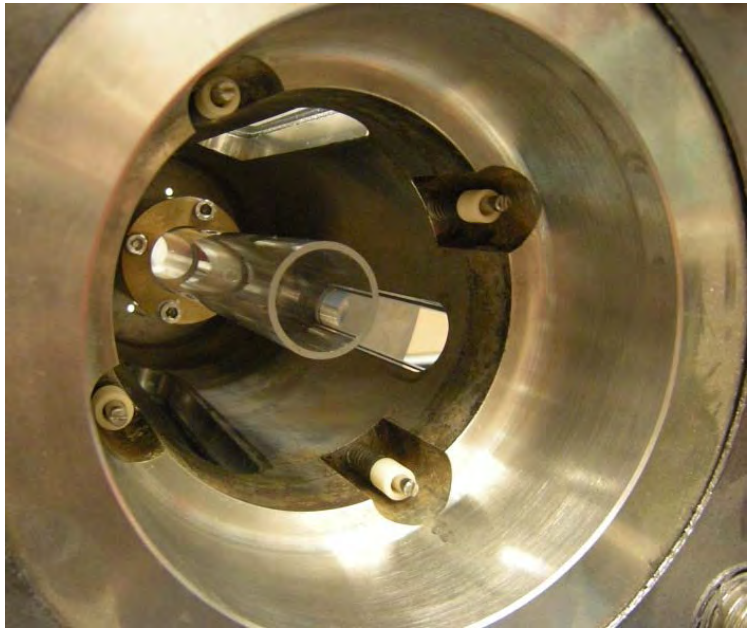
Flashback-Tests: *NOx-Emissionen*



Flashback-Tests: *NOx-Emissionen*

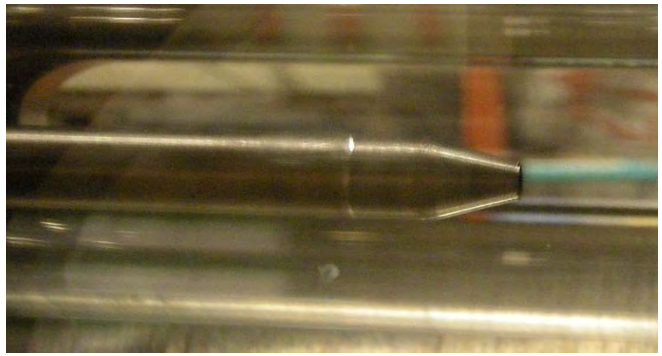
Flashback-Tests: *Versuche mit optischem Zugang*

- **Bedingungen**
  - P = 8 bar
  - U_{ox} = 50 m/s
  - T_{ox} = 550 °C
  - Re_{ox} ≈ 91’000

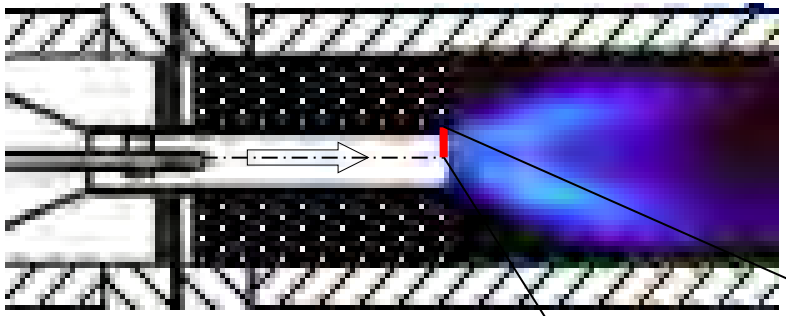


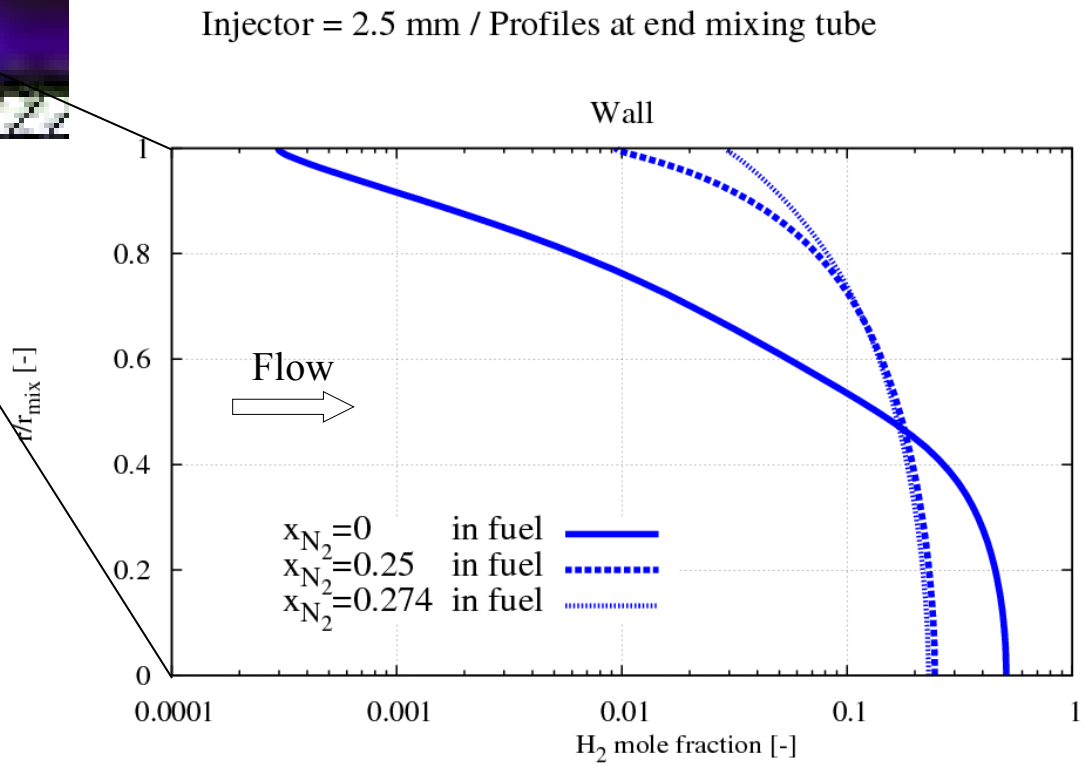
- **Eindüsung (Innen-Ø 2.5 mm)**

Verdünnung mit N_2 um Turbulenz/Mischung zu variieren



Numerische Simulation

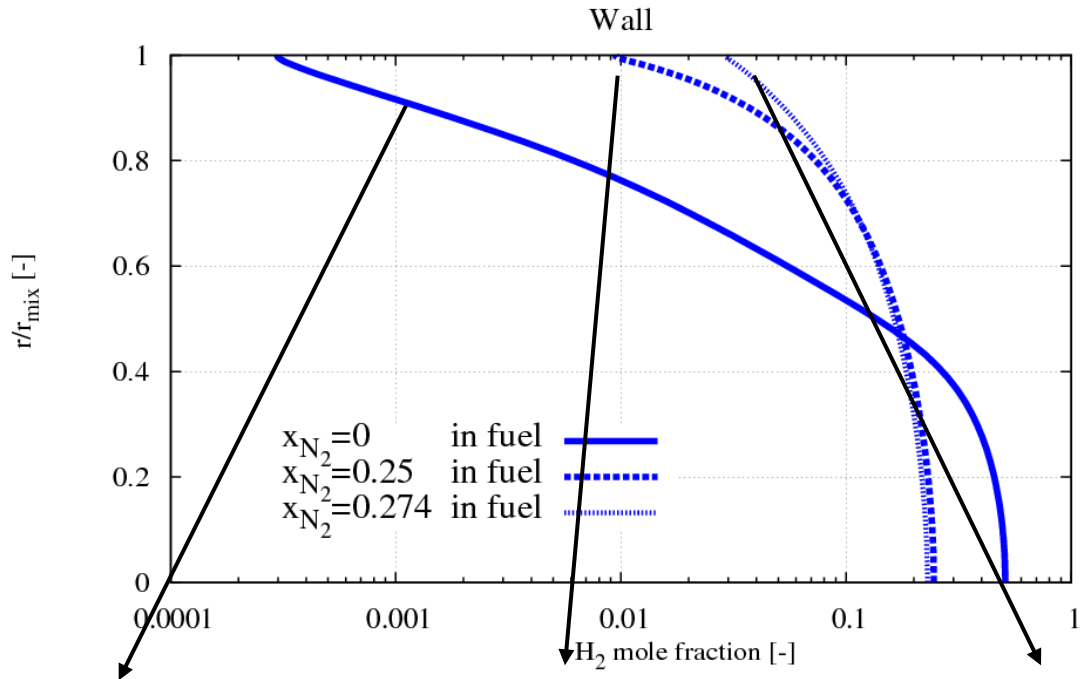




Glass Mixer - T_{ox} = 550 °C, T_{ad} = 1750 K, P = 8 bar, velocity = 50 m/s, H_2/N_2

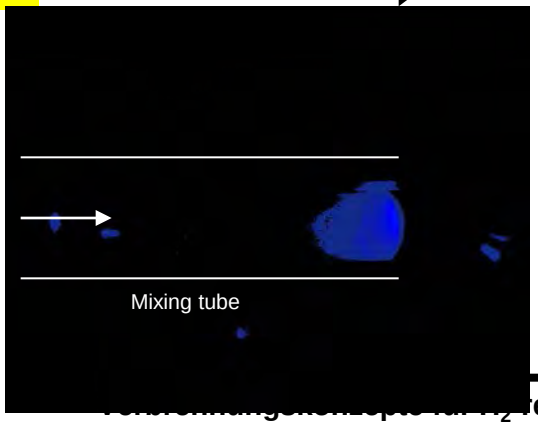
Injector = 2.5 mm / Profiles at end mixing tube

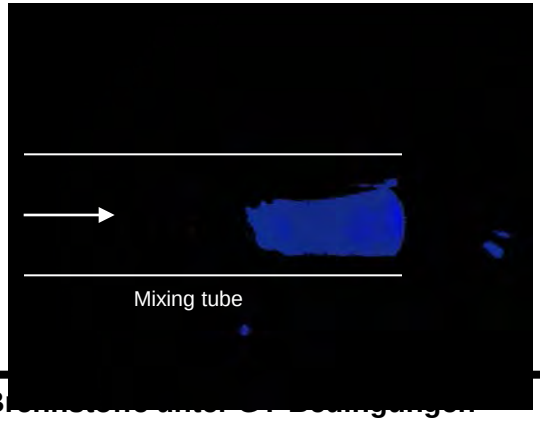
OH*-Chemielumineszenz mit UV-Kamera

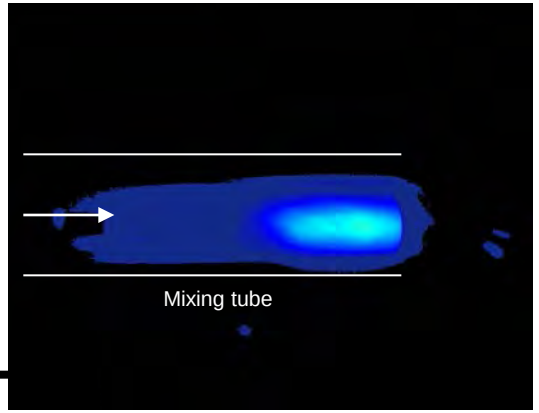


Problem:

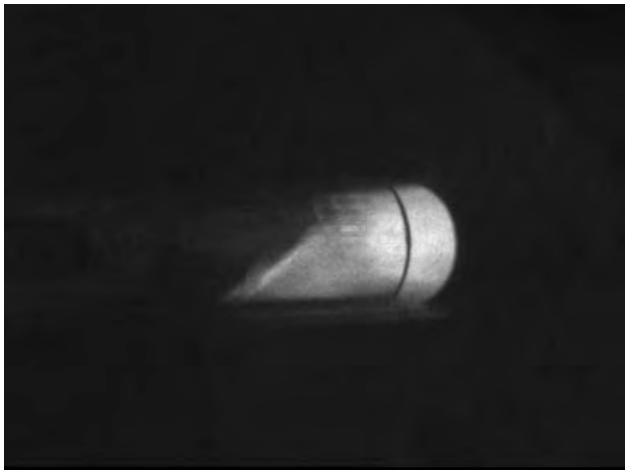
bessere Mischung führt zu höherer Flashbackgefahr



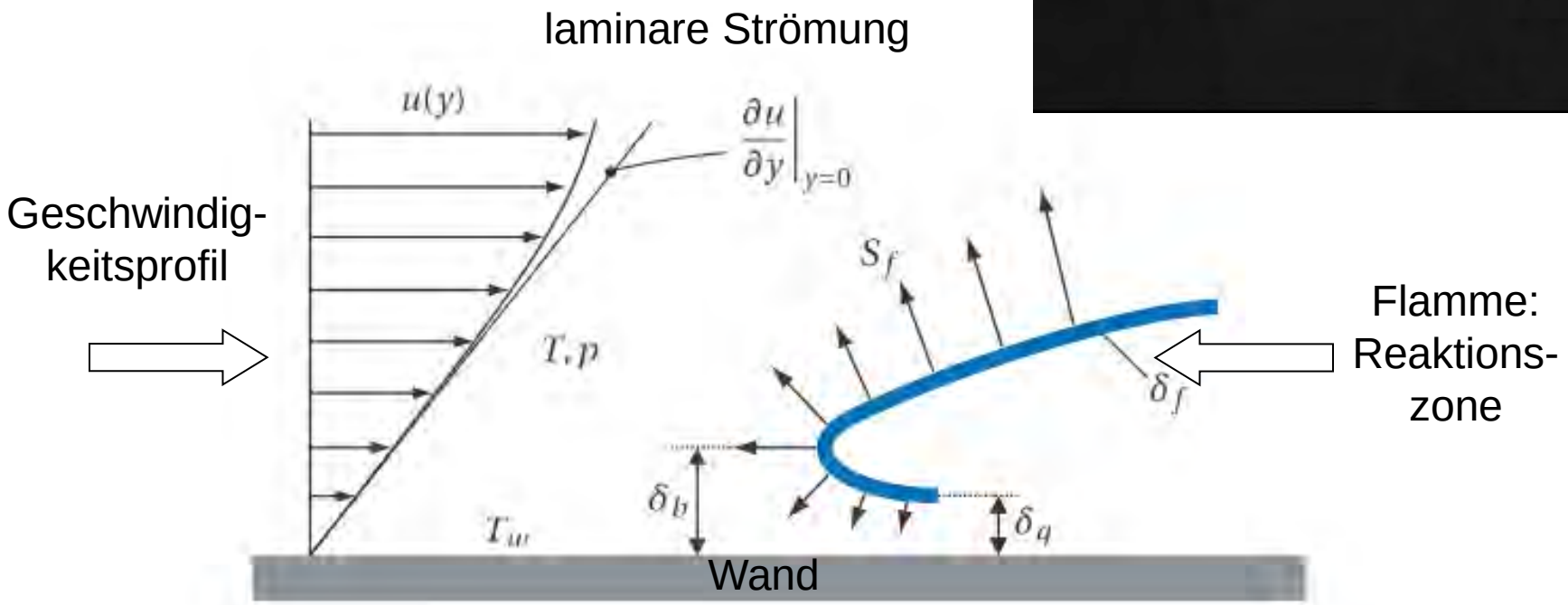




Flashback-Mechanismen



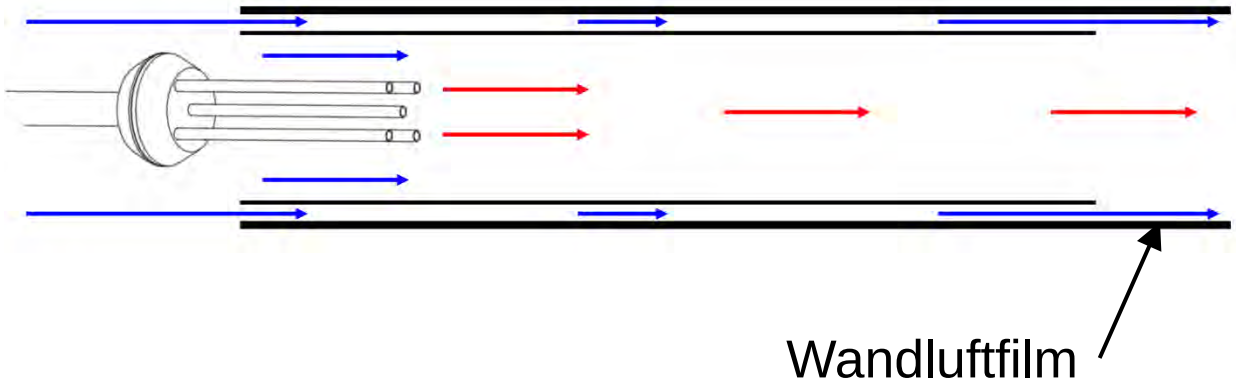
- **Ausbreitung der Grenzschicht**

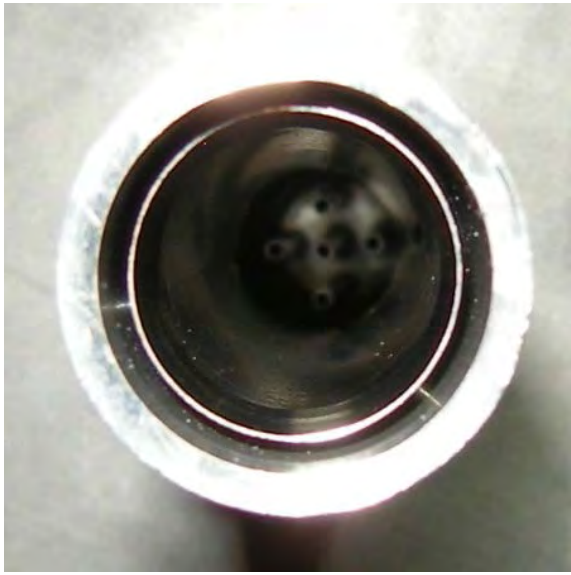


Quelle: Eichler and Sattelmayer, ASME Turbo Expo 2010

Variante zur Minderung der Flashback-Gefahr

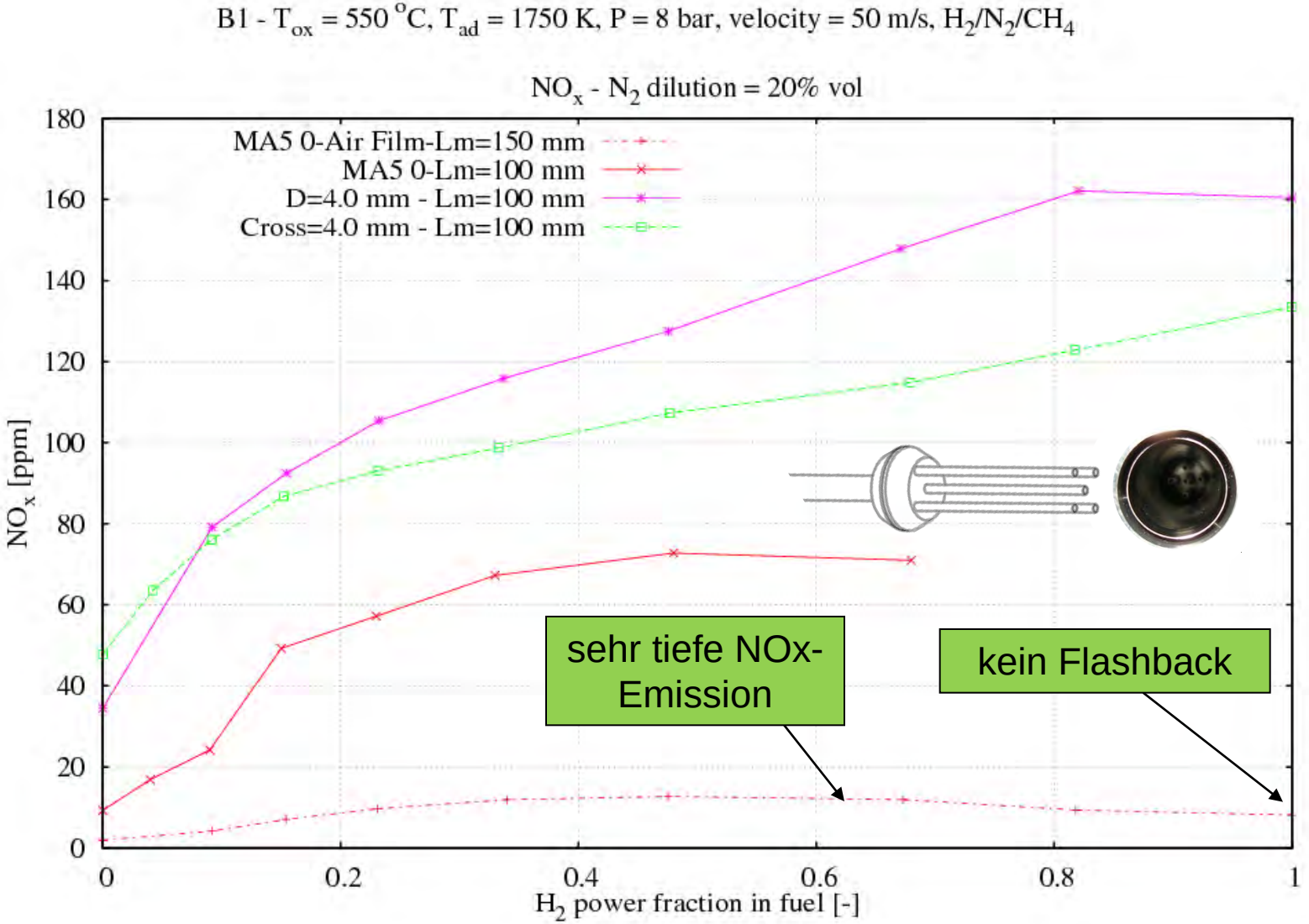
Idee: Mischrohr am Austritt mit einem Wandluftfilm versehen, um Brennstoff von der Wandgrenzschicht fern zu halten





Ausführung

Minderung der Flashback-Gefahr: *Versuche*



Gestuftes Konzept

Ziel: stabile und saubere Verbrennung von Wasserstoff

Stabil = keine/geringe Flashbackgefahr

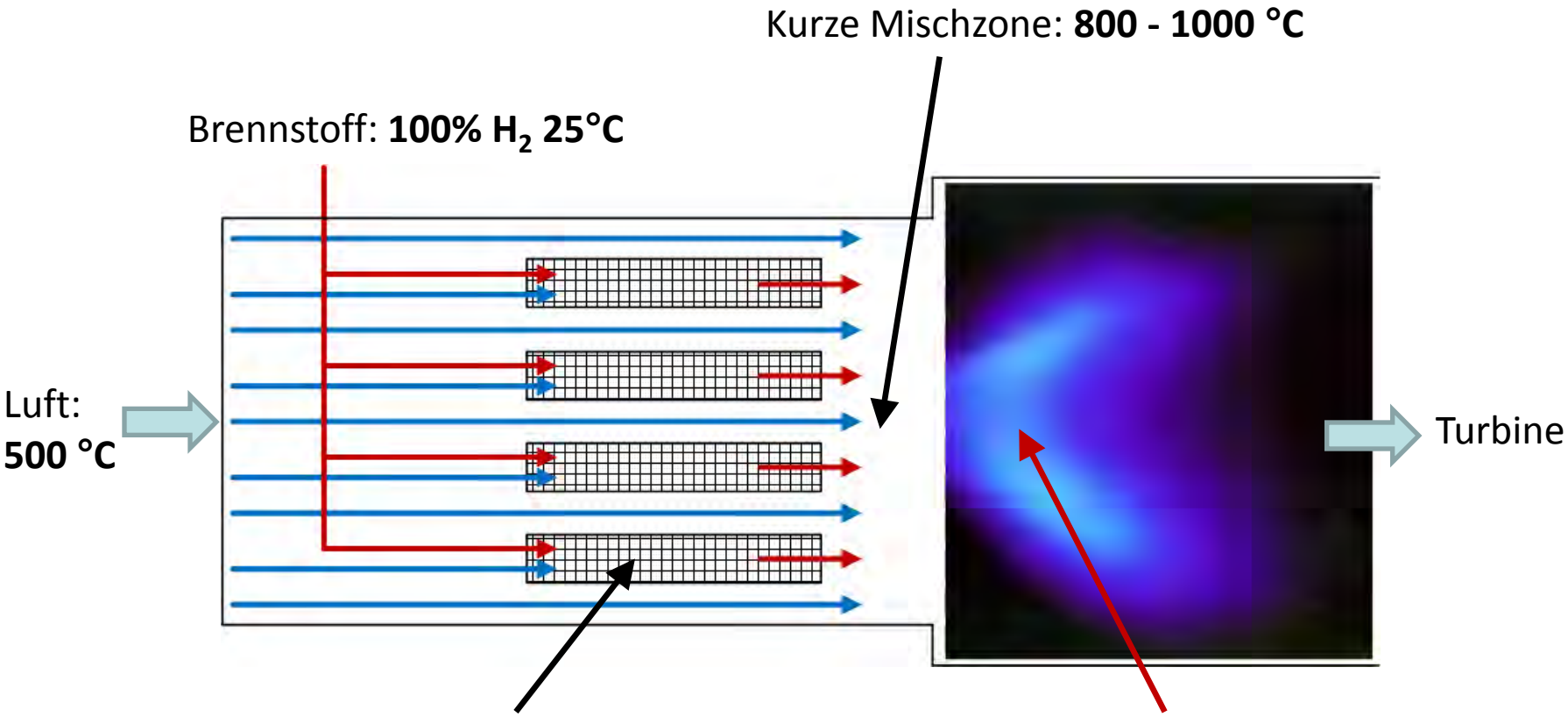
Sauber = tiefe NO_X-Emissionen

Vorgehen?

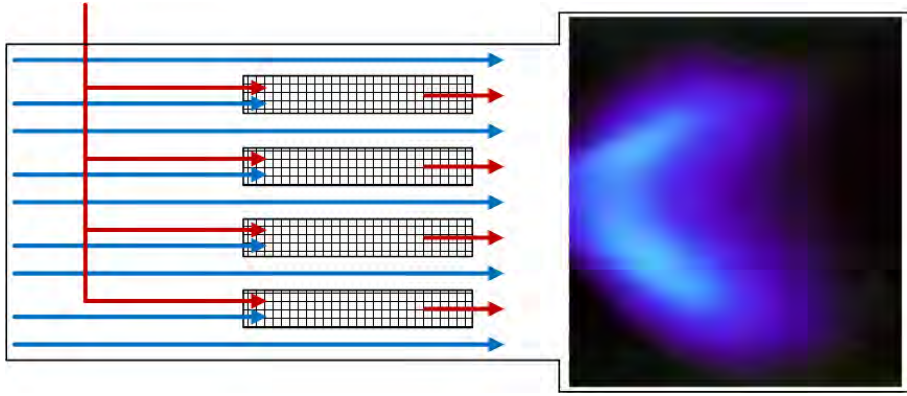
1. **Realisierbarkeit eines gestuften Verbrennungskonzept untersuchen → «In-situ Verdünnung» erzeugen**

2. **Versuche durchführen mit verschiedenen Umsätzen in der Vorstufe**

Gestuftes Verbrennungskonzept



Vorteile

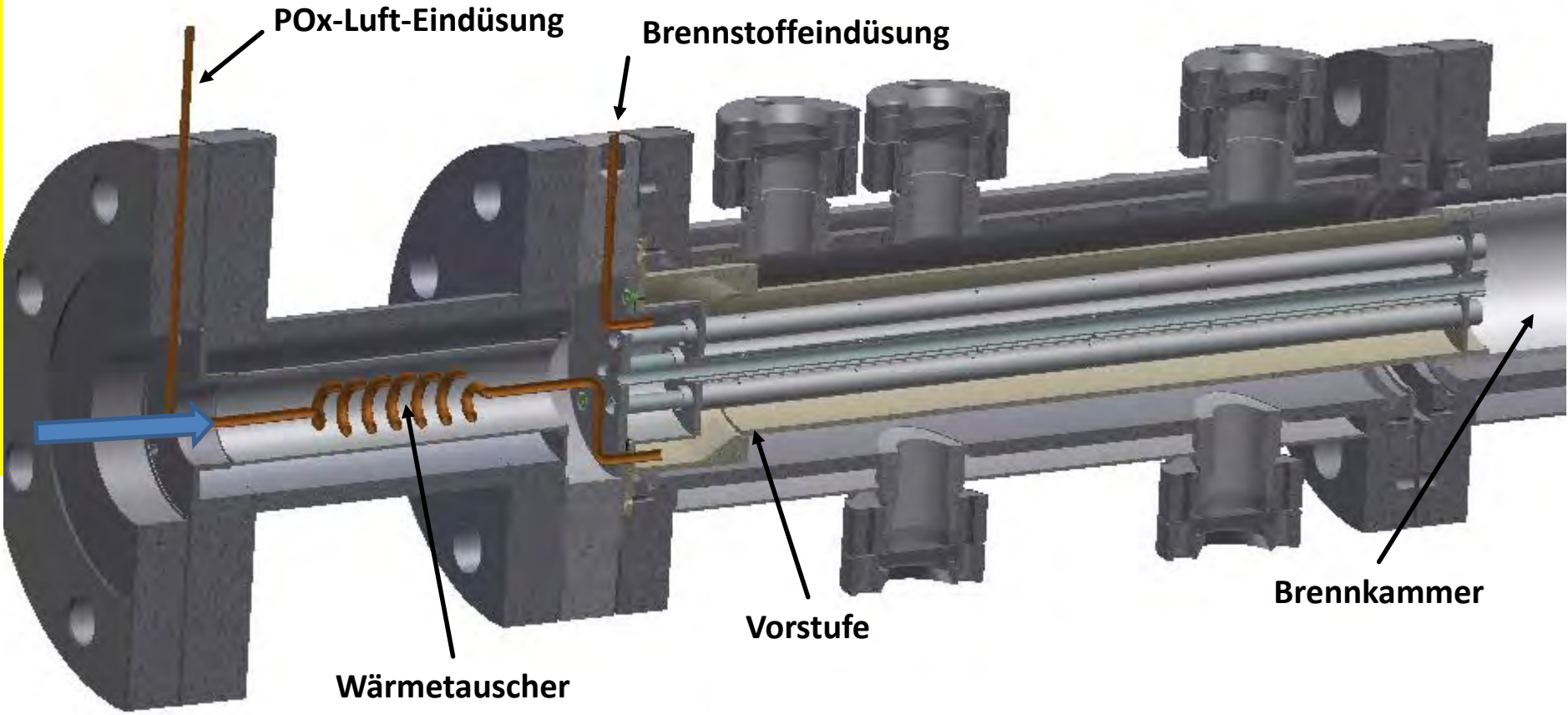


- Rohrbündel ermöglicht eine verteilte Eindüsung.
- Wegen der Vorreaktionen in der ersten Stufe ist eine **geringere Brennstoffkonzentration** in der Brennkammer vorhanden.
- Die in der ersten Stufe freigesetzte Enthalpie wird durch Wärmetausch zwischen den Kanälen gleichmässig verteilt.
- Am Austritt der ersten Stufe ist der Wasserstoff **mit Stickstoff und Wasserdampf verdünnt** und somit stark entschärft.

λ_{POx} [ ]	H_2 [Vol%]	N_2 [Vol%]	H_2O [Vol%]
0.5	26	48	26

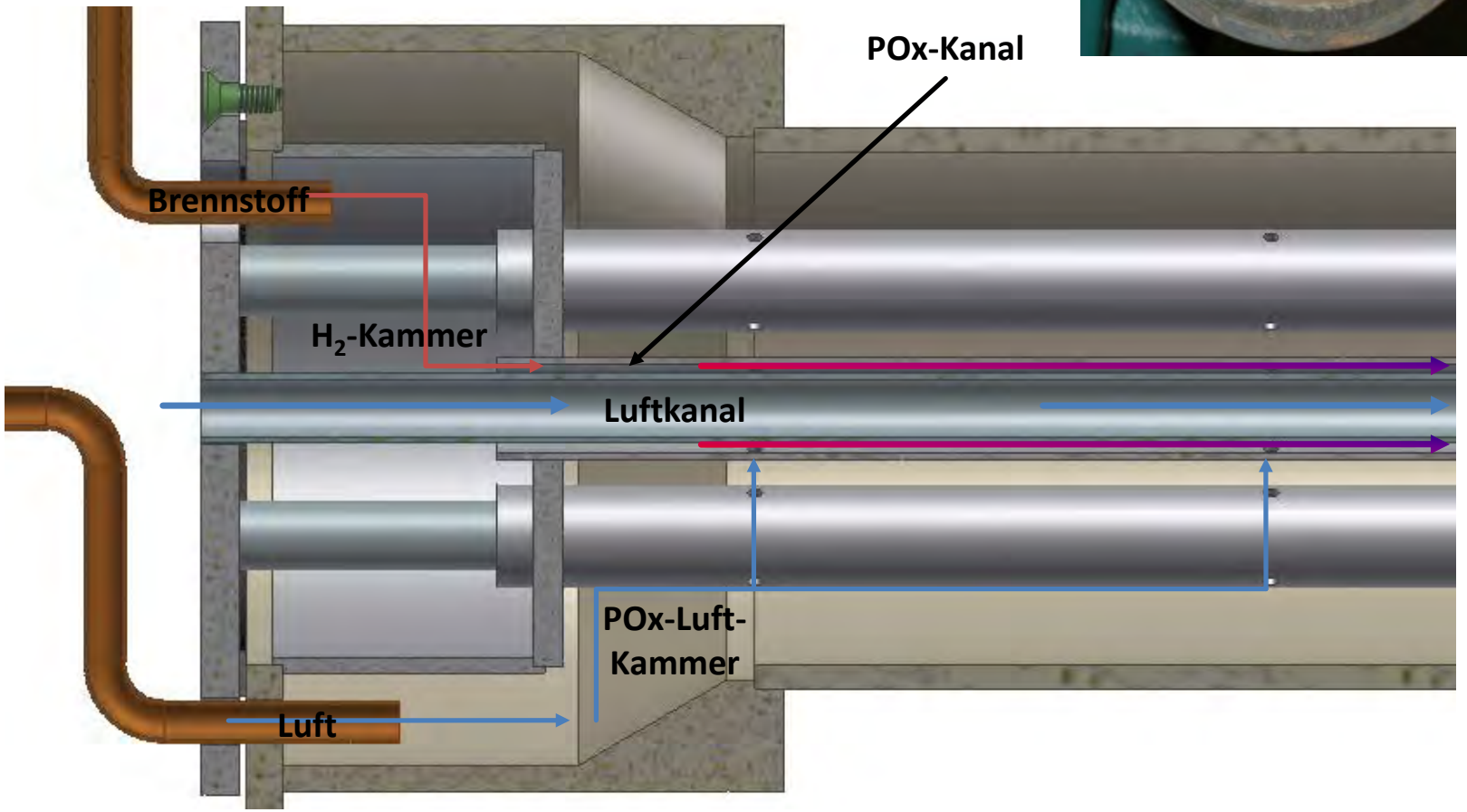
Der Brenner

- POx-Luft wird separat zugeführt, um Bedingungen besser steuern zu können.
- Im Brenner: 7 Rohre mit katalytischer Beschichtung.



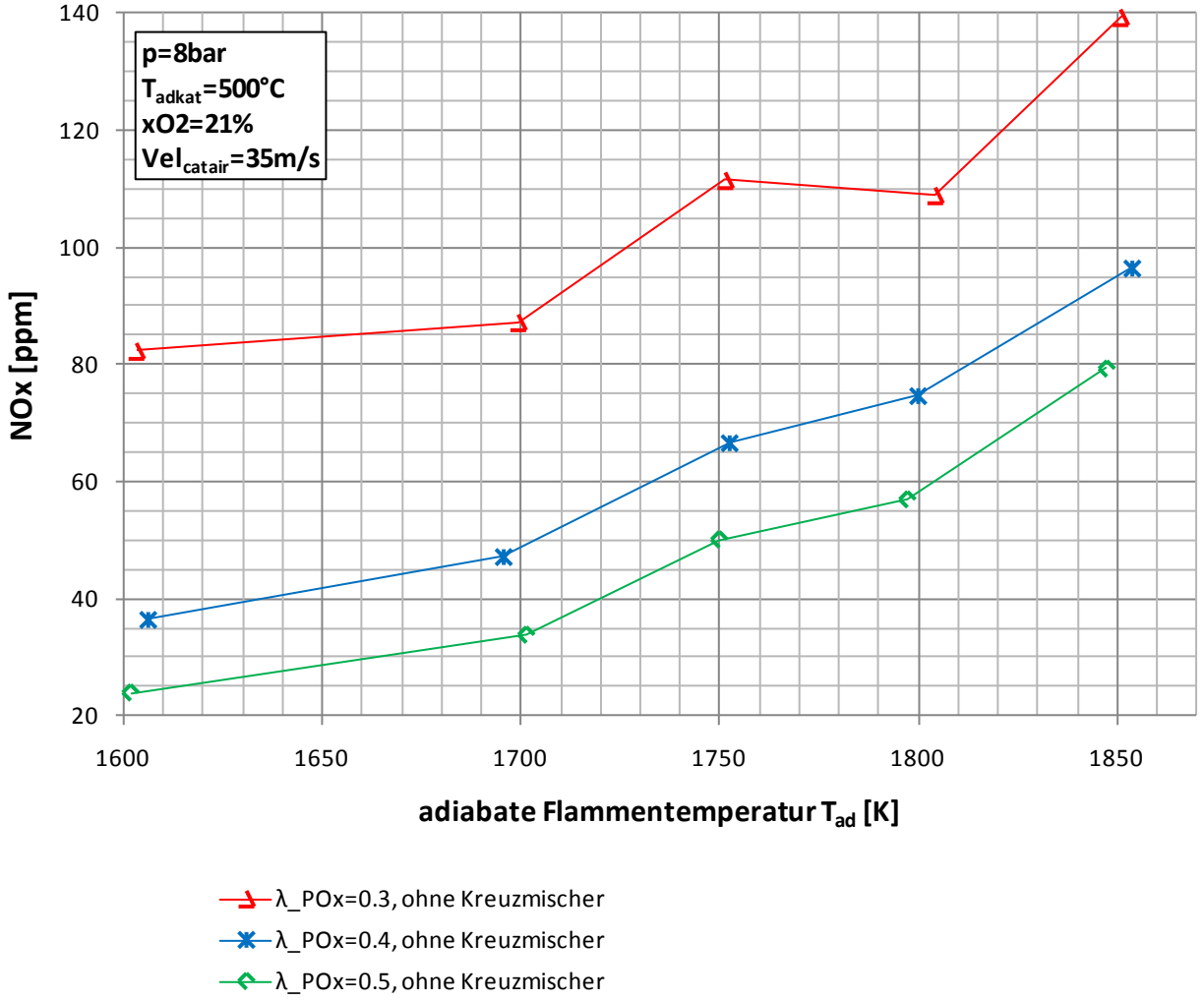
Der Brenner: *Kanäle*

- „Rohr im Rohr“ Struktur
- Luftkanal: Kühlung
- POx-Kanal: bis zu 50% Brennstoffumsatz



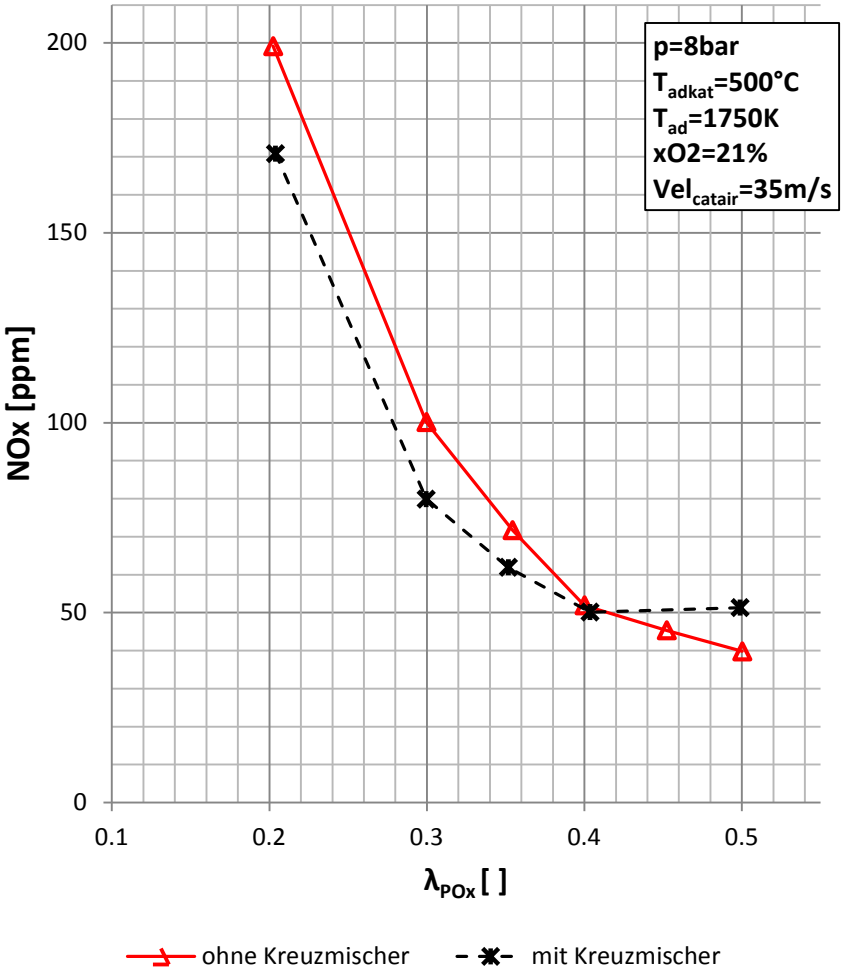
Messergebnisse: *NOx-Emission*

- Bei theoretisch 30, 40 und 50% Umsatz im POx-Kanal



Messergebnisse: *NOx-Emission*

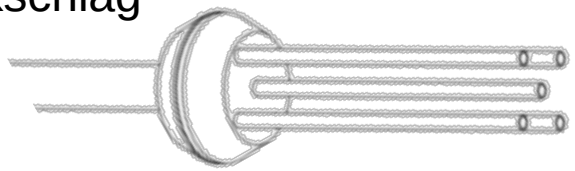
- Bei $\lambda_{POx} = 0.5$ (ohne Kreuzmischer) nur 40 ppm NOx



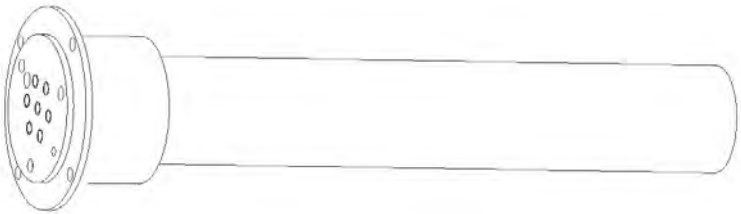
Fazit

Bei 8 bar Druck, 1750 K adiabater Flammentemperatur und 500 - 550 °C Luft-Eintrittstemperatur wurden folgende Ergebnisse erzielt:

1. **MA 5 mit Wandluftfilm**
   - 80% H_2 und 20% N_2 → 10 ppm NOx ohne Rückschlag
   - 100% H_2 mit erhöhter Rückschlaggefahr



2. **Gestuftes Konzept**
   - 100% H_2-Verbrennung ohne Rückschlag möglich
   - NOx sinkt mit steigendem Umsatz in der 1. Stufe
   - < 50 ppm NOx möglich in einem Konzept ohne Vormischung



Ausblick

1. **Konzept mit Wandluftfilm**
   - Verbesserung des Konzepts, so dass mit 100% H_2 bei guter Vormischung tiefe NOx-Emission bei gleichzeitig geringem Flashback-Risiko erreicht werden

2. **Gestuftes Verbrennungskonzept**
   - Mischung der Brennstoffmischung aus der ersten Stufe mit der Restluft verbessern
   - Untersuchen, ob auf Verwendung des Katalysators verzichtet werden kann
   - Integration der beiden Konzepte?

Danksagung

- **Swisselectric Research**
- **Bundesamt für Energie (BFE)**
- **Alstom (Schweiz)**

PAUL SCHERRER INSTITUT

PSI

Wir schaffen Wissen – heute für morgen

Paul Scherrer Institut
Marco Schultze

Catalytic combustion of fuel-rich hydrogen/air mixtures

EU Project H_2-IGCC

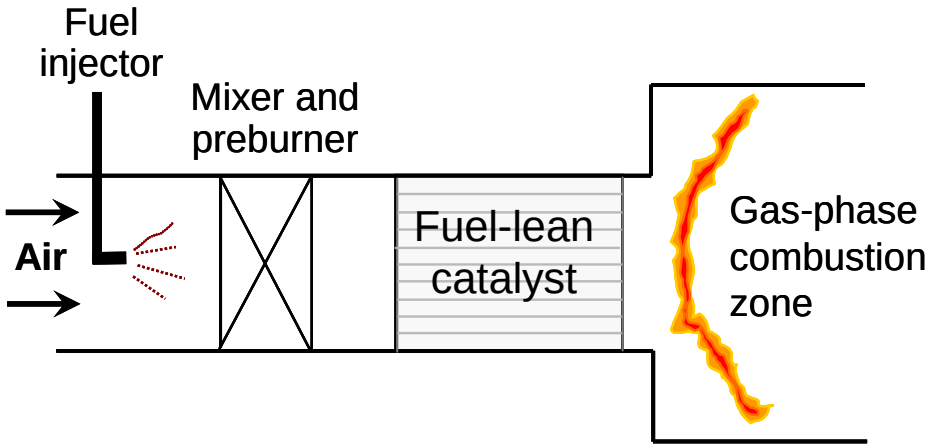
H_2IGCC Energy without CO_2

Outline

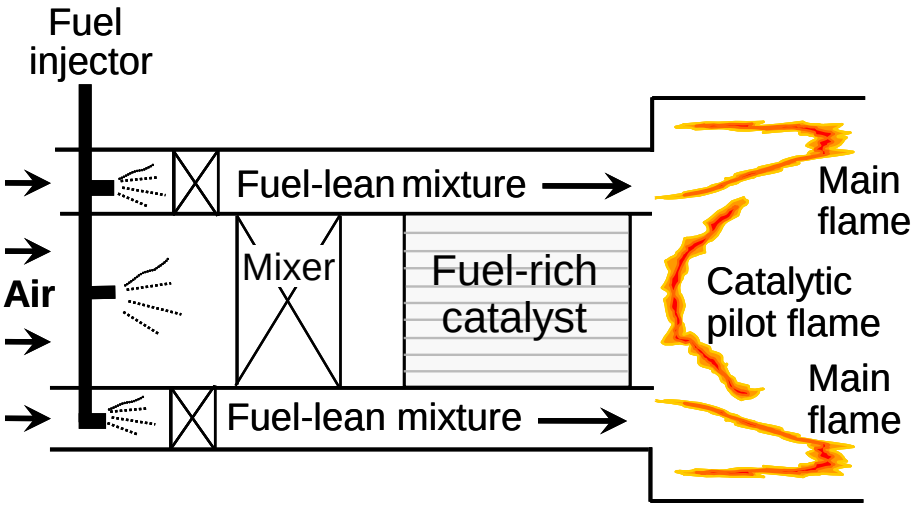
- Motivation / objectives
- Method of approach
  - Experimental
  - Numerical
- Results
  - Catalytic conversion
  - Homogeneous ignition
- Conclusions / outlook

Motivation: Lean versus rich combustion of hydrogen

(a) Fuel-lean combustion (conventional)



(b) Fuel-rich combustion (newer concept)

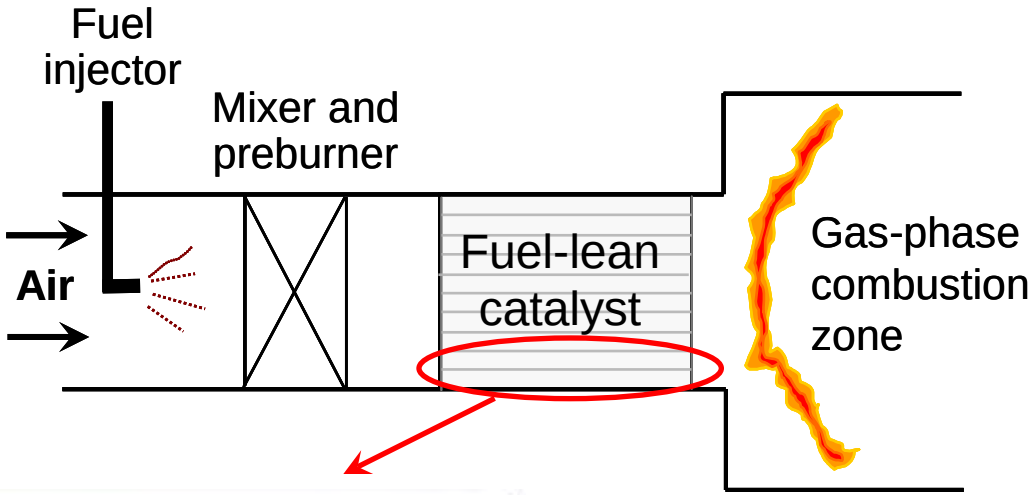


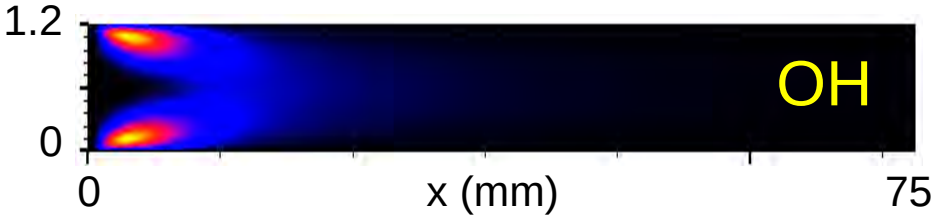
for natural gas:

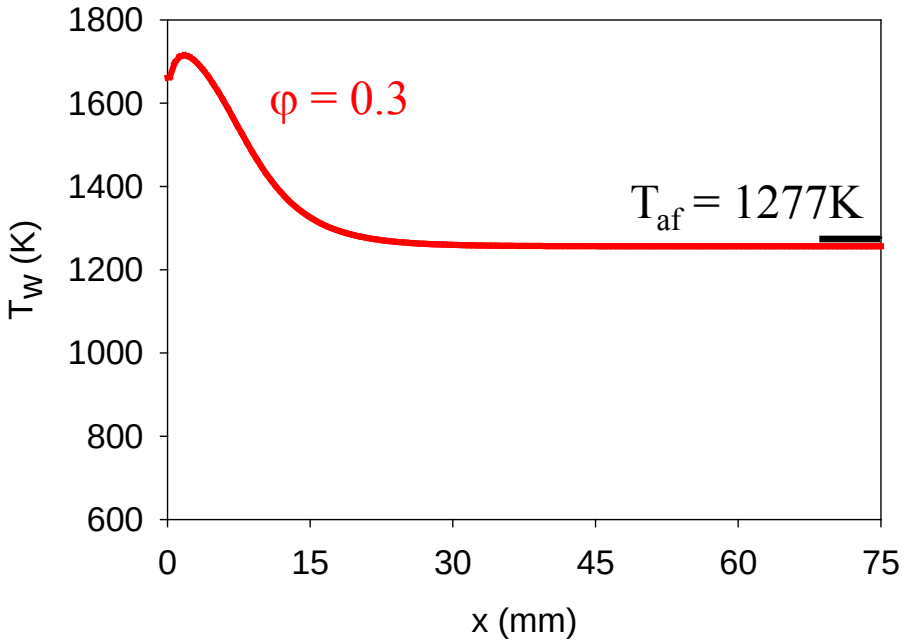
- Light-off easier
- Better control of homogeneous combustion

Motivation: Lean versus rich combustion of hydrogen

Fuel-lean combustion concept





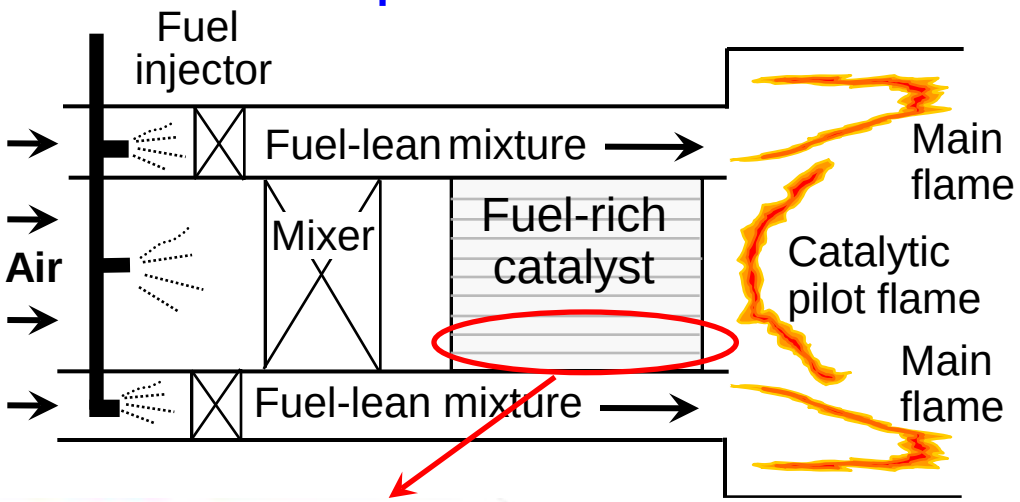


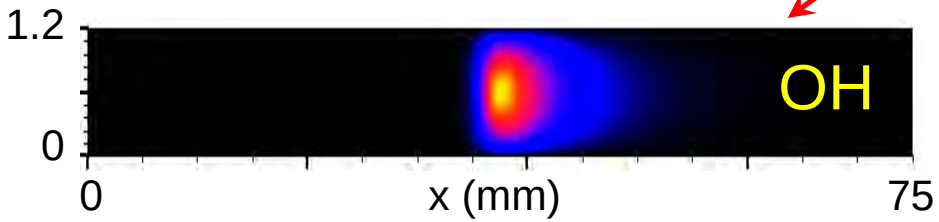
$T_w = T_{in} + (\Delta T)_c \, Le^{-1/3}$

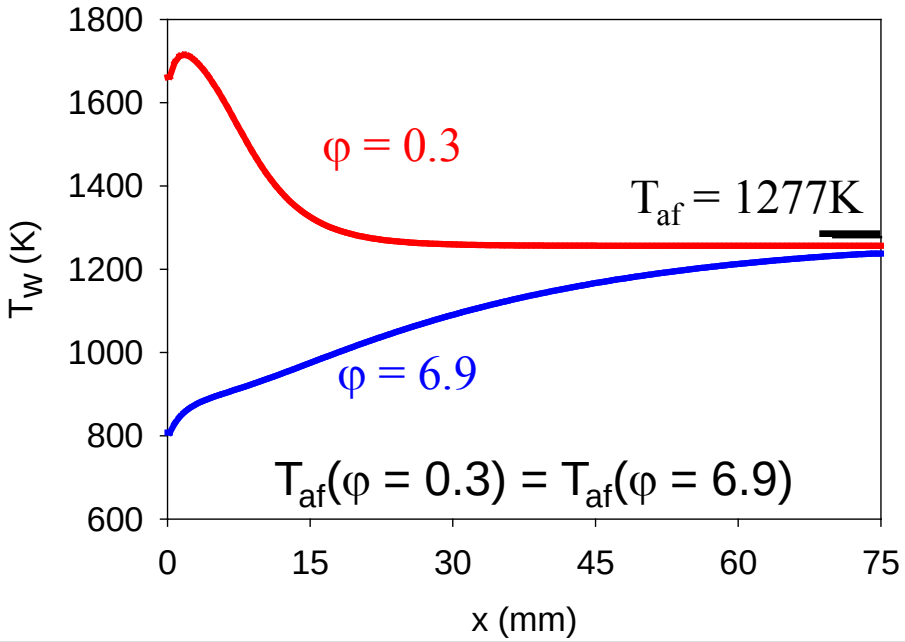
$Le_{H2} \sim 0.3$ for lean H_2/air

Motivation: Lean versus rich combustion of hydrogen

Fuel-rich combustion concept







$T_w = T_{in} + (\Delta T)_c \, Le^{-1/3}$

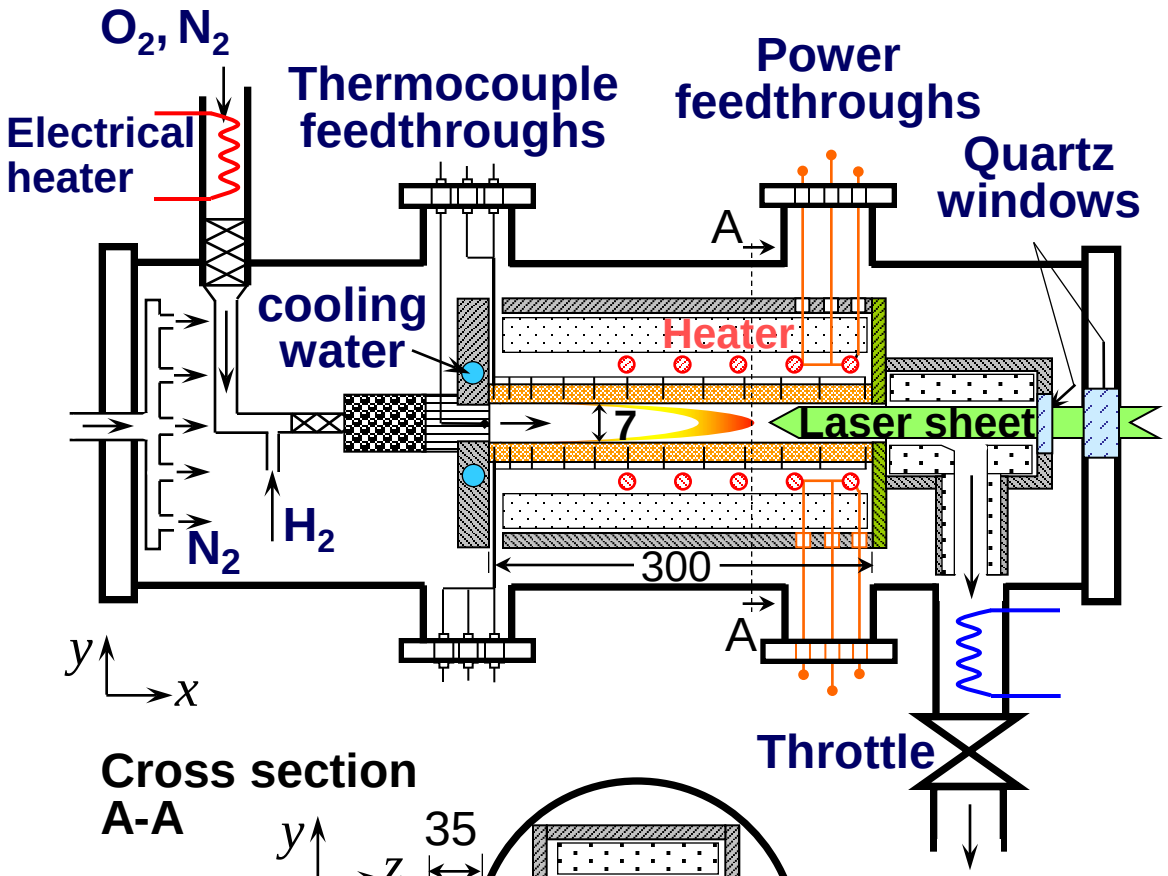
$Le_{O2} \sim 2.0$ for rich H_2/air

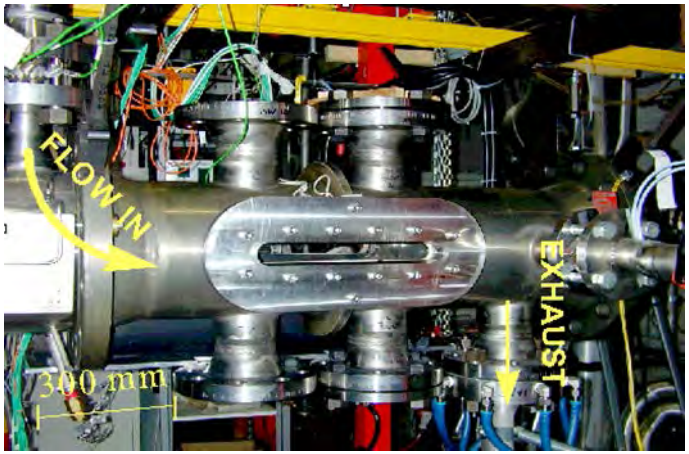
Objectives

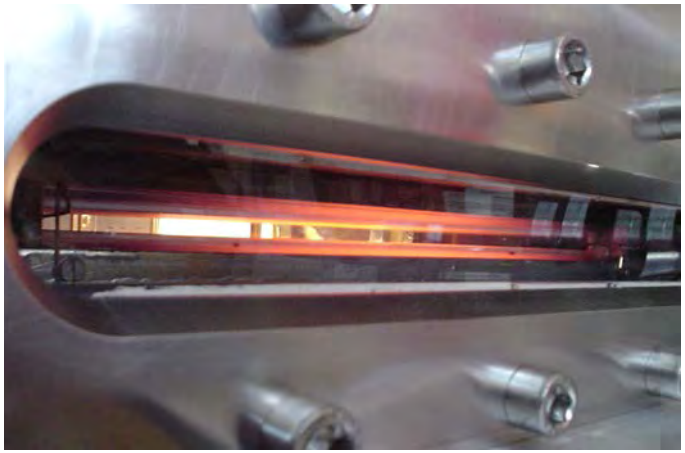
- Assess applicability of hetero-/homogeneous chemical reaction schemes in fuel-rich ($2 < \varphi < 7$) combustion of H_2/air on platinum
- Determine conditions leading to onset of homogeneous ignition
- Investigate catalytic processes upstream of homogeneous ignition
- Assess reactor thermal management issues at fuel-rich conditions
- Investigate hetero-/homogeneous chemistry coupling
- Compare fuel-lean and fuel-rich combustion concepts

Experimental: high-pressure, optically accessible, catalytic channel flow reactor

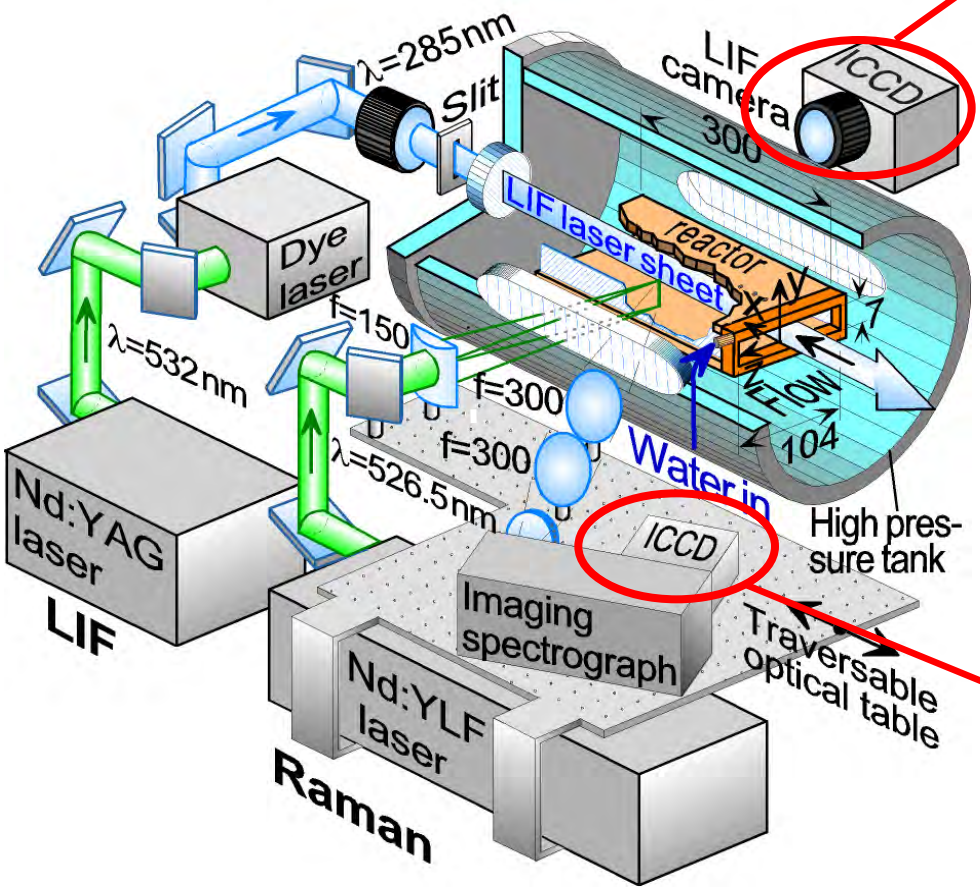
p < 20 bar

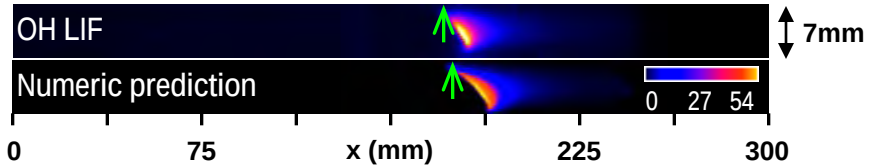






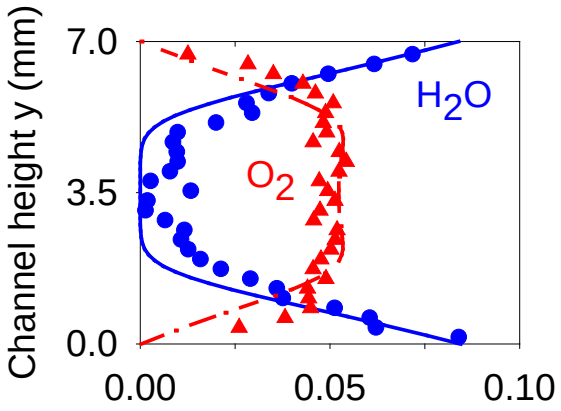
Experimental: in situ laser measurements





H_2-rich combustion

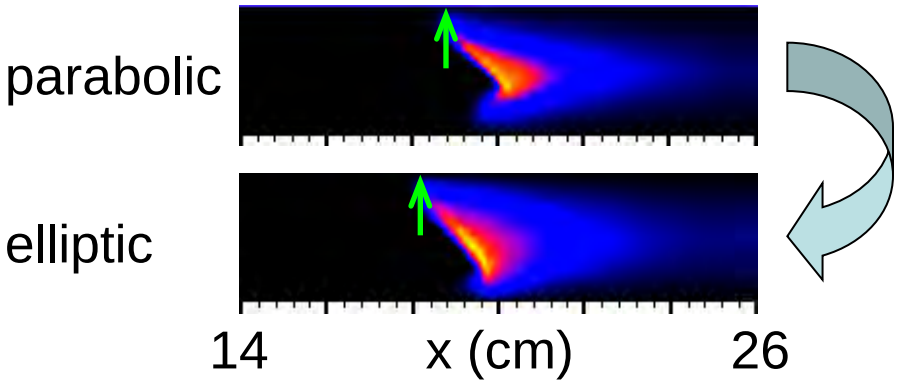
H_2-rich combustion



Appel, Mantzaras et al., CNF 128, 2002;
Reinke et al., CNF 136, 2004; CNF 141, 2005
Ghermay, Mantzaras et al., PCI 33, 2011

Numerical approach

- 2-D parabolic (boundary layer) code
  - for initial guess to full elliptic code runs
- 2-D elliptic (Navier Stokes) code
  - Finite volume approach
  - Mixture-average species transport
  - Prescribed wall temperature as energy boundary condition (TE measurements)



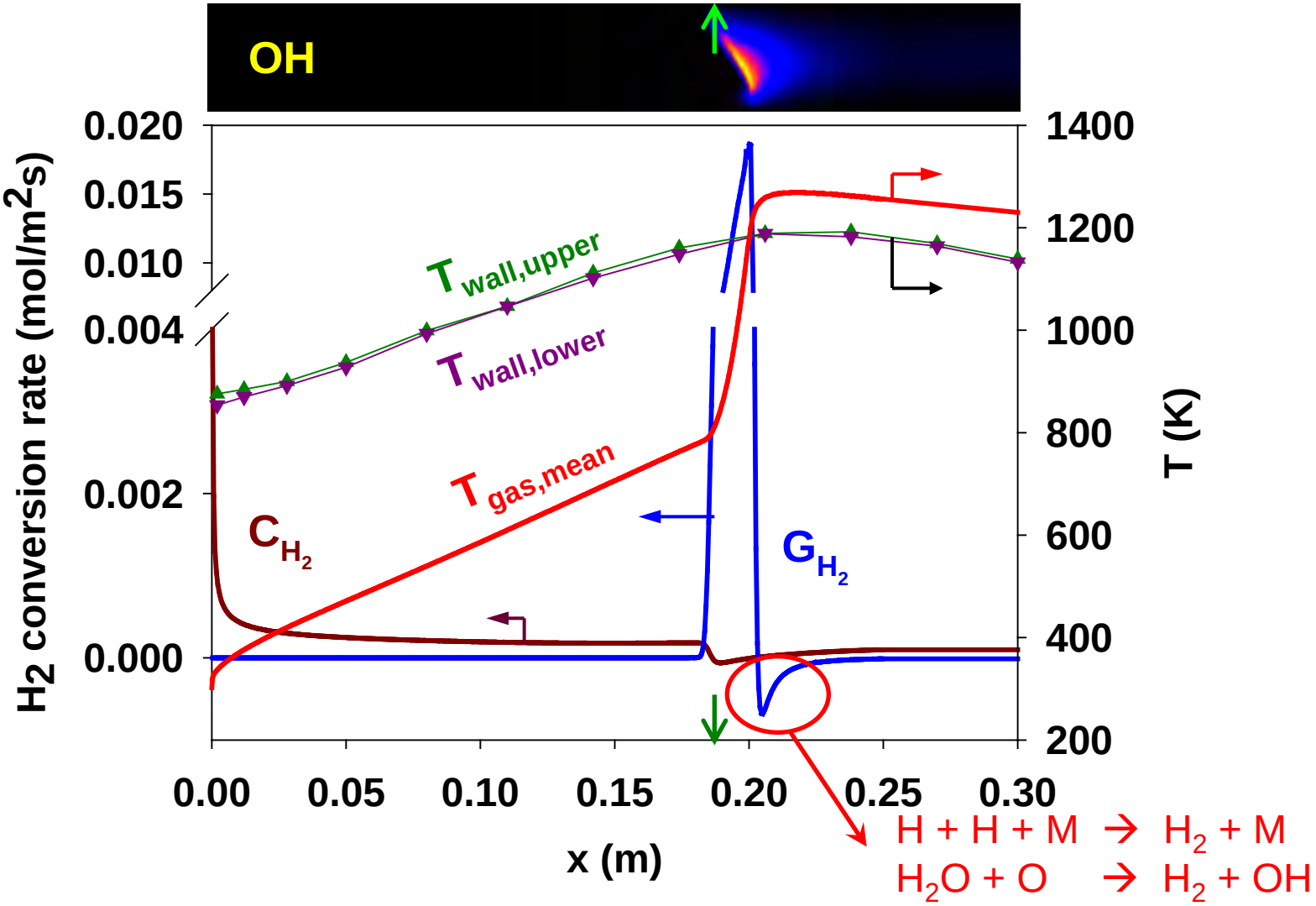
- Detailed heterogeneous chemical reaction scheme
  - Deutschmann et al., 2000
    - 11 irreversible and 3 reversible reactions
    - 5 surface and 6 gaseous reactions
- Elementary gas-phase reaction scheme
  - Li et al., 2004 (Princeton mechanism)
    - 21 reversible reactions
    - 9 species

Appel, Mantzaras et al., CNF 128, 2002
Karagiannidis, Mantzaras et al., PCI 31, 2007; 32, 2009
Ghermay, Mantzaras et al., PCI 33, 2011

Experimental conditions

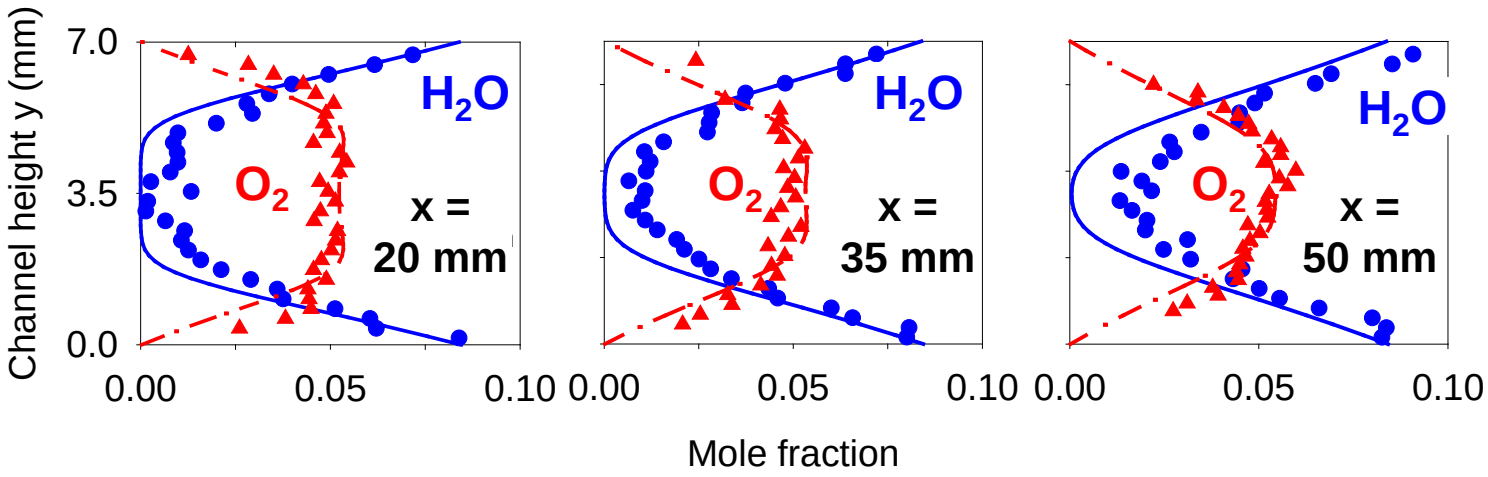
Fuel-to-air equivalence ratio:	φ = 2.0 ... 7.0
Pressure:	p = 1.0 ... 5.0 bar
Inlet temperature:	T_{in} ~ 300 K
Inlet velocity:	u_{in} ~ 4.8 ... 0.8 m/s
Inlet Reynolds number:	Re_{in} ~ 1200 ... 1400

Numerical predictions (φ = 6.0; p = 1bar)



Results: catalytic conversion

- catalytic conversion of deficient reactant is mass transport limited
  - p = 5.0 bar; φ = 6.5



Mass transport limited catalytic conversion of limiting reactant (O_2), captured by the catalytic mechanism

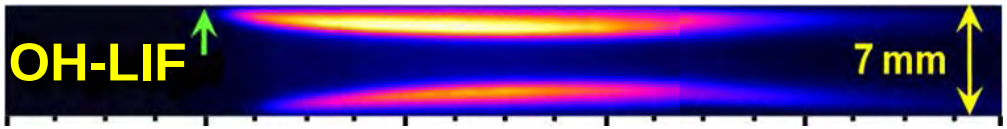
Results: homogeneous ignition

(a) LIF measurements and (b) numerical prediction

p = 1bar

φ = 2.0

Fuel-lean combustion



Mantzaras, Bombach, Schaeren, PCI 32, 2009

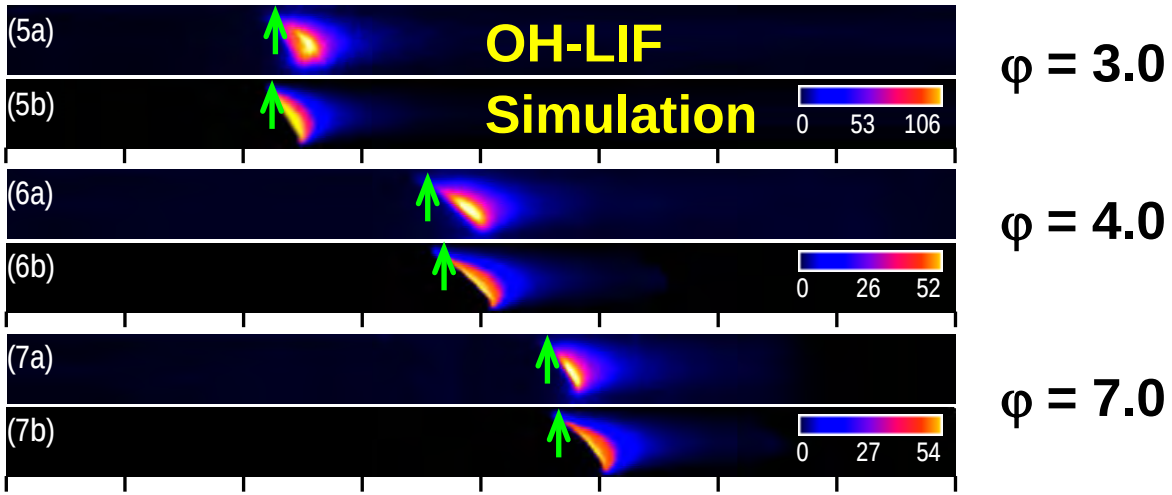
→ Implications on reactor thermal management

Employed schemes capture onset of homogeneous ignition

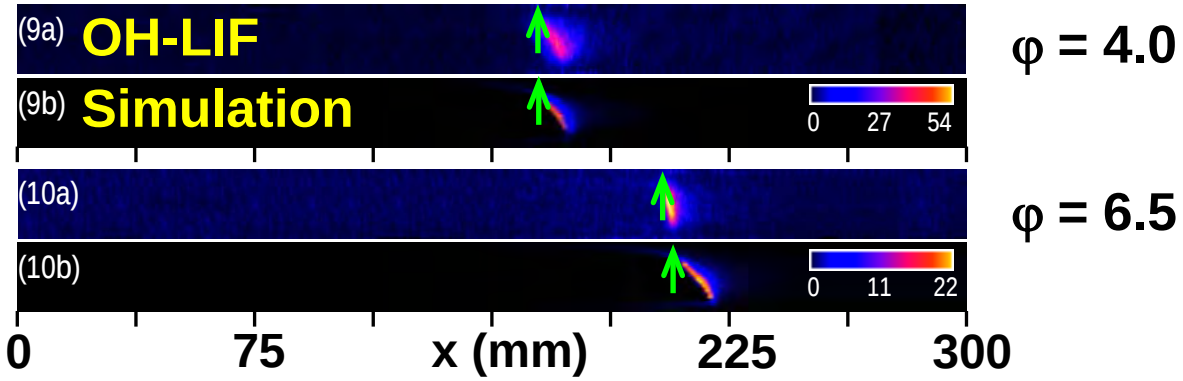
Results: homogeneous ignition

LIF measurements (a) vs. numeric prediction (b)

p = 2 bar



p = 5 bar



Conclusions

- Experimental investigation of catalytic combustion of fuel-rich H_2 mixtures over Pt: LIF and Raman measurements at moderate pressures completed
- Hetero-/homogeneous chemical reaction schemes are suitable for rich catalytic combustion at atmospheric pressure and microreactor-relevant pressures
- Good prediction of homogeneous ignition and upstream catalytic conversion
- Structure of rich flames markedly different from lean flames; implications for reactor thermal management

Outlook

- Investigate pressures up to 15 bar
- Investigate coupling of heterogeneous and homogeneous pathways
- Influence of catalytically produced H_2O on homogenous reactions
- Extend investigations to syngas fuels

Acknoledgements

I. Mantzaras, R. Bombach, R. Kaufmann, K. Boulouchos

Einsatz von 3D-CFD Simulationen

zur Optimierung des Verbrennungssystems und zur Gestaltung des Abgasstranges von Off-Road Dieselmotoren

Tagung „Verbrennungsforschung in der Schweiz“

ETH Zürich, 28.10.2011

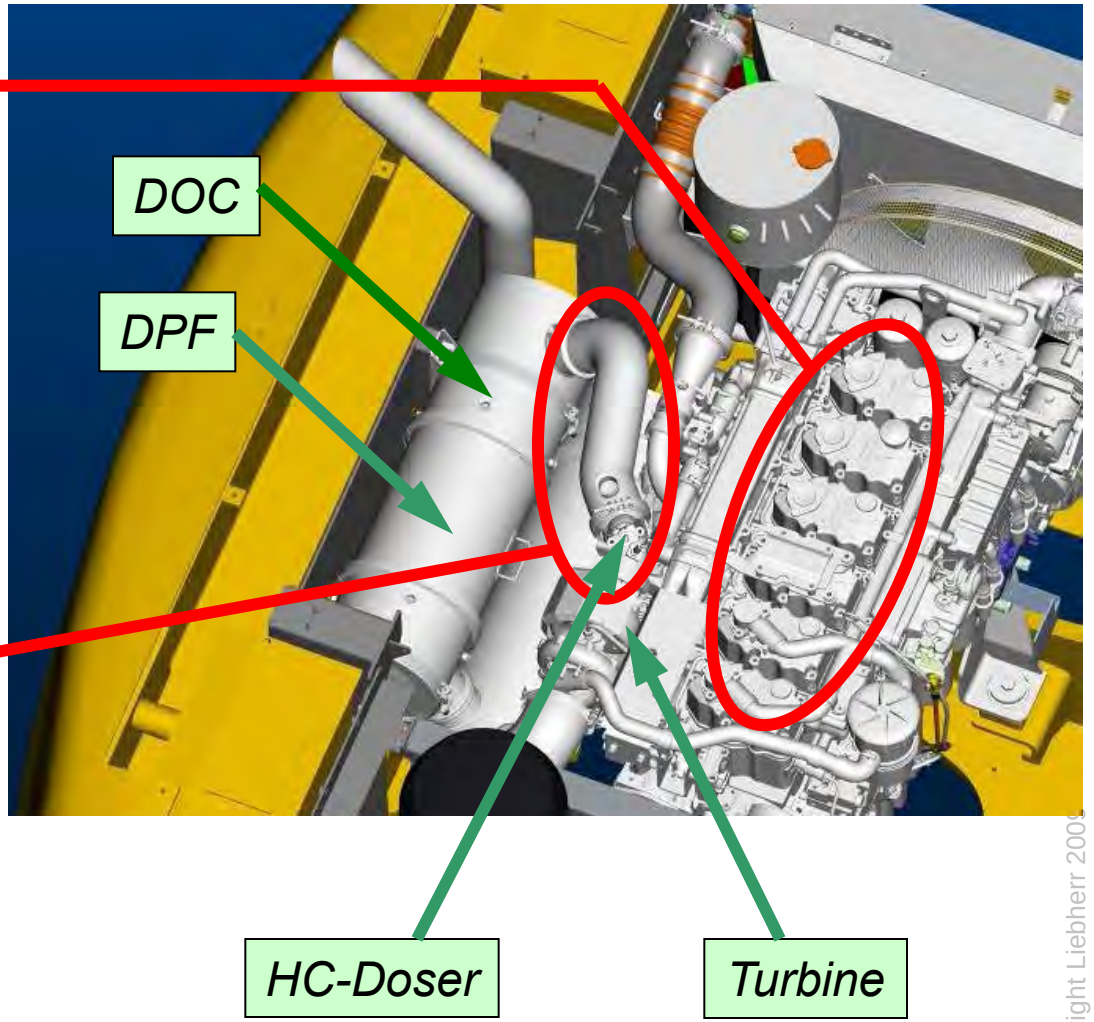
Inhalt

- **Einführung**
- **Verbrennungsentwicklung**
  - Überblick
  - Modellierung Spray und Verbrennung
  - Ergebnisse
- **HC-Eindüsung**
  - Motivation
  - Experimentelle Validierung
  - Ergebnisse
- **Zusammenfassung**

Einführung

- **CFD Ziel 1:**
  Optimierung Verbrennungsparameter
  - Kolbenmulde
  - Einspritzdüse
  - Einspritzverlauf
  - Drallniveau
  - Verdichtungsverhältnis

- **CFD Ziel 2:**
  Design Abgasrohr
  - Optimierung HC-Uniformität vor DOC
  - Minimierung Wandfilmregionen



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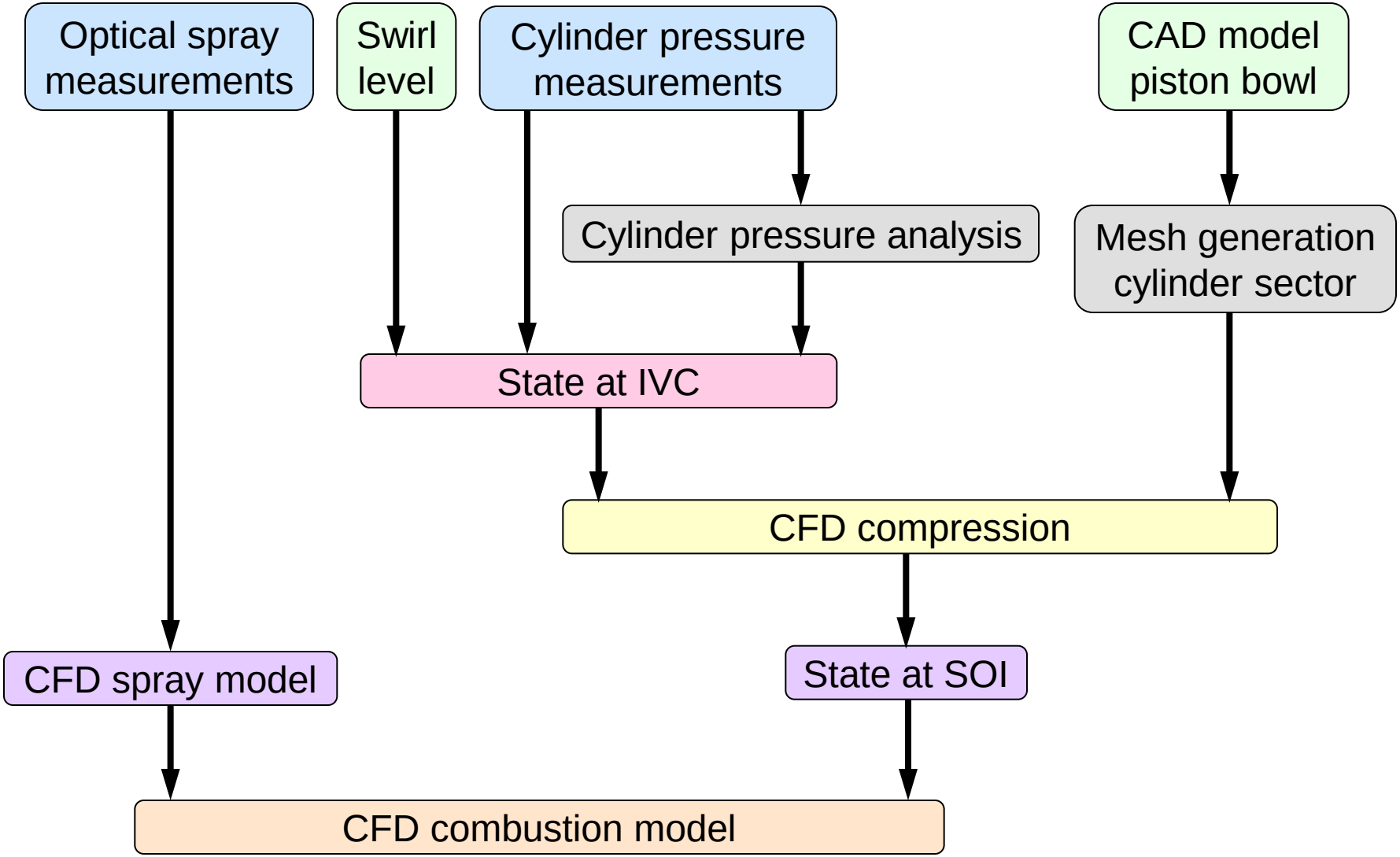
Überblick Verbrennungsentwicklung



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Beschreibung Simulationen

- **Motor**
  - R-6 Zylinder, 10.5 Liter Hubraum, 270kW
  - Gekühlte Hochdruck-AGR
- **CFD-Simulationen**
  - Kompressibel, Netz beweglich
  - Zylindersektor ➔ entspricht 1 Einspritzstrahl
- **Modellierung**
  - Verbrennung: Shell/CTC-Modell
  - Turbulenzmodell: modifiziertes RNG k-epsilon gemäss Han und Reitz
  - Modell Wandwärmeverluste: modifizierte Version gemäss Han und Reitz
  - Spray-Zerstäubung: Huh-Gosman
  - Spray-Aufbruch: wave (Kelvin-Helmoltz)
  - Kraftstoff: C14H30 (Tetradekan)

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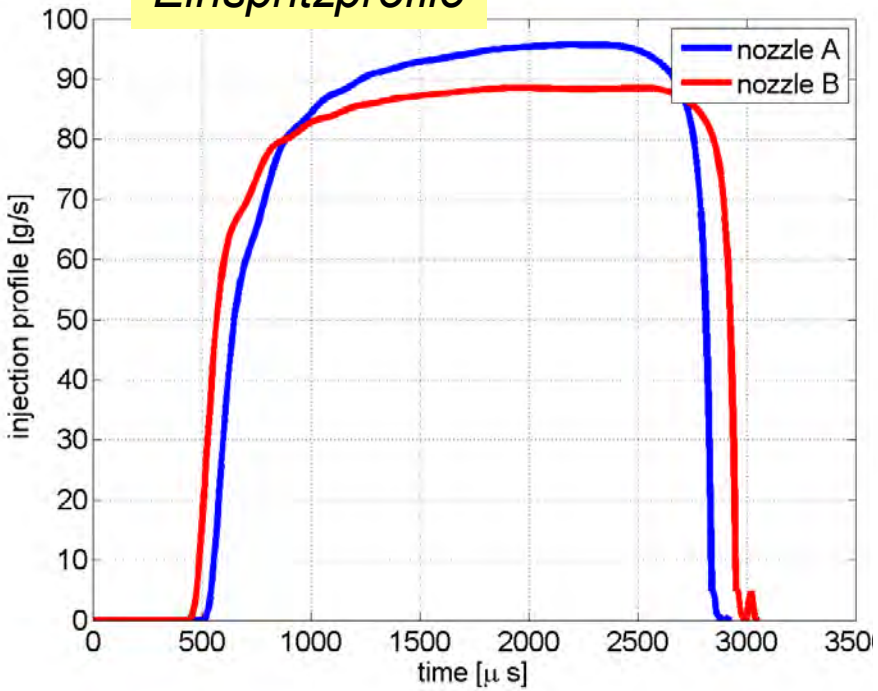
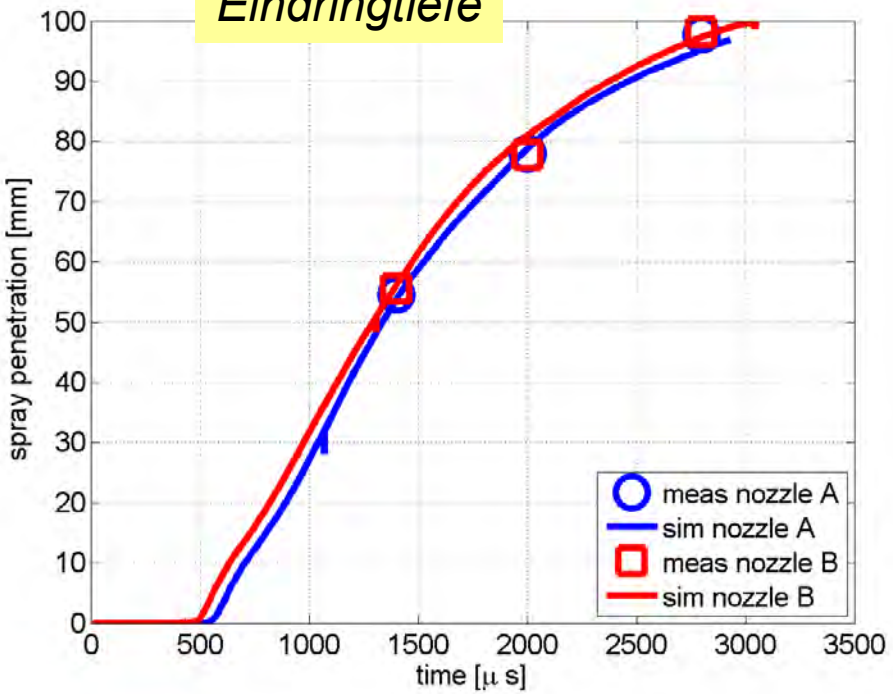
Modellierung Spray (2000 bar, 2 ms)

Einspritzprofile



Eindringtiefe



Düse	**[-]**	A	B
Lochanzahl	**[-]**	8	9
Durchfluss	**[ml/30s @ 100bar]**	710	650
Winkel	**[deg]**	138	146
K-Faktor	**[-]**	0.0	1.5

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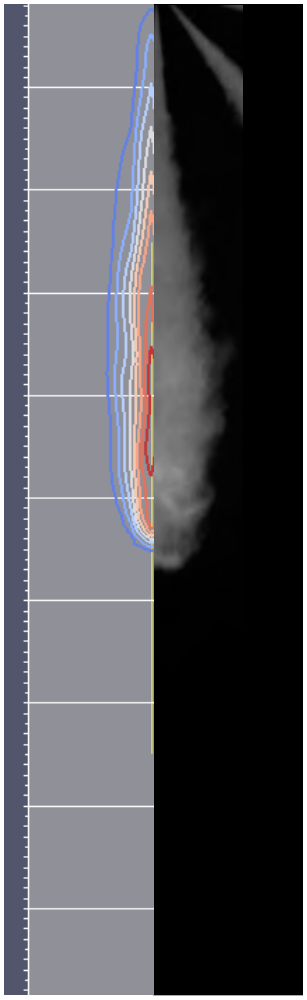
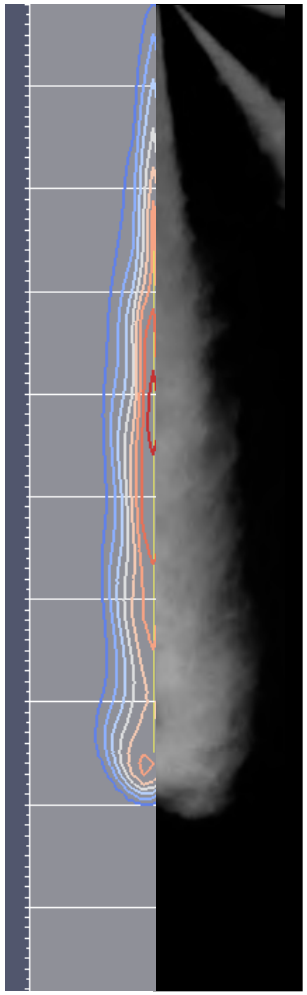
Ergebnisse für Düse B

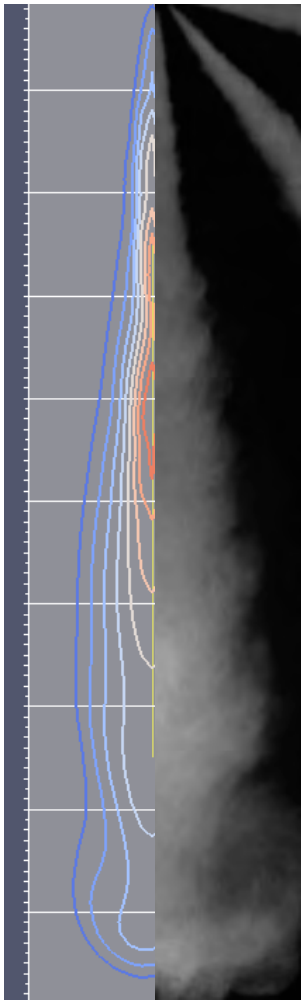
t = 1400 µs



t = 2000 µs



t = 2800 µs



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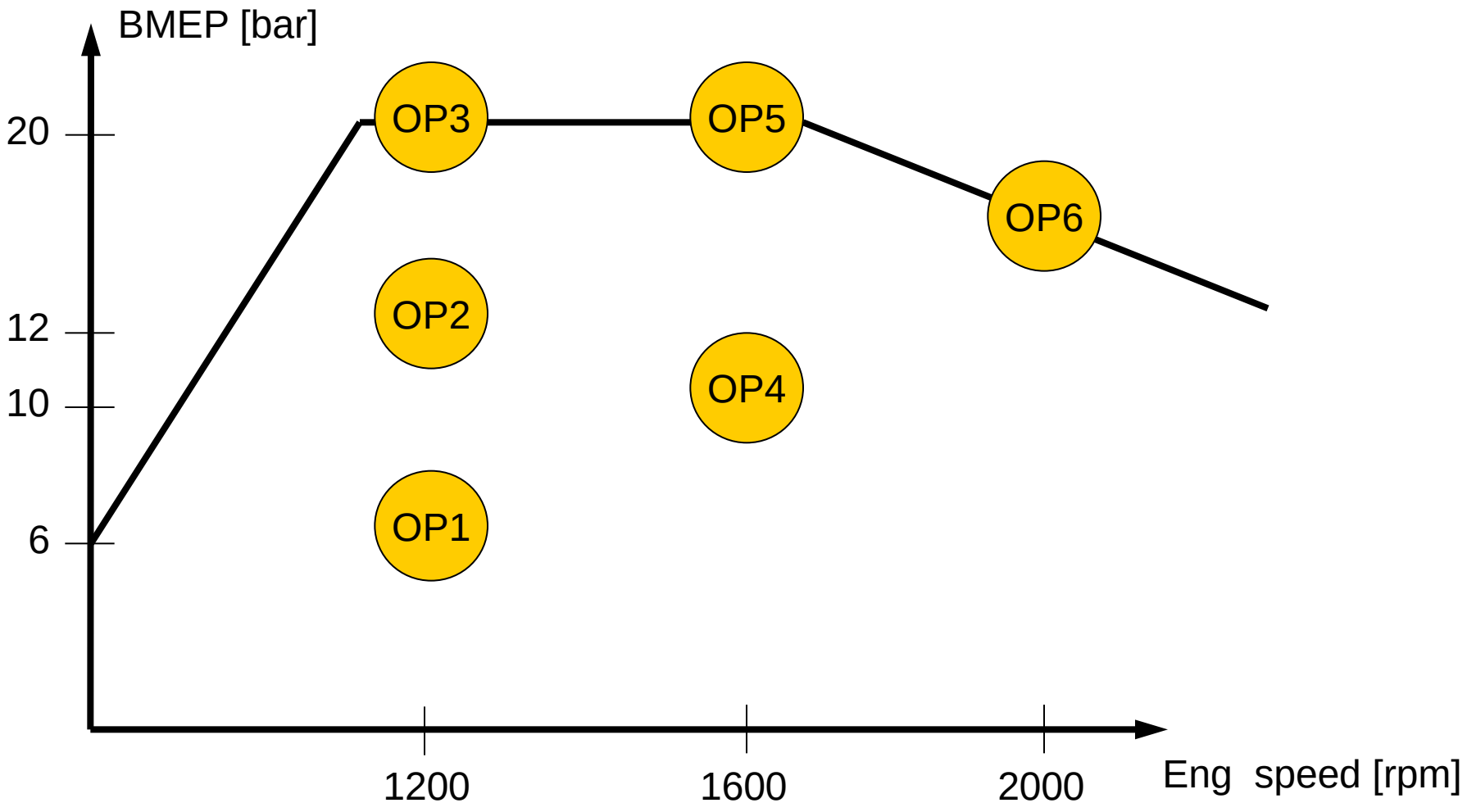
Modellierung Verbrennung – Betriebspunkte



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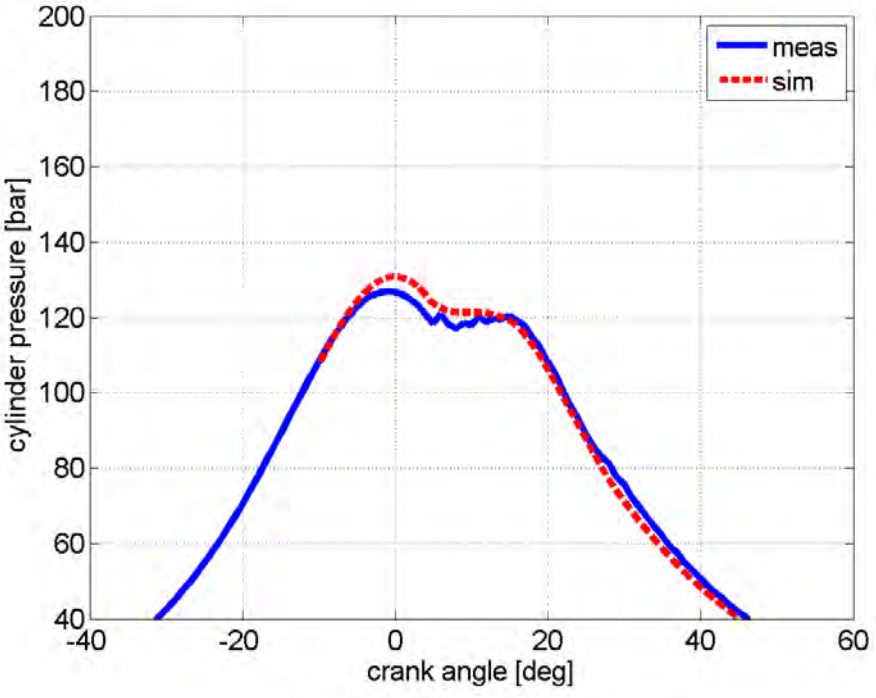
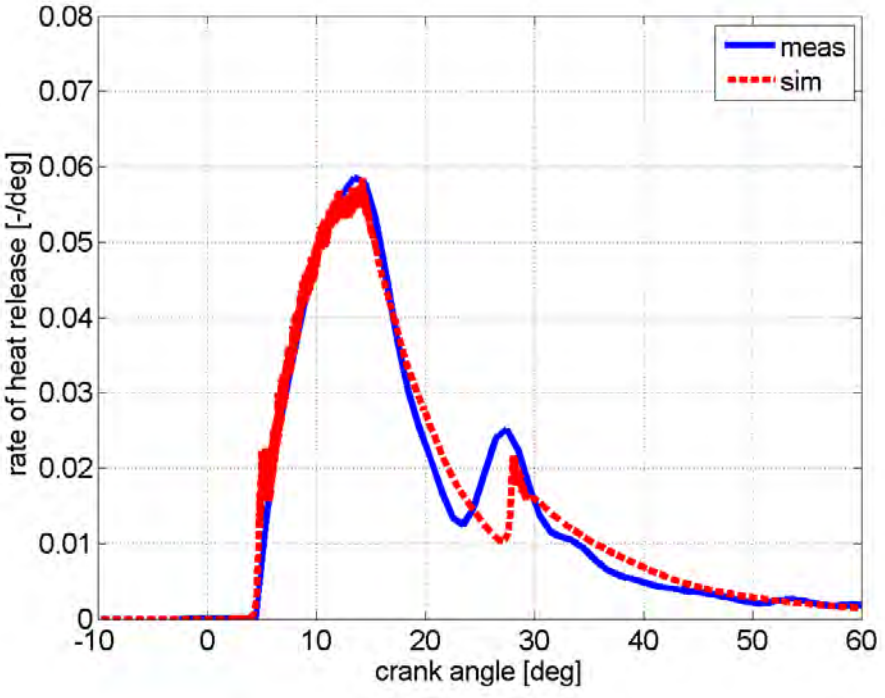
Ergebnisse für Düse A: OP4 – 1600 rpm, 10 bar BMEP

Zylinderdruck



Wärmeentwicklungsrate



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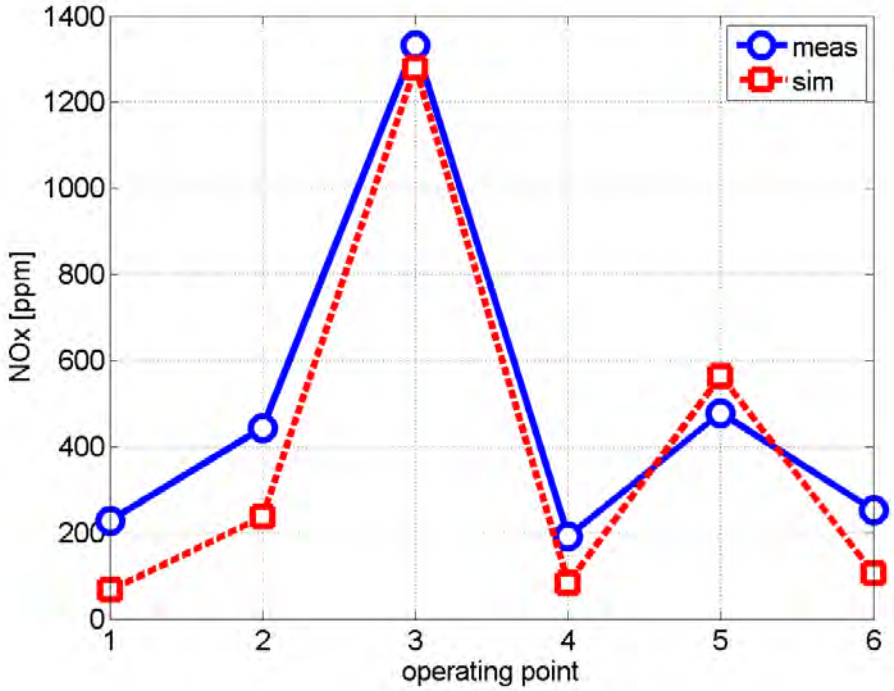
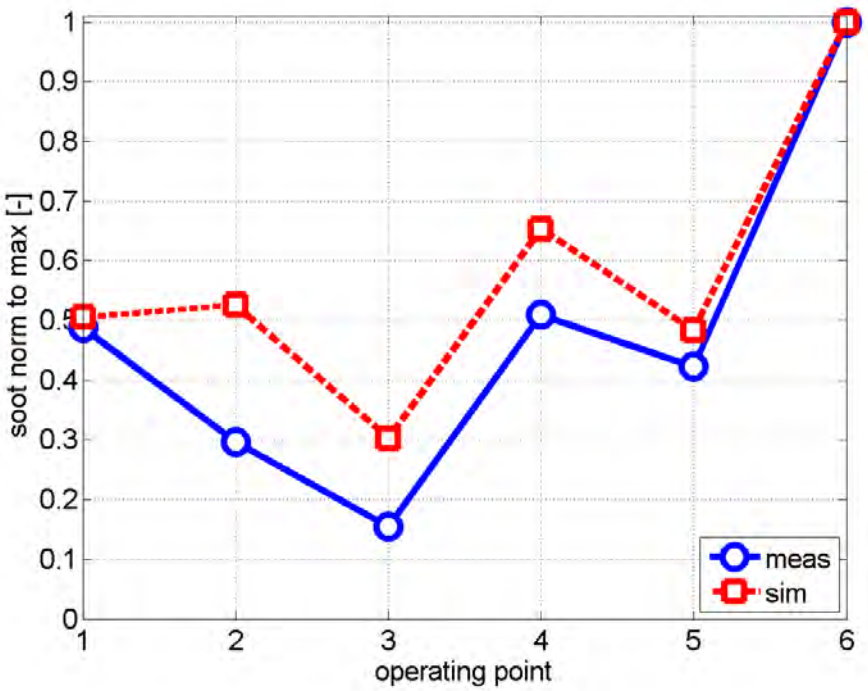
Ergebnisse für Düse A: OP1-OP6, NOx und Russ

NOx



Russ



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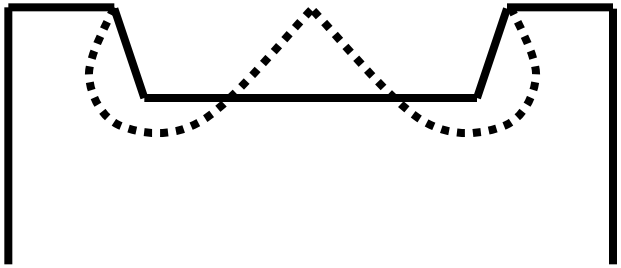
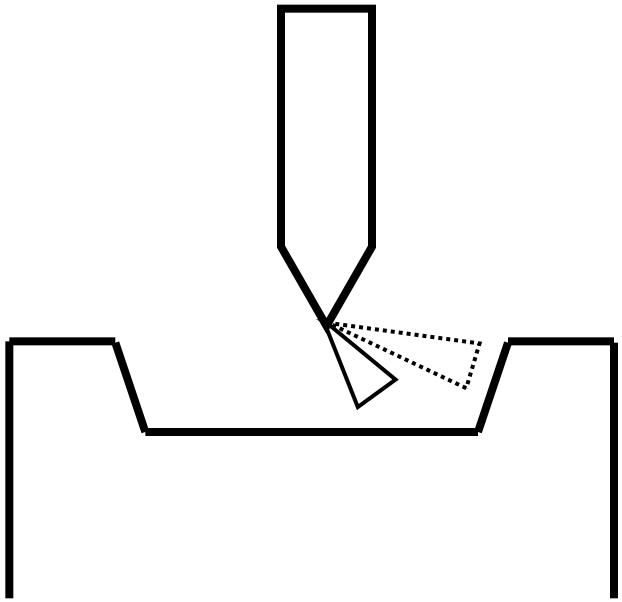
Untersuchungen

1) Variation Kolbenmulde



2) Variation Einspritzwinkel



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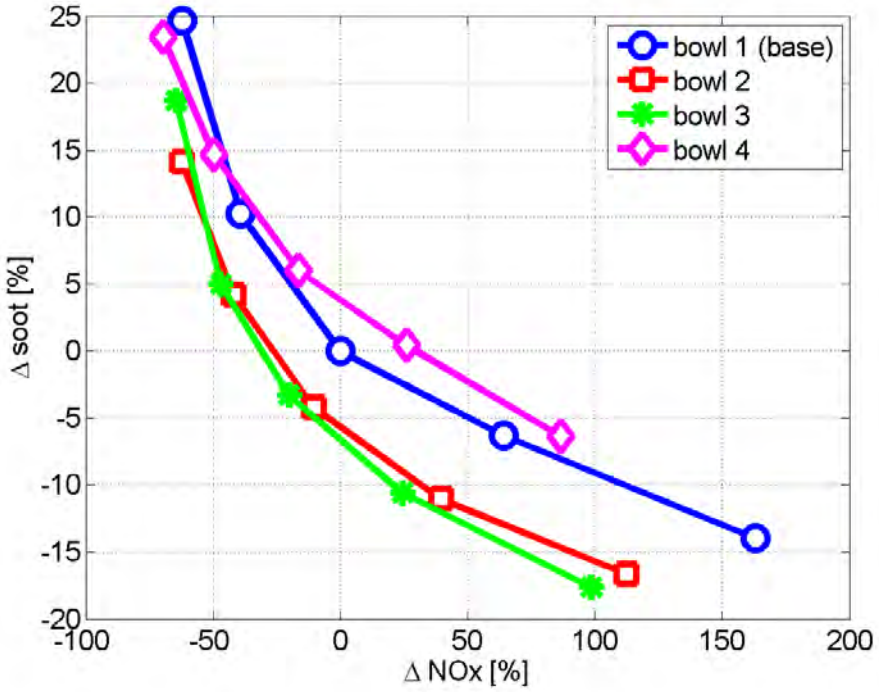
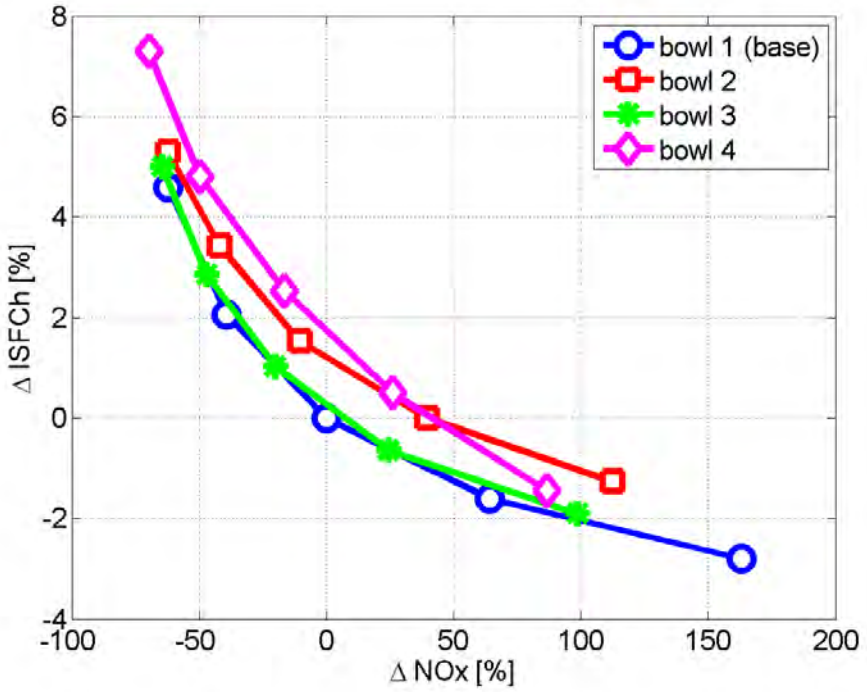
Simulation Variation Kolbenmulde

NOx-Russ



NOx-ISFCh



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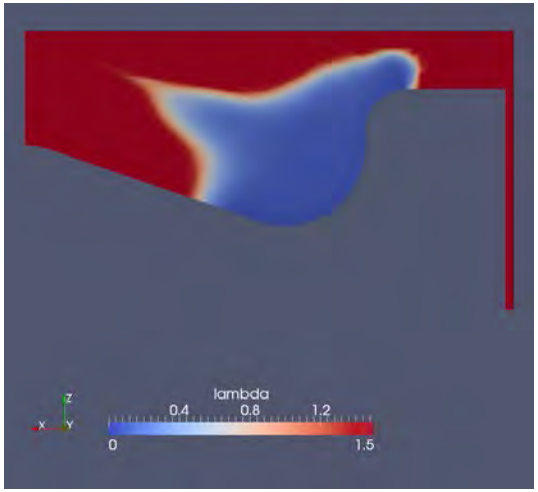
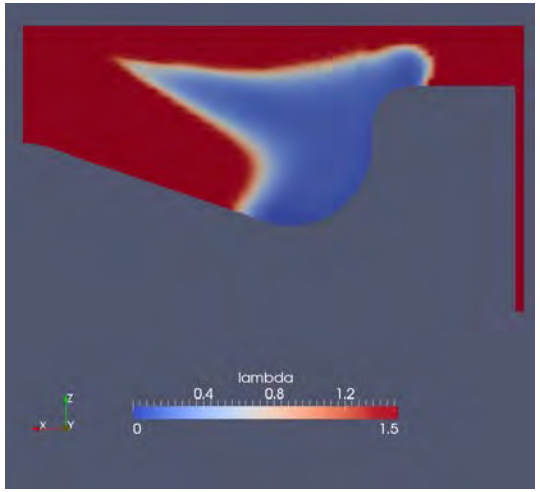
Simulation Variation Einspritzwinkel – lambda

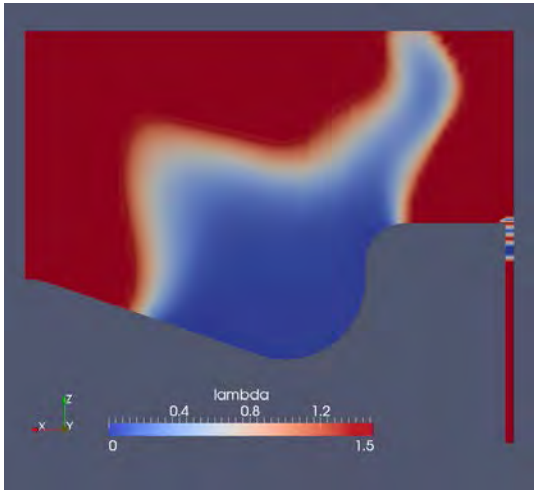
Winkel = 138°



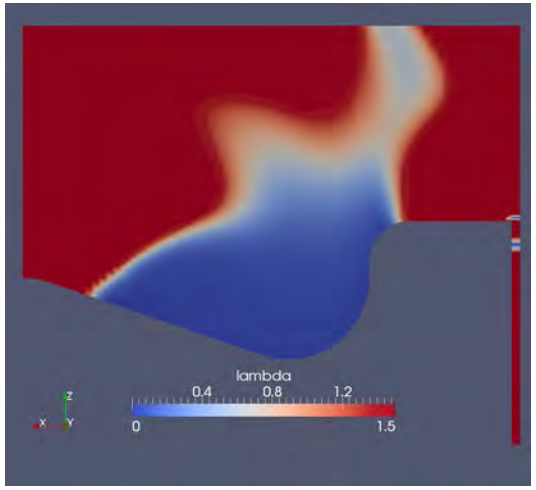
20° KW nOTP

Winkel = 146°





40° KW nOTP



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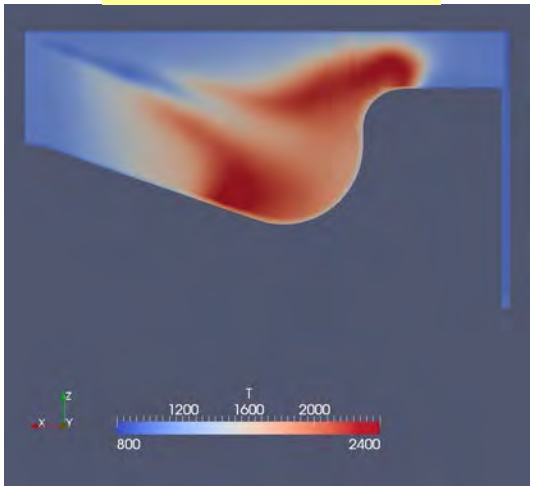
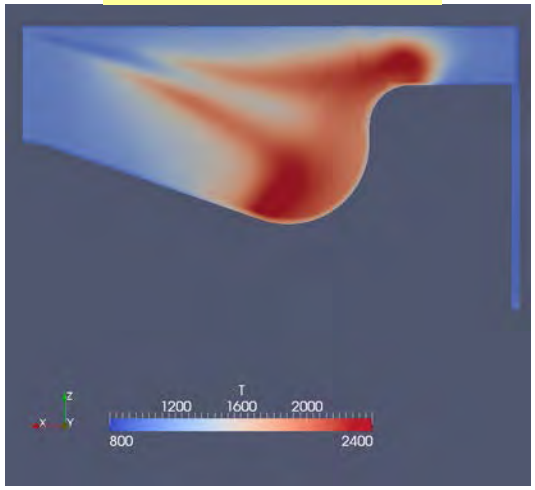
Simulation Variation Einspritzwinkel – Temperatur

Winkel = 138°

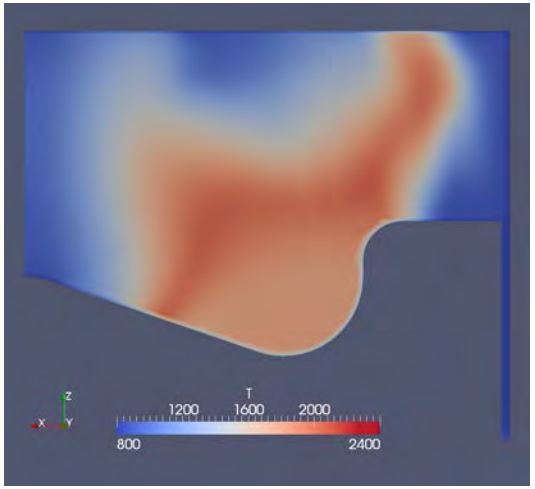


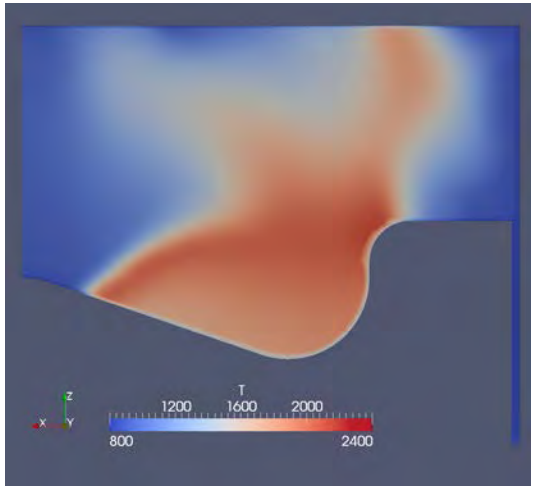
Winkel = 146°



20° KW nOTP

40° KW nOTP





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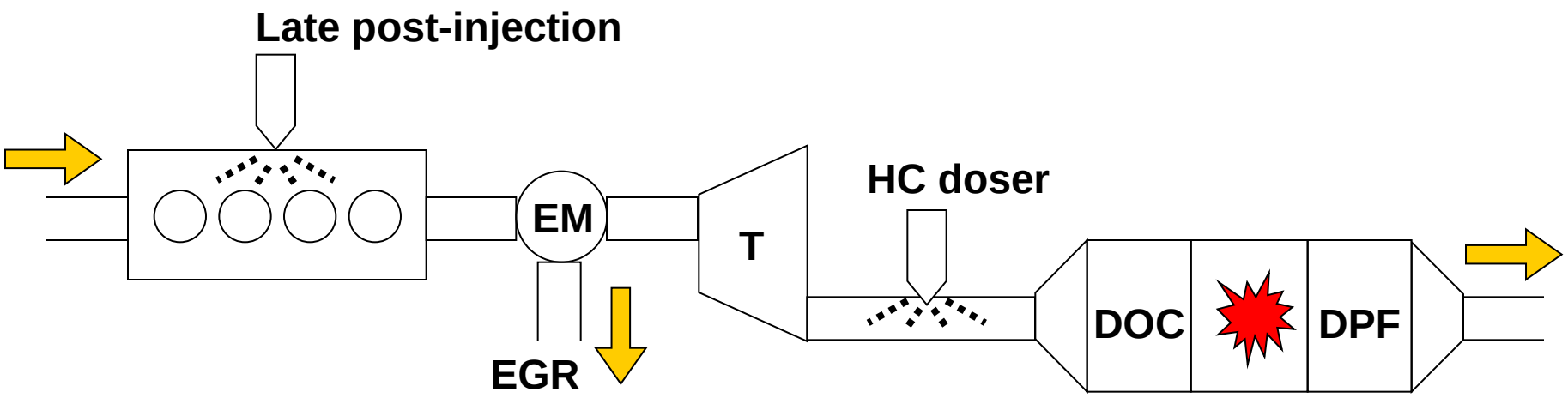
Aktive DPF-Regeneration und HC-Eindüsung

- Thermomanagement ➔ Ziel: Temperatur vor DOC > 350 °C
- Wärmeabgabe nach DOC wegen späte Nacheinspritzung oder HC-Einsdüsung ➔ Ziel: Temperatur vor DPF > 650 °C

$$4HC + 5O_2 \rightarrow 2H_2O + 4CO_2$$

- Aktive Regeneration (Abgastemperatur > 550 °C):

$$C + \left(1 - \frac{\sigma_{CO}}{2}\right) O_2 \rightarrow \left(\sigma_{CO}\right) CO + \left(1 - \sigma_{CO}\right) CO_2$$



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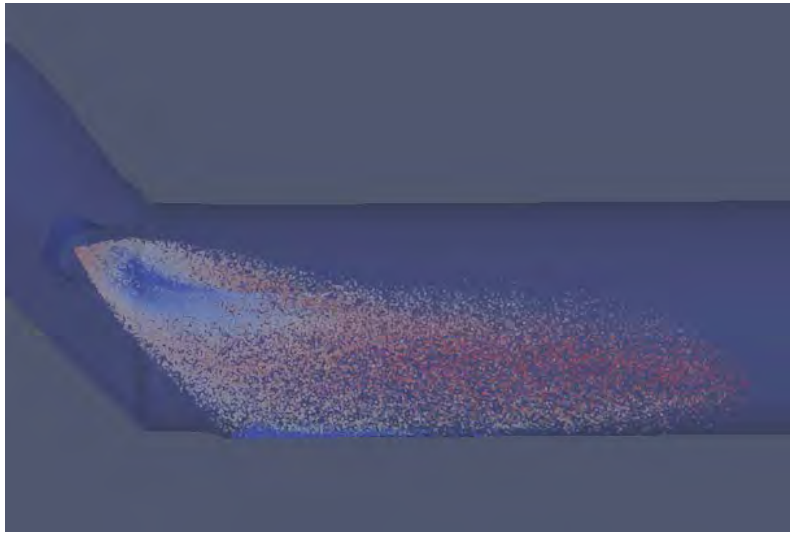
Beschreibung Simulationen

- **Modellierung**
  - Turbulenzmodell: k-epsilon
  - Tropfenmassenverteilung: Hohl-Kegel
  - SMD-Tropfenverteilung: Rosin-Rammler ➔ Parameter eingestellt basierend auf Messdaten
  - Aufbruchsmodell: KH-RT
  - Düsendurchmesser eingestellt um angegebene Einspritzgeschwindigkeit zu erzielen



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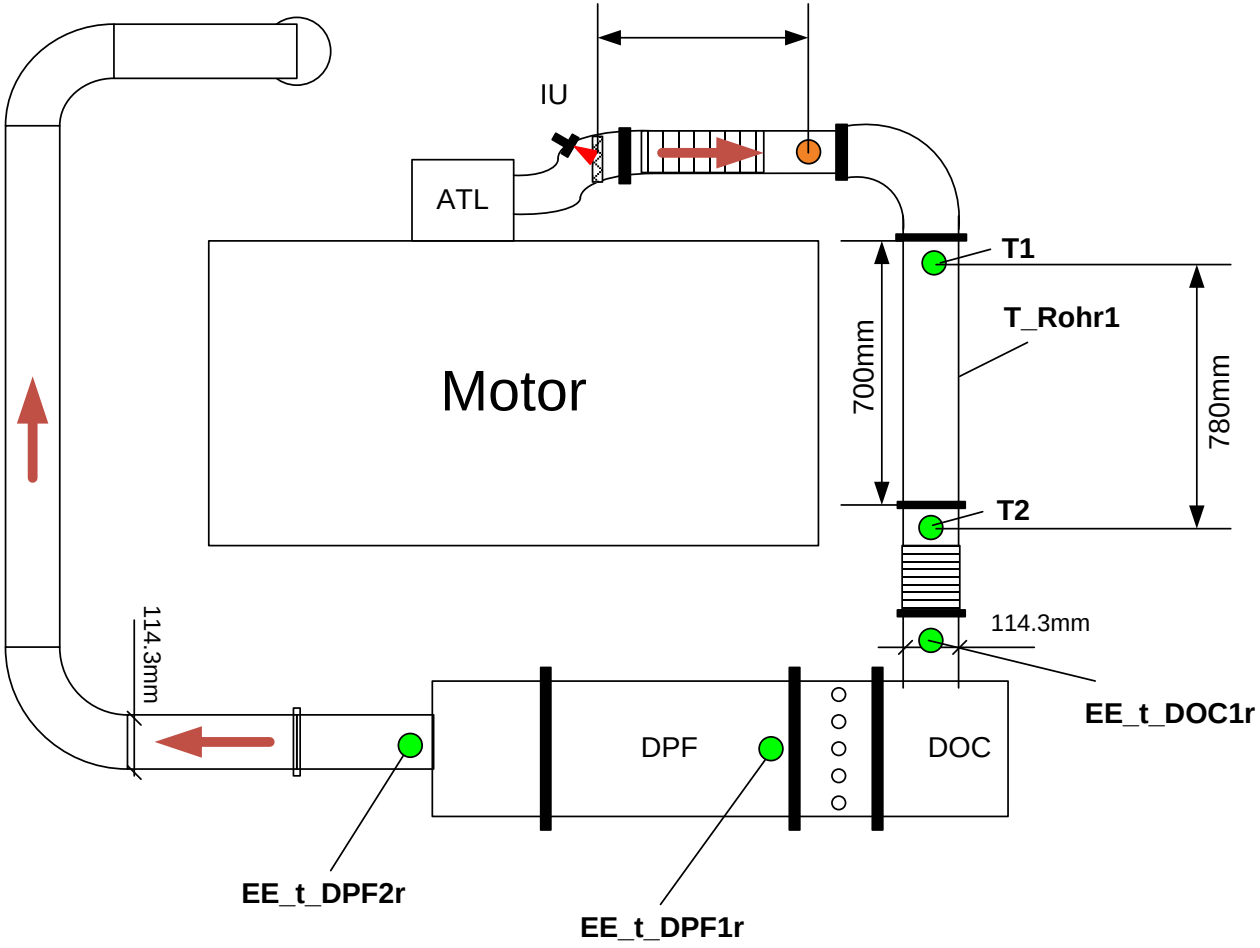
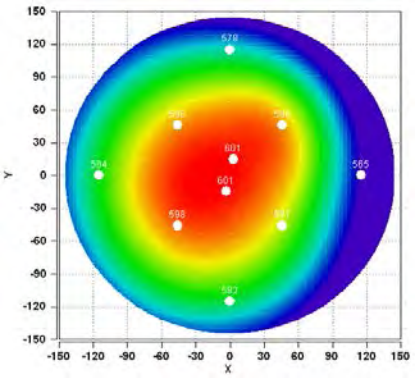
Experimentelle Charakterisierung der HC-Uniformität





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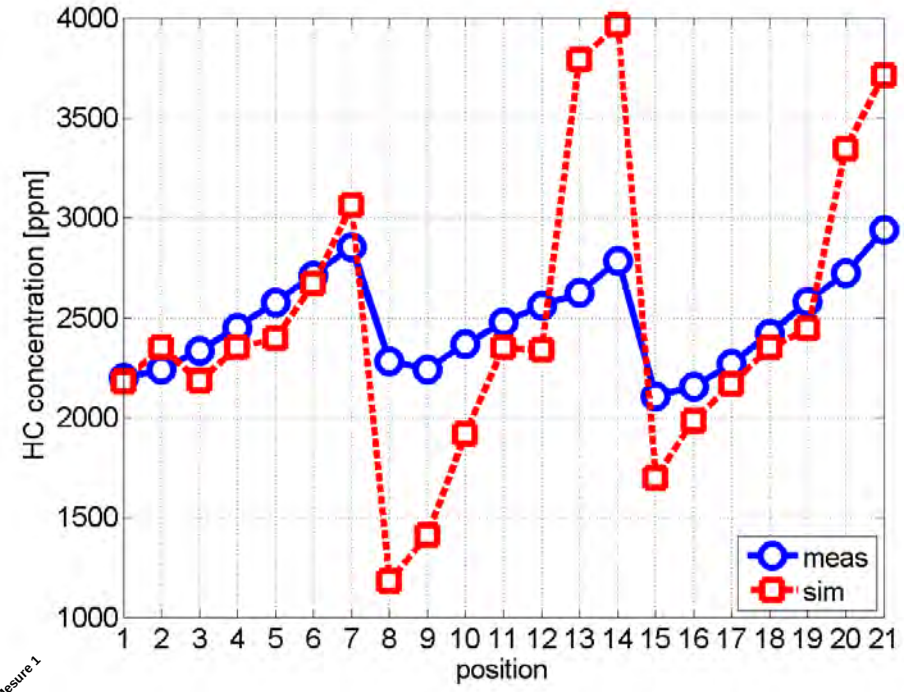
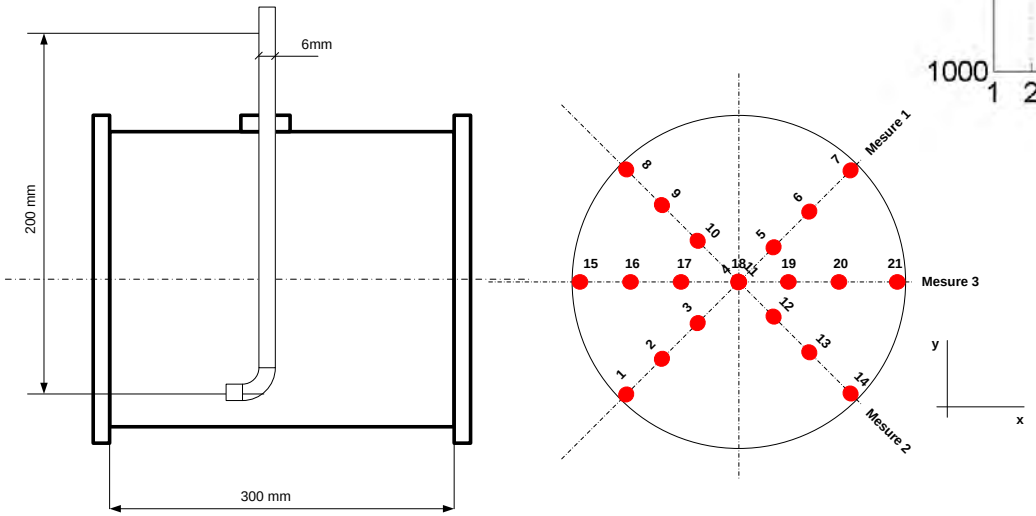
Messungen und Simulationen der HC-Konzentration





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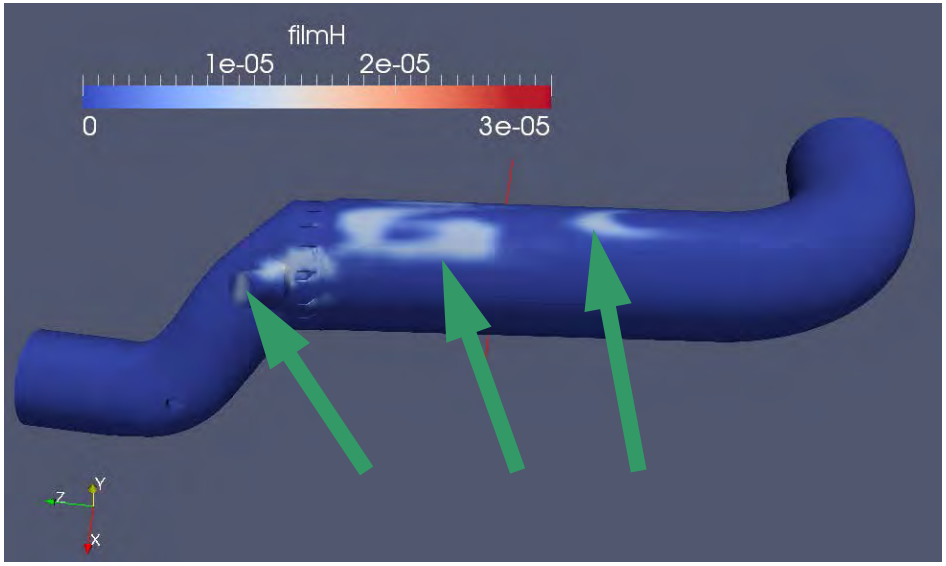
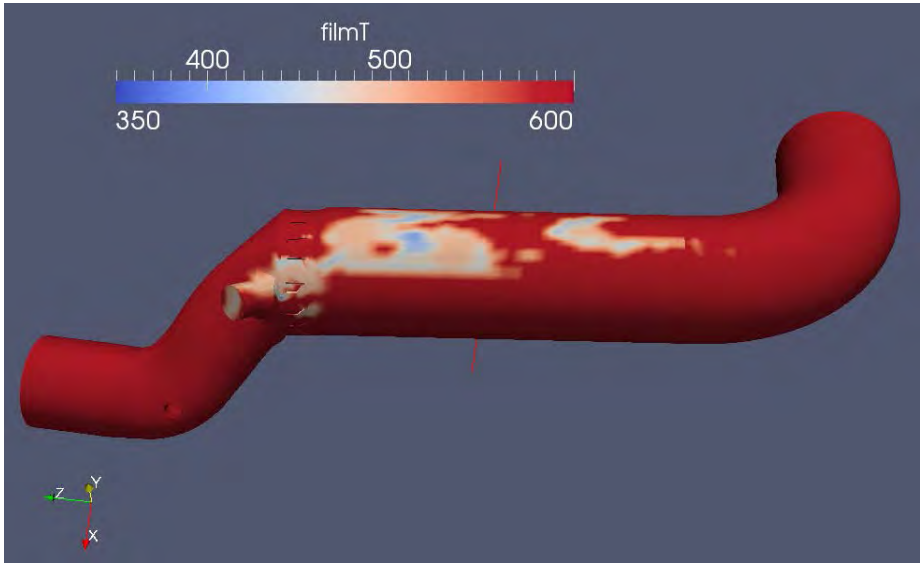
Simulation: Wandfilm auf Abgasrohrwände (t=0.45 s)

Höhe Wandfilm [m]



Temperatur Wandfilm [K]



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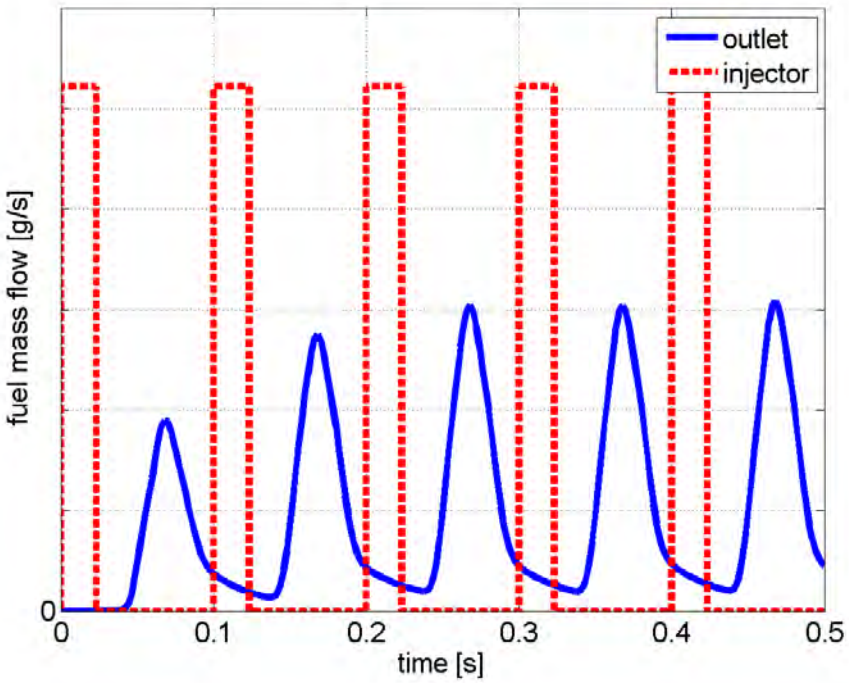
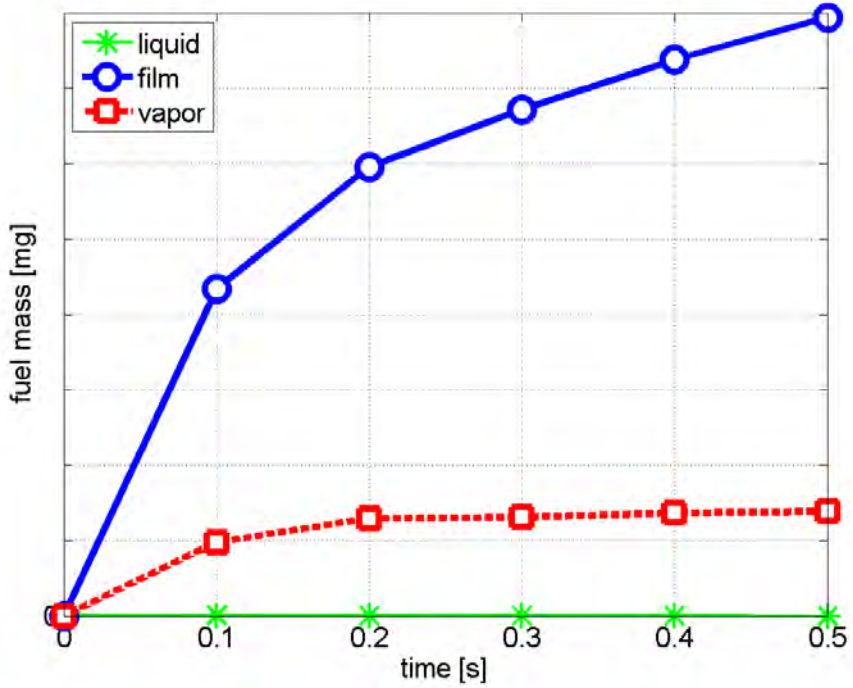
Simulation HC-Eindüsung bei realen Motorbedingungen

HC-Massenströme



HC-Mengen



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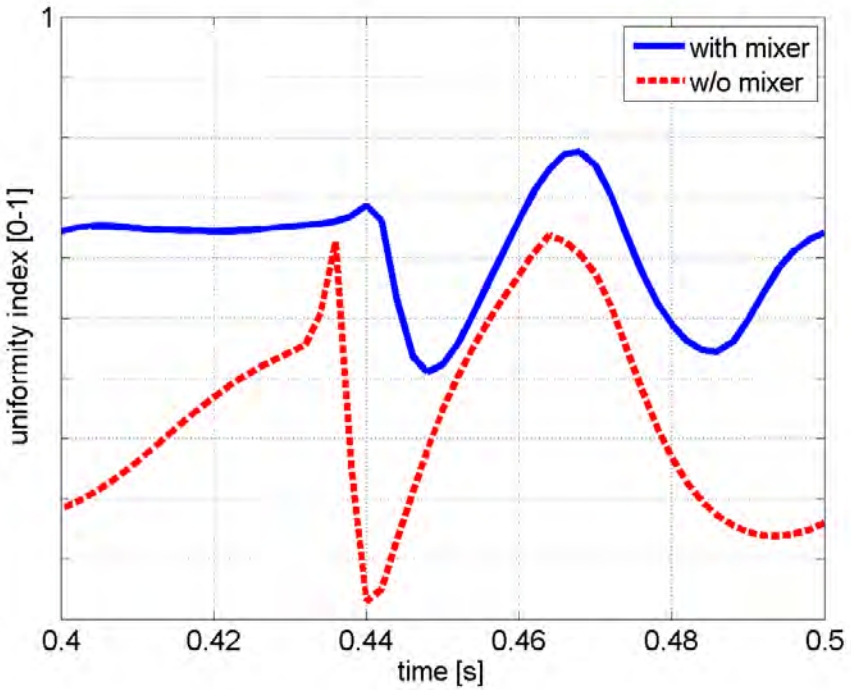
Simulationsergebnisse: Uniformitätsindex



$$UI(t) = 1 - \frac{\sum_i \left(\left| Y_{HC,i} - \bar{Y}_{HC} \right| \cdot \dot{m}_i \right)}{2 \cdot \sum_i \left(Y_{HC,i} \cdot \dot{m}_i \right)}$$

UI = uniformity index
Y_{HC} = HC mass fraction
m = mass flow*
i = cell index

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Zusammenfassung

- **Verbrennungsentwicklung**
  - Kalibriertes Spray-Modell unumgänglich
  - Verwendete Verbrennungsmodell sehr gut hinsichtlich Vorausberechnung des Verbrennungsprozesses und der NOx-Emissionen
  - Hingegen, gute Vorausberechnung der Russemissionen ist schwieriger
  - Deshalb: neben berechneten globalen Parameter, Einblick in lokalen Strömungsphänomene ist empfehlenswert
  - Gezeigtes Beispiel: Wahl Kolbenmulde und Düsenkonfiguration

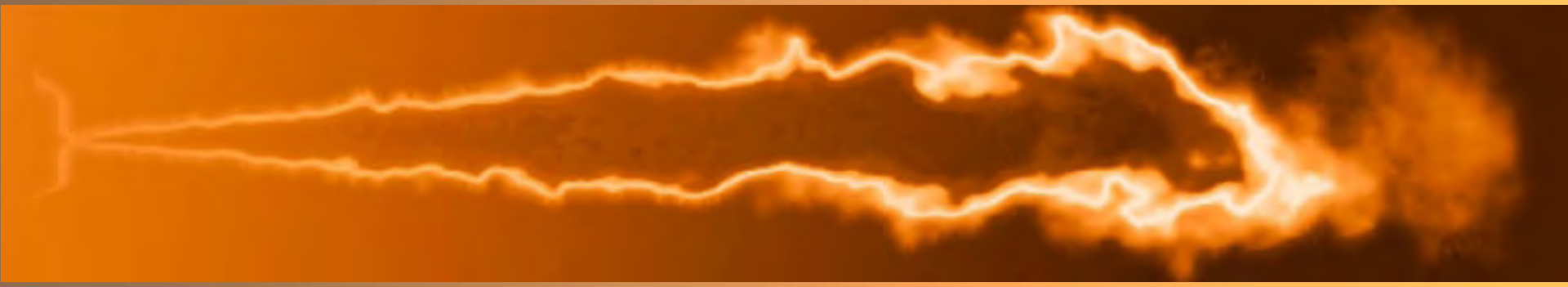
- **HC-Eindüsung**
  - Model validiert mit Messdaten
  - Simulationen geben wichtige Informationen, für welche eine direkte Ermittlung zu schwierig oder zeitaufwendig ist, wie z.B. Wandfilmbildung und HC-Uniformität
  - Gezeigtes Beispiel: Einfluss eines Mixers auf die HC-Uniformität

Vielen Dank für Ihre Aufmerksamkeit

ETH
Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo

Verbrennungstagung, ETH Zurich, 28th October 2011

Soot formation modeling of n-Heptane sprays under diesel engine conditions using the Conditional Moment Closure approach



M. Bolla, Y.M. Wright and K. Boulouchos

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ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory, Switzerland

Outline

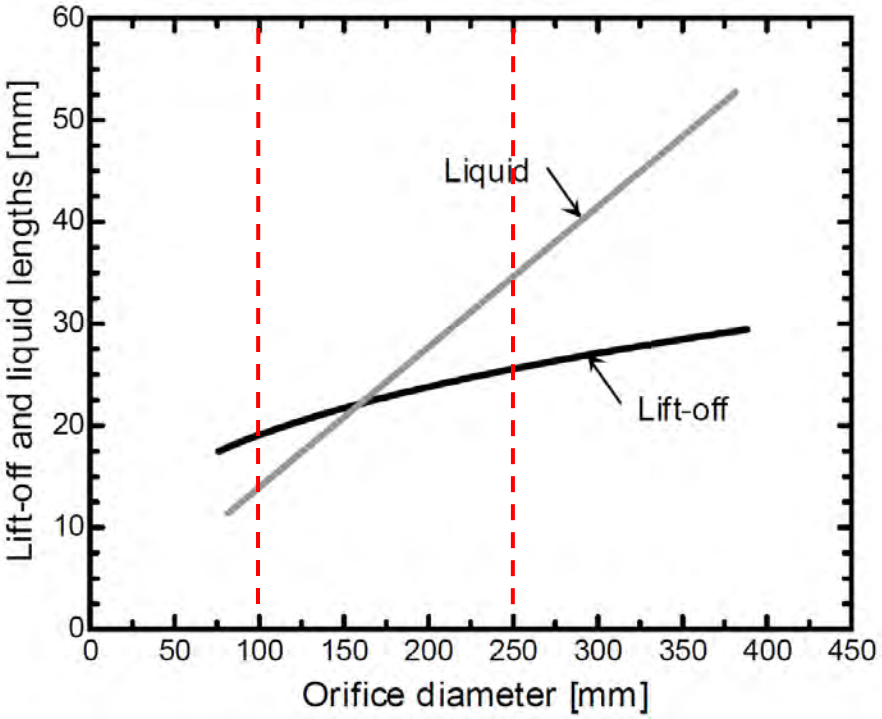
- **Introduction**
  - Spray combustion: concept
  - Experimental setup: Sandia constant-volume combustion chamber
  - Test cases
- **Numerical methodology**
  - CMC formulation
  - Soot model
- **Results**
  - Ignition delay & lift-off height
  - Flame structure
  - Soot distribution
- **Conclusions and Outlook**

Spray combustion - concept

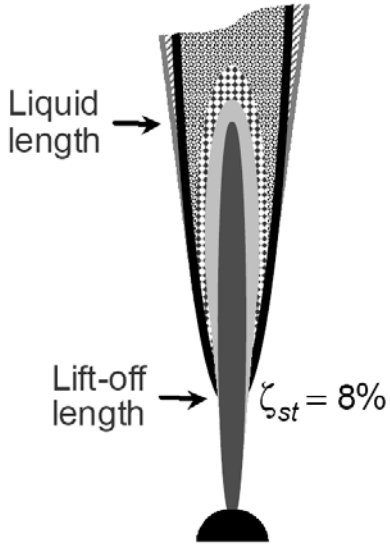
- Influence orifice diameter:

n-Heptane fuel

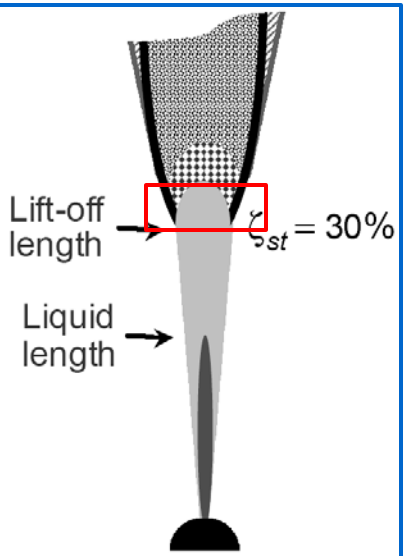
T=1000K;p=42bar;Δp_{inj}=1380bar



Fuel droplets, fuel vapor, and air
Vaporized fuel and air
Rich "premixed" combustion
Stoichiometric diffusion flame
Soot formation/growth region
Combustion products



d_0=250 μm



d_0=100 μm

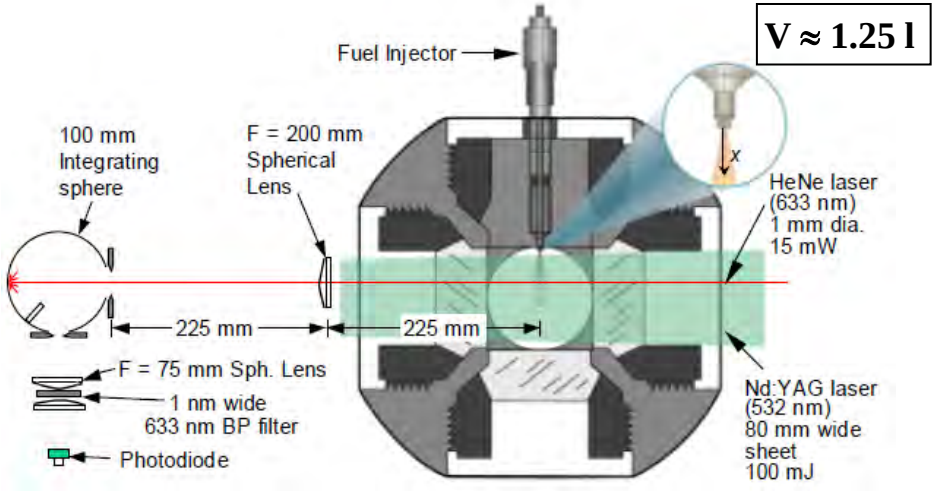
Convective-reactive balance at lift-off

Source: Siebers & Higgins, *SAE Technical Paper* **2001-01-0530** (2001)

Experimental setup

Sandia constant-volume chamber with optical access

Fuel type	n-Heptane
Orifice pressure drop	1500 bar
Injection duration	7 ms
Nozzle diameter	0.100 mm
Air pressure	42 bar / 85 bar
Oxygen content («EGR»)	21, 15, 12, 10, 8 %
Air temperature	1000 K



Measurement techniques:

- Ignition delays (pressure trace)
- Lift-off heights (OH* chem.)
- Soot volume fraction (PLII)

Test cases:

- **42 bar: 21/15/12/10/8% O_2**
- **85 bar: - /15/12/10/8% O_2**

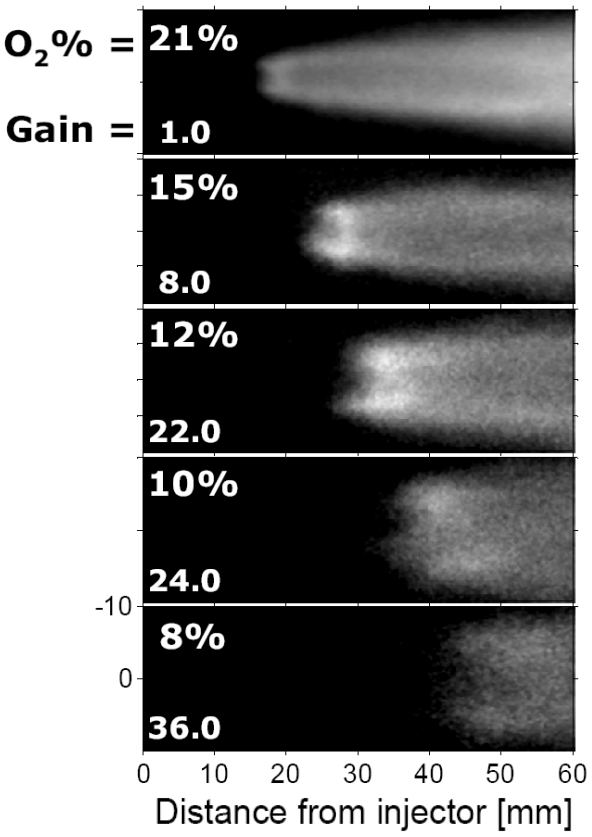
9 different cases

Source: C.A. Idicheria and L.M. Pickett, *SAE Technical Paper* **2005-01-3834** (2005)

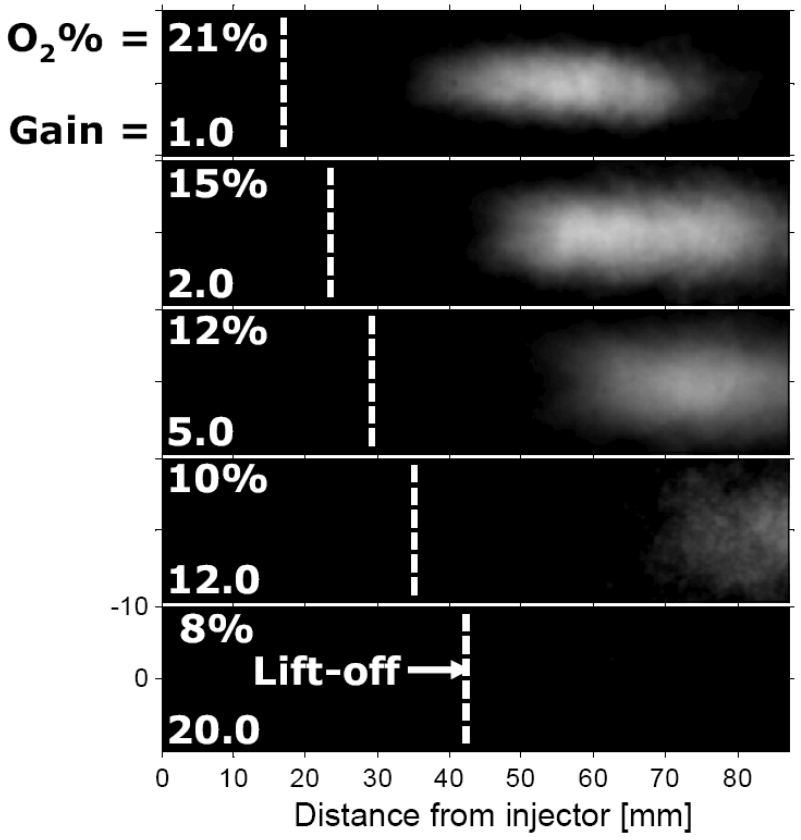
Experimental results: validation data

- **Experimental conditions: 42 bar, 1000 K, (21/15/12/10/8% O_2)**

- **Flame region (OH* chem.)**

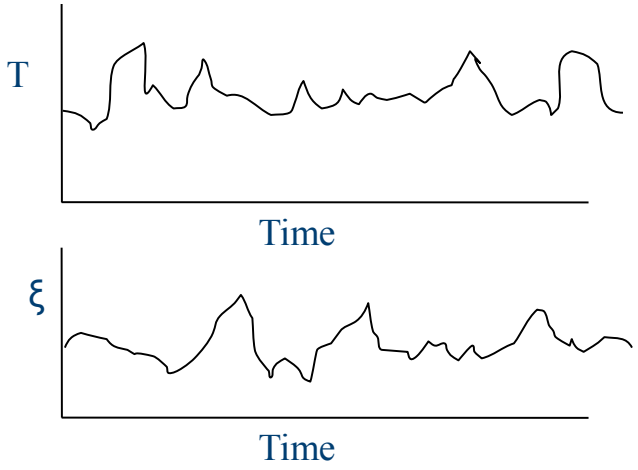


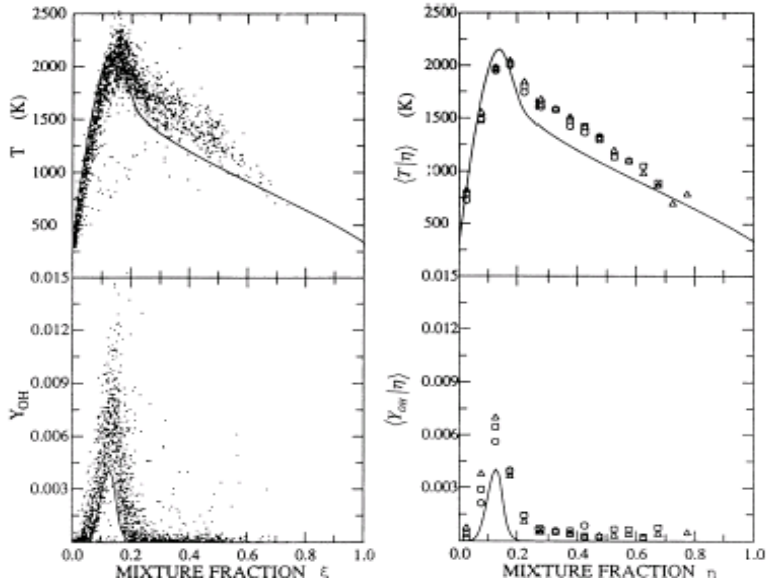
- **Soot region (PLII)**



Source: C.A. Idicheria and L.M. Pickett, *SAE Technical Paper* **2005-01-3834** (2005)

Conditional averaging – concept





Piloted diffusion flame of methanol
Source: R.W. Bilger, Physics of Fluids (1993)

- **Conservation equations:**

$$\rho \frac{\partial Y_i}{\partial t} + \rho v \cdot \nabla Y_i - \nabla \cdot (\rho D_i \nabla Y_i) = \dot{\omega}_i$$

- **‚Bilger-approach' – consider:**

$$Y(\underline{x},t) = Q\left(\xi(\underline{x},t), \underline{x}, t\right) + y'(\underline{x},t) \quad \textit{where} \quad Q = \left\langle Y(\underline{x},t) \middle| \xi(\underline{x},t) = \eta \right\rangle$$

- **Increased dimensionality of the problem: Q(x,η,t)**
- **But Qs have weaker spatial dependence than unconditional values**

Multi-Dimensional-CFD
Conditional Moment Closure Equations

$Le = 1$

$$Q_\alpha = \langle Y_\alpha \,|\, \xi = \eta \rangle$$

Species

$$\frac{\partial Q_\alpha}{\partial t} + \underbrace{\langle u_i \,|\, \eta \rangle \cdot \nabla Q_\alpha}_{\text{Conditional velocity}} = \underbrace{\langle N \,|\, \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2}}_{\text{Molecular mixing}} - \underbrace{\frac{\nabla \cdot \left(\langle u_i'' Y_\alpha'' \,|\, \eta \rangle \langle \rho \rangle \tilde{P}(\eta) \right)}{\langle \rho \rangle \tilde{P}(\eta)}}_{\text{Conditional turbulent flux}} + \underbrace{\langle w_\alpha \,|\, \eta \rangle}_{\text{Chemistry}}$$

Temperature

$$\frac{\partial Q_T}{\partial t} + \langle u_i \,|\, \eta \rangle \cdot \nabla Q_T = \langle N \,|\, \eta \rangle \frac{\partial^2 Q_T}{\partial \eta^2} + \langle N \,|\, \eta \rangle \left[\frac{1}{\langle c_p \,|\, \eta \rangle} \left(\frac{\partial \langle c_p \,|\, \eta \rangle}{\partial \eta} + \sum_{\alpha=1}^{N} \langle c_{p,\alpha} \,|\, \eta \rangle \frac{\partial Q_\alpha}{\partial \eta} \right) \right] \frac{\partial Q_T}{\partial \eta}$$

$$- \frac{\nabla \cdot \left(\langle u_i'' T'' \,|\, \eta \rangle \langle \rho \rangle \tilde{P}(\eta) \right)}{\langle \rho \rangle \tilde{P}(\eta)} + \underbrace{\frac{1}{\langle c_p \,|\, \eta \rangle} \left\langle \frac{1}{\rho} \frac{\partial P}{\partial t} \,|\, \eta \right\rangle}_{\text{Time-varying pressure}} + \frac{\langle w_H \,|\, \eta \rangle}{\langle \rho \,|\, \eta \rangle \langle c_p \,|\, \eta \rangle} + \underbrace{\frac{\langle w_{RAD} \,|\, \eta \rangle}{\langle \rho \,|\, \eta \rangle \langle c_p \,|\, \eta \rangle}}_{\text{Radiation}} + \underbrace{\frac{\langle w_{WALL} \,|\, \eta \rangle}{\langle \rho \,|\, \eta \rangle \langle c_p \,|\, \eta \rangle}}_{\text{Wall heat transfer}}$$

Source: De Paola, Mastorakos, Wright & Boulouchos, Comb. Sci. and Techn. 180 (2008)

Submodels in the CMC equations

$$\left\langle u_j'' y_\alpha'' \,\middle|\, \eta \right\rangle = -D_t \frac{\partial Q_\alpha}{\partial x_j}$$

Gradient flux

Bilger & Klimenko, Progress in Energy and Combustion Science (1999)

$$\left\langle u_j \,\middle|\, \eta \right\rangle = \tilde{u}_j - \frac{D_t}{\widetilde{\xi''^2}} \frac{\partial \tilde{\xi}}{\partial x_j} \left(\eta - \tilde{\xi} \right)$$

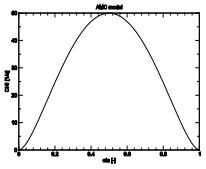
Linear model for conditional velocities

Bilger & Klimenko, Progress in Energy and Combustion Science (1999)
model comparison presented in I.S. Kim, PhD Thesis, Uni Cambridge (2004)

$$\left\langle w_\alpha \,\middle|\, \eta \right\rangle = \dot{\omega}_\alpha \left(Q_\alpha, Q_T, P \right)$$

First order closure for the source terms

$$\left\langle N \,\middle|\, \eta \right\rangle = \frac{\tilde{\chi}}{2 \int_0^1 G(\eta) \tilde{P}(\eta) \, d\eta} \underbrace{\exp\left(-2 \left[erf^{-1}(2\eta - 1) \right]^2 \right)}_{G(\eta)}$$



AMC model for the scalar dissipation rate

O'Brien & Jiang, Physics of Fluids (1991)

$$\left\langle w_{RAD} \,\middle|\, \eta \right\rangle = -4 \sigma \alpha_{soot} \left[\left\langle T \,\middle|\, \eta \right\rangle^4 - T_{Wall}{}^4 \right]$$

$$with \;\; \alpha_{soot} = 2370 \frac{1}{mK} \cdot f_{V_{SOOT}} \cdot \left\langle T \,\middle|\, \eta \right\rangle$$

Optical thin model for radiation heat transfer

Widmann et al., Combustion Science Technology (2003)

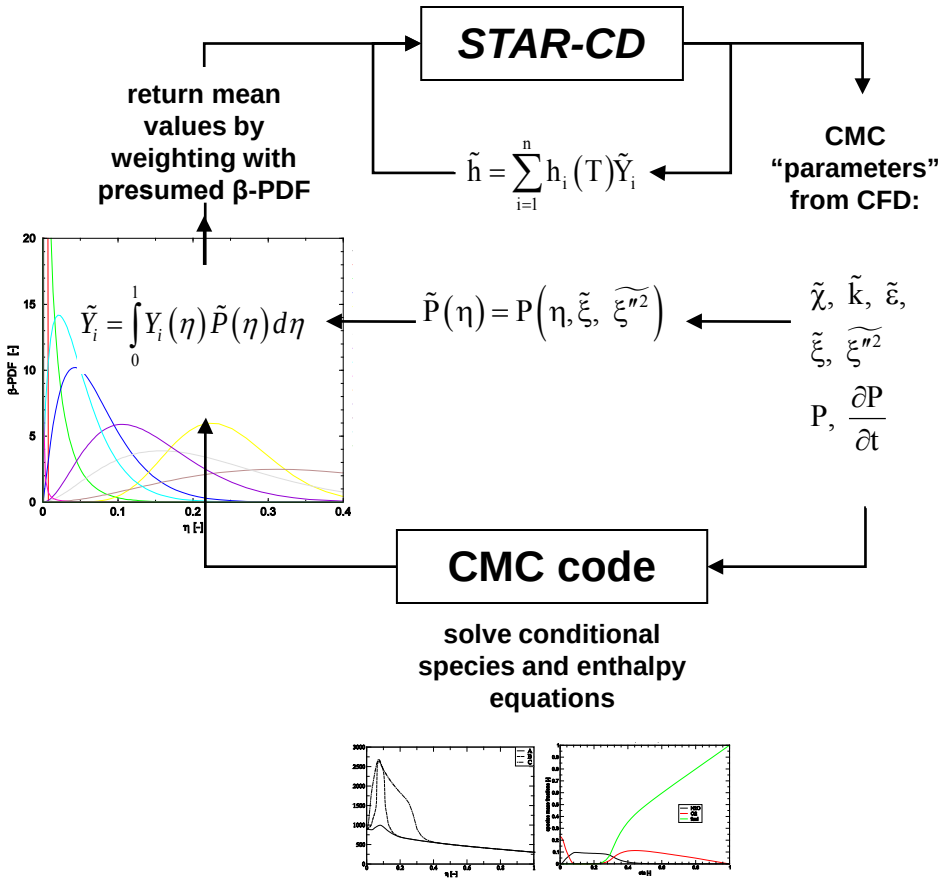
$$\left\langle w_{WALL} \,\middle|\, \eta \right\rangle = h \left(Q_T - \tilde{T}_{WALL} \right) \; with \; h = \frac{\tilde{w}_{WALL}}{\int_0^1 \left(Q_T - \tilde{T}_{WALL} \right) P(\eta) \, d\eta}$$

Wall heat transfer

Hergart & Peters, Journal of Engineering for Gas Turbines and Power (2001)

Numerical set-up

- Interfacing STAR-CD / CMC code



- **3D CFD code STAR-CD v4.16**
  - Quasi-2D grid (0.5mm size)
- **Turbulence model:** κ-ε-RNG
- **Spray model: Lagrangian**
  - Atomisation: Reitz-Diwakar
  - Break-up: Reitz-Diwakar
- **Combustion model:**
  - Conditional Moment Closure
  - Reduced C_7H_{16} mechanism
    - Liu* 22/44 species
- **Soot model:**
  - 2-eq model by Leung**

Wright, de Paola, Mastorakos & Boulouchos, Comb. Flame 143 (2005)

*) Mechanisms: Liu et al., Comb. Flame 137 (2004) **) Soot model: Leung et al., Comb. Flame 87 (1991)

2-equation soot model into CMC framework

$$\frac{\partial Q_\alpha}{\partial t} = -\langle u_i | \eta \rangle \cdot \nabla Q_\alpha + \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} - \frac{\nabla \cdot \left(\langle u_i'' Y_\alpha'' | \eta \rangle \langle \rho | \eta \rangle \widetilde{P}(\eta) \right)}{\langle \rho | \eta \rangle \widetilde{P}(\eta)} + \langle w_\alpha | \eta \rangle$$

Y_S [-]

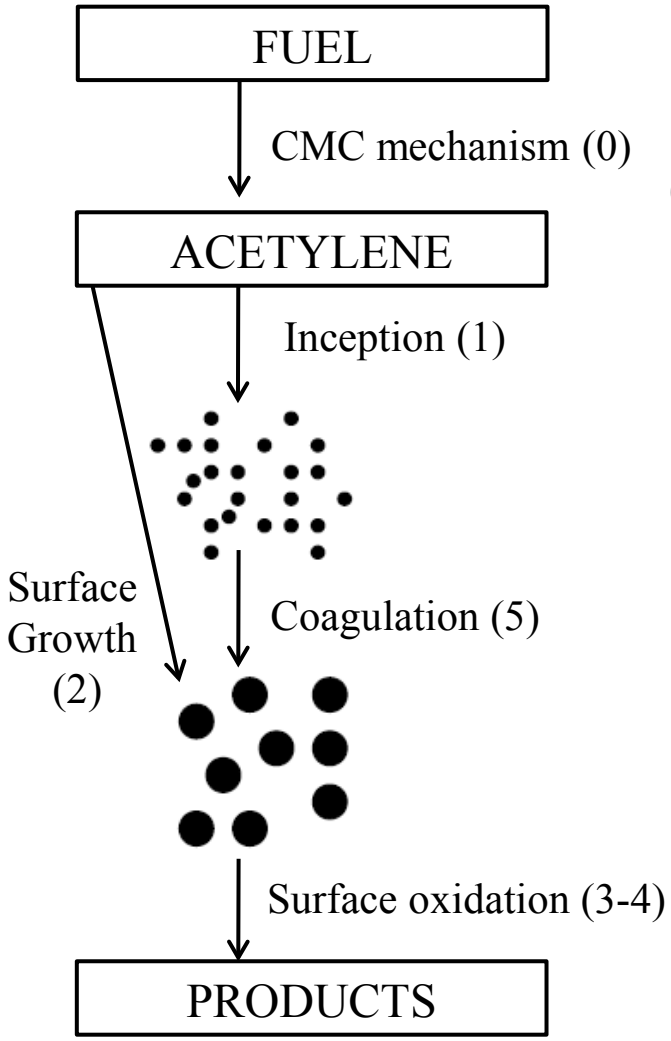
$$\langle w_{Y_S} | \eta \rangle = \langle w_{Y_S,inception} | \eta \rangle + \langle w_{Y_S,growth} | \eta \rangle + \langle w_{Y_S,oxidation} | \eta \rangle$$

$N_S \left[\frac{\#}{m^3} \right]$

$$\langle w_{N_S} | \eta \rangle = \langle w_{N_S,inception} | \eta \rangle + \langle w_{N_S,coagulation} | \eta \rangle$$

- Solve transport equation for soot mass fraction and number density
- Accounts for nucleation, surface growth, coagulation and surface oxidation
- Calibrated soot source terms
- Mono-disperse spherical soot particles assumed

2-equation soot model (Leung, C&F 1991)



(1) Particle Inception

$$C_2H_2 \rightarrow 2C_{(S)} + H_2 \qquad \dot{\omega}_1 = 10^4 [C_2H_2] e^{-\frac{21100}{T}}$$

(2) Particle Surface Growth

$$C_2H_2 + nC_{(S)} \rightarrow (n+2)C_{(S)} + H_2 \qquad \dot{\omega}_2 = 6 \cdot 10^3 [C_2H_2] e^{-\frac{12100}{T}} \cdot \sqrt{A_{soot}}$$

(3) Particle Oxidation by O_2

$$C_{(S)} + \tfrac{1}{2} O_2 \rightarrow CO \qquad \dot{\omega}_3 = 10^4 [O_2] e^{-\frac{19000}{T}} \cdot \sqrt{T} \cdot A_{soot}$$

(4) Particle Oxidation by OH

$$C_{(S)} + OH \rightarrow CO + H \qquad \dot{\omega}_4 = 0.36 [OH] \cdot \sqrt{T} \cdot A_{soot}$$

(5) Particle Coagulation

$$nP \rightarrow P_n \qquad \dot{\omega}_5 = -c_a \left(\frac{24R}{\rho_S N_A} \right)^{\frac{1}{2}} \left(\frac{6}{\pi \rho_S} \right)^{\frac{1}{6}} T^{\frac{1}{2}} (\rho Y_S) N_S^{\frac{11}{6}}$$

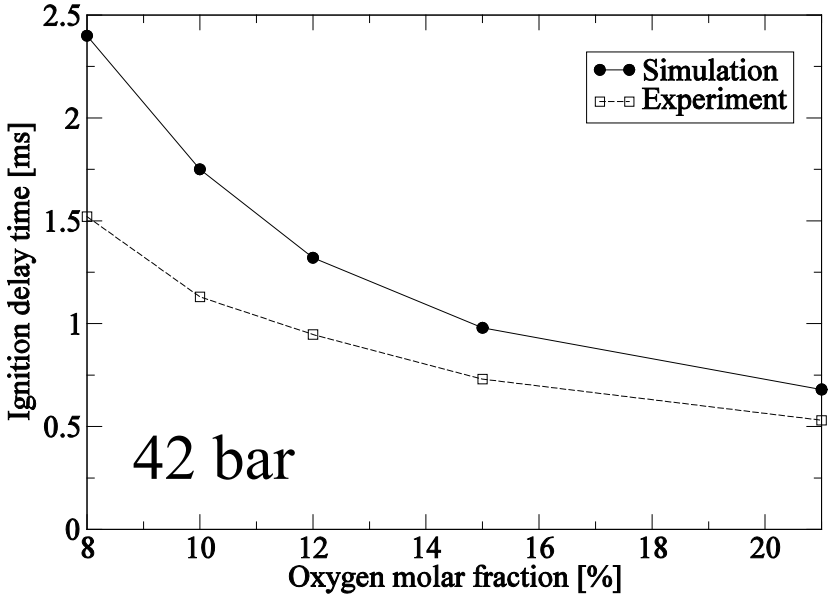
$$A_{soot} = \pi N_S^{1/3} \left(\frac{6}{\pi} \frac{\rho}{\rho_S} Y_S \right)^{2/3}$$

Figure modified from Tao et al., SAE2005-01-0121

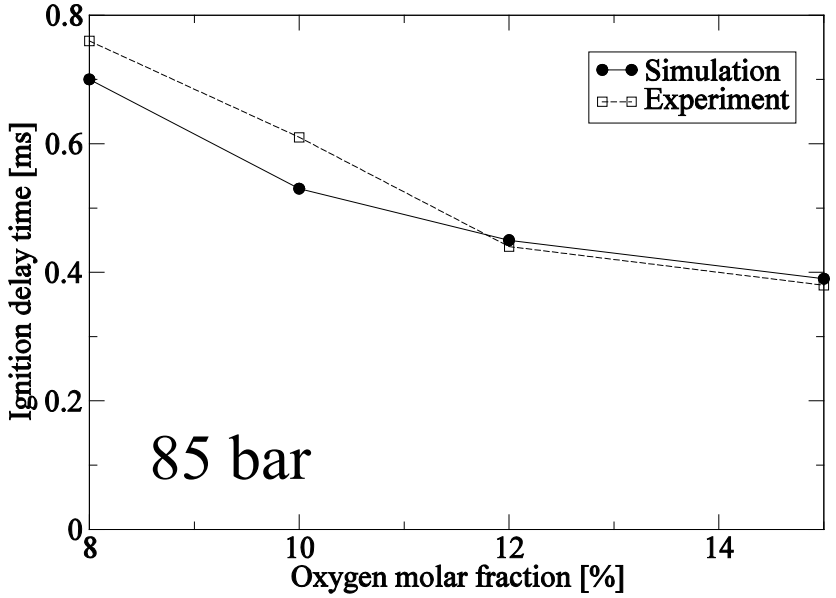
Bolla, Wright and Boulouchos., *in preparation for Comb. Sci. Techn.* (2011)

Ignition delay time

- **14.8 kg/m³**



- **30 kg/m³**

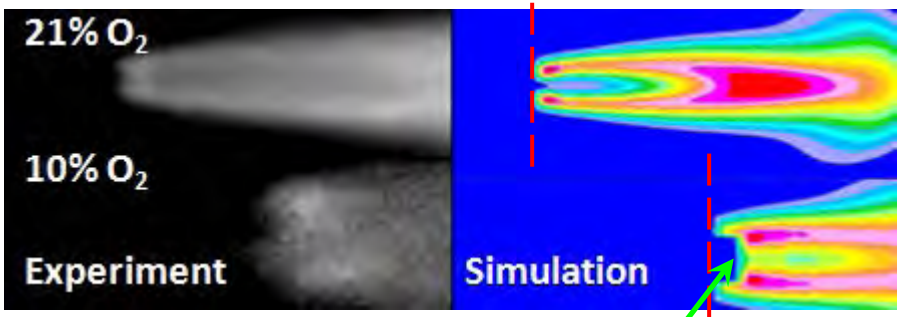


- **Over-prediction for 42 bar at lower oxygen concentration**
- **Well agreement at 85 bar**

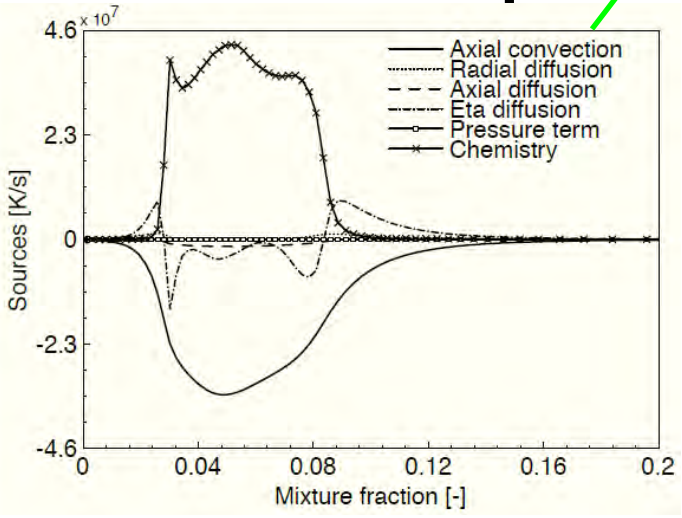
Source: Bolla, Wright and Boulouchos., *in preparation for Comb. Sci. Techn.* (2011)

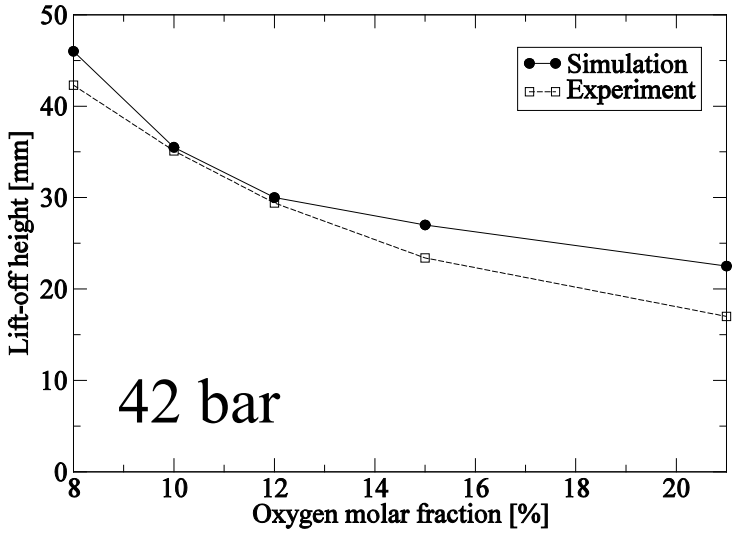
Flame lift-off heights

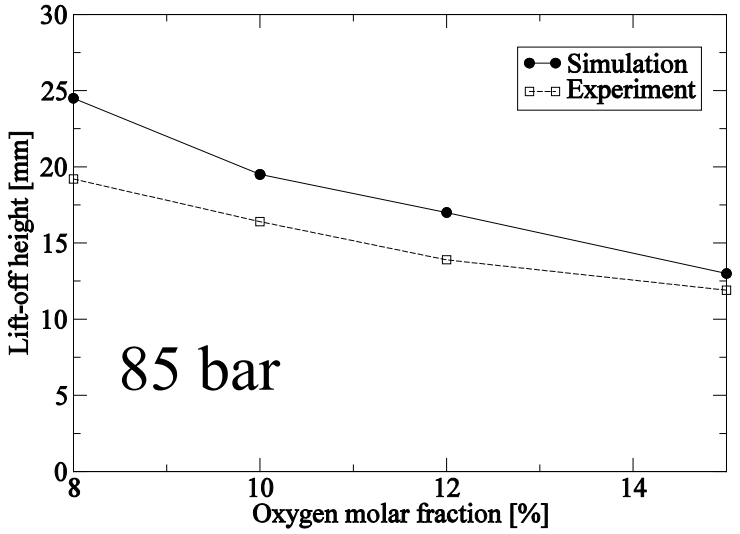
- **Good predictions of lift-off heights**



- **Convective-reactive balance in conditional temperature equation**





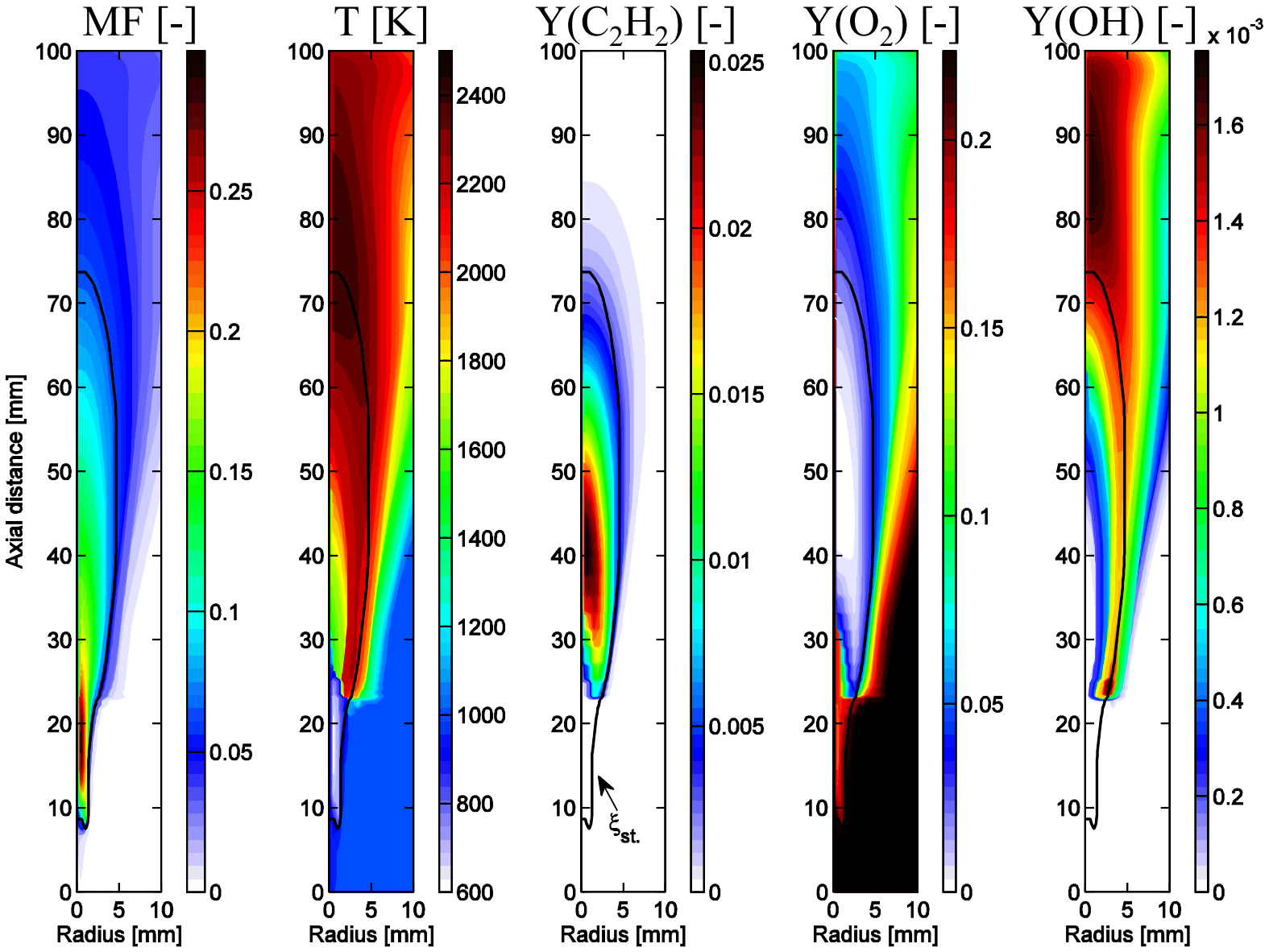


Source: Borghesi et al., *Comb. Theory Model.* (2011)

Bolla, Wright and Boulouchos., *in preparation for Comb. Sci. Techn.* (2011)

Flame structure

Soot relevant quantities-(21% O_2, 42 bar, 5ms)



Source: Bolla, Wright & Boulouchos, *in preparation for Comb. Sci. Techn.* (2011)

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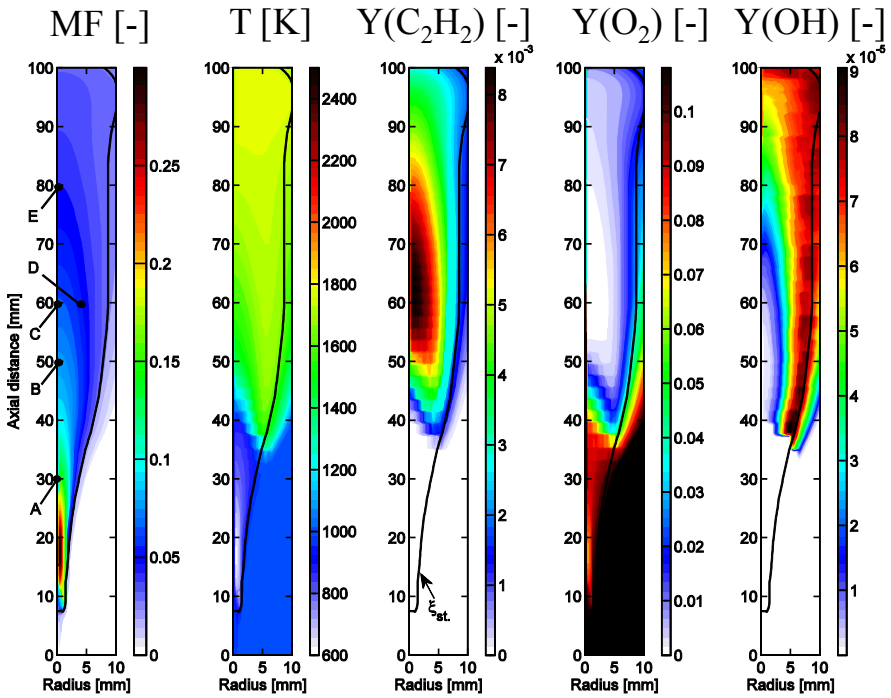
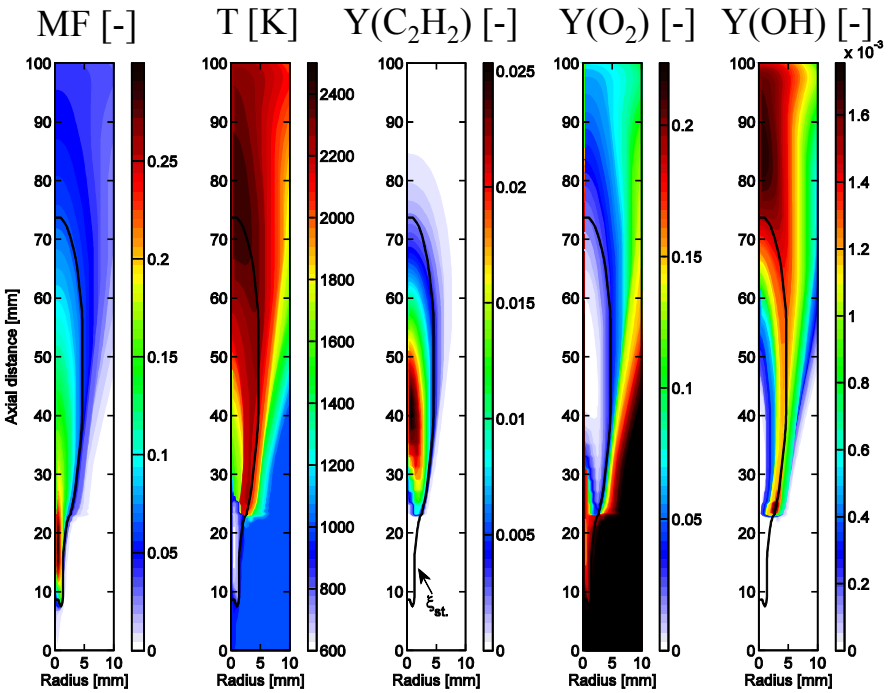
Swiss Federal Institute of Technology Zurich

Flame structure
Influence of O_2 concentration ('EGR' effect)

- **10% O_2 ($\xi_{st.}$=0.03)**
- **21% O_2 ($\xi_{st.}$=0.062)**





- **With lower oxygen:**
  - τ_{id} ↗ $H_{lift\text{-}off}$ ↗
  - $\xi_{st.}$ ↘ T_{flame} ↘ $Y(C_2H_2)$ ↘ $Y(O_2)$ ↘ $Y(OH)$ ↘

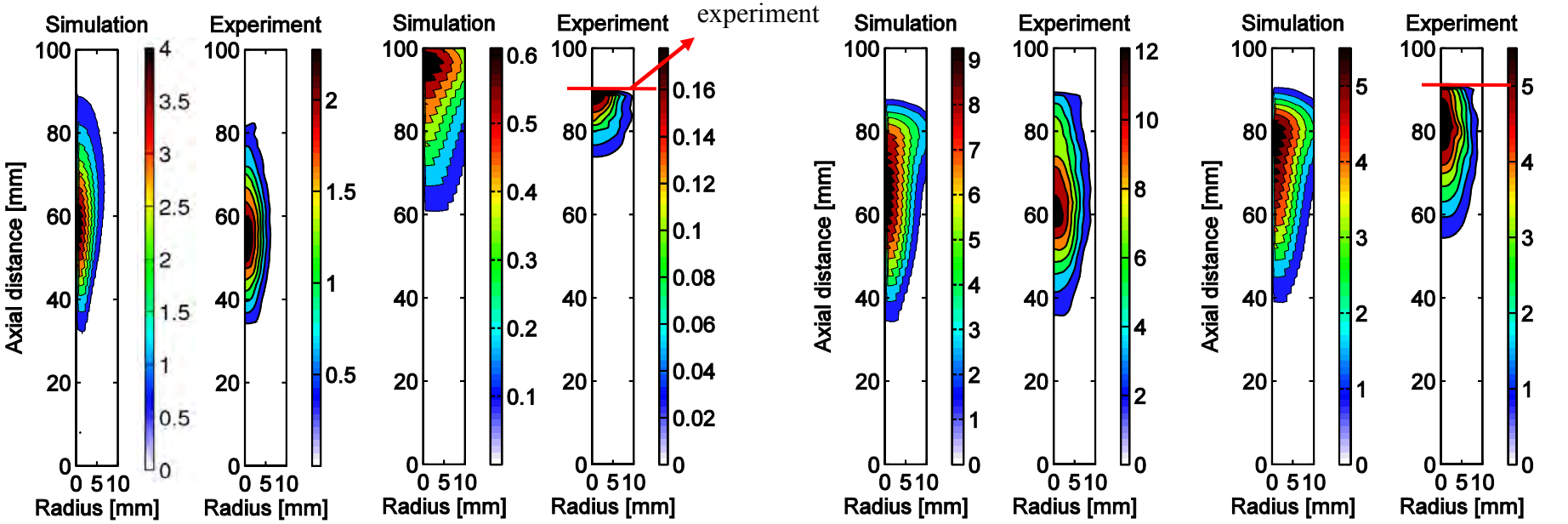
Source: Bolla, Wright & Boulouchos, *in preparation for Comb. Sci. Techn.* (2011)

Soot results: soot volume fraction [ppmv] spatial distribution

- **Good predictions for all 9 conditions (2 pressures, 5 EGR rates)**

42 bar | **85 bar**

21 % O_2 | **10 % O_2** | **15 % O_2** | **10 % O_2**

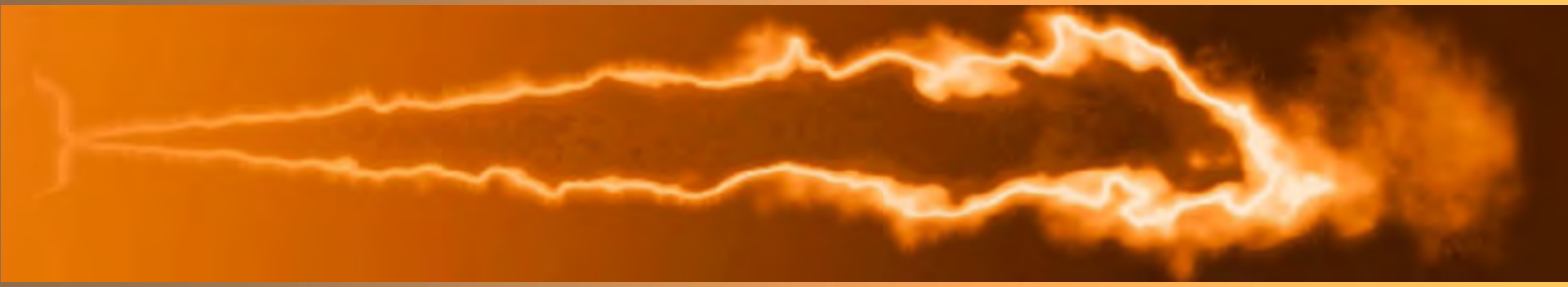


Source: Bolla, Wright & Boulouchos, *in preparation for Comb. Sci. Techn.* (2011)

Conclusions & Outlook

- First attempt of soot modeling with two-phase multi-dimensional CMC
- Good predictions of ignition delay and lift-off heights for 5 'EGR' levels at 2 pressures without changes in model parameters and rxn rates.
- Influence of oxygen concentration on soot relevant quantities was shown
- Soot formation well described for all 9 cases with standard model
- CMC was found to be a promising framework for soot modeling under diesel engine conditions
- Outlook
  - Soot model:
    - Investigate influence of soot differential diffusion effects [Kronenburg, C&F 2000]
    - Method of Moments for particle dynamics [Frenklach 2002]
    - Explore different PAH inception paths
  - Application:
    - Chemical mechanism for diesel surrogates (70%n-Heptane+30%Toluene) [Chen et al., FUEL 2009]
    - Soot model applied in a diesel engine

Thank you.



M. Bolla, Y.M. Wright and K. Boulouchos

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ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory, Switzerland

Regenerationsvorgänge und Emissionen verschiedener DPF-Systeme mit RME

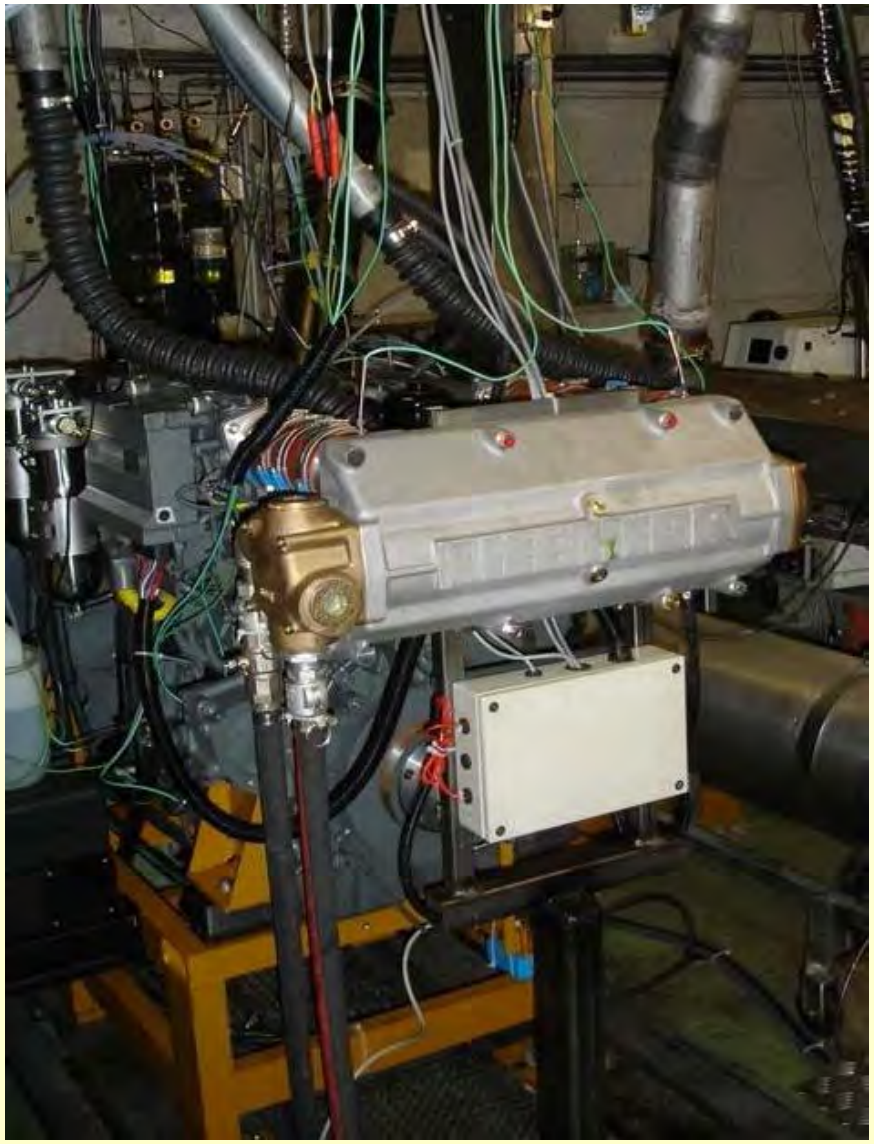
J. Czerwinski, P. Bonsack, S. Bürki, A. Krasniqi
University of Applied Sciences, Biel-Bienne, CH, (AFHB)

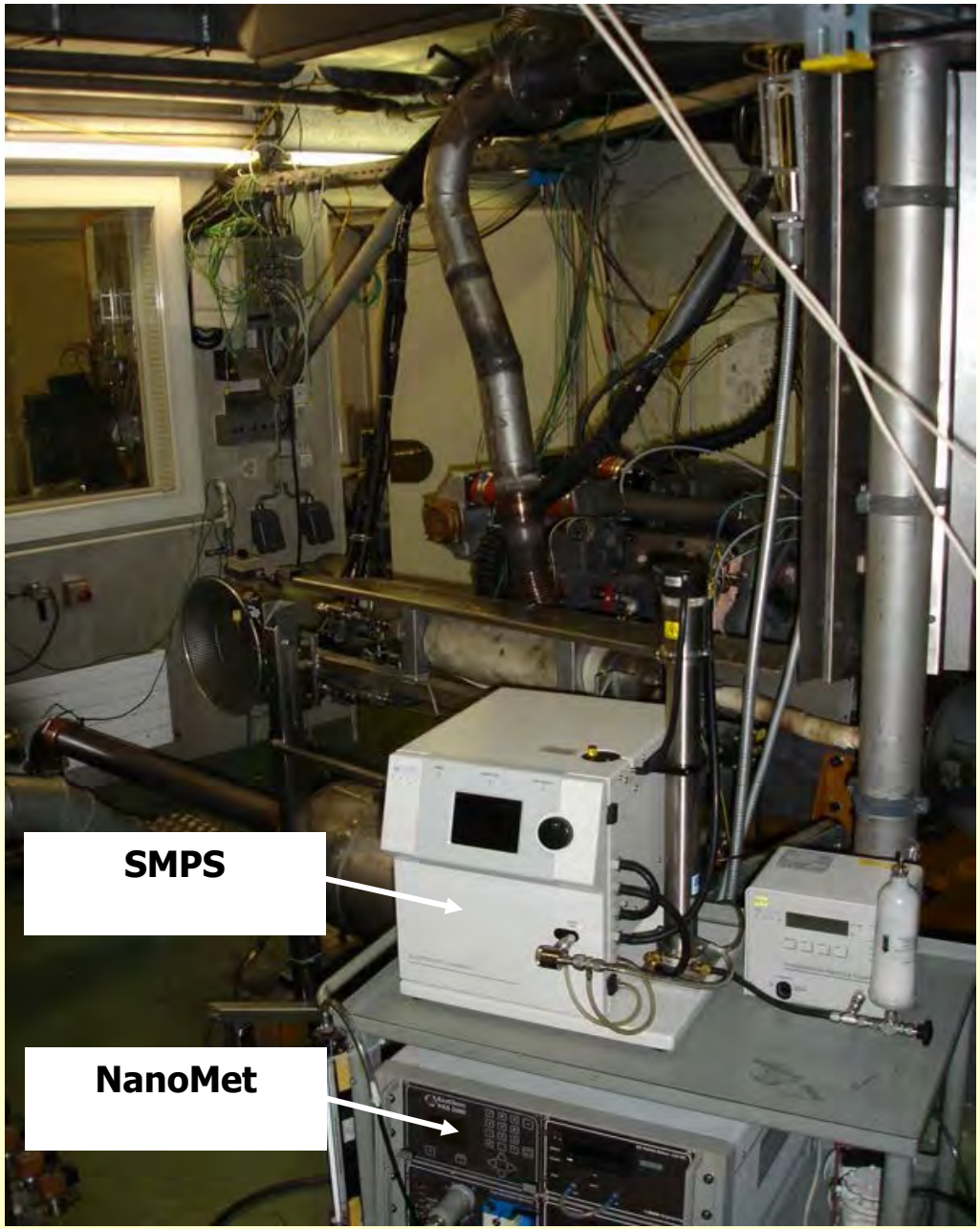
Verbrennungstagung 2011, ETH Zürich

Measuring Set-up

TEST ENGINE

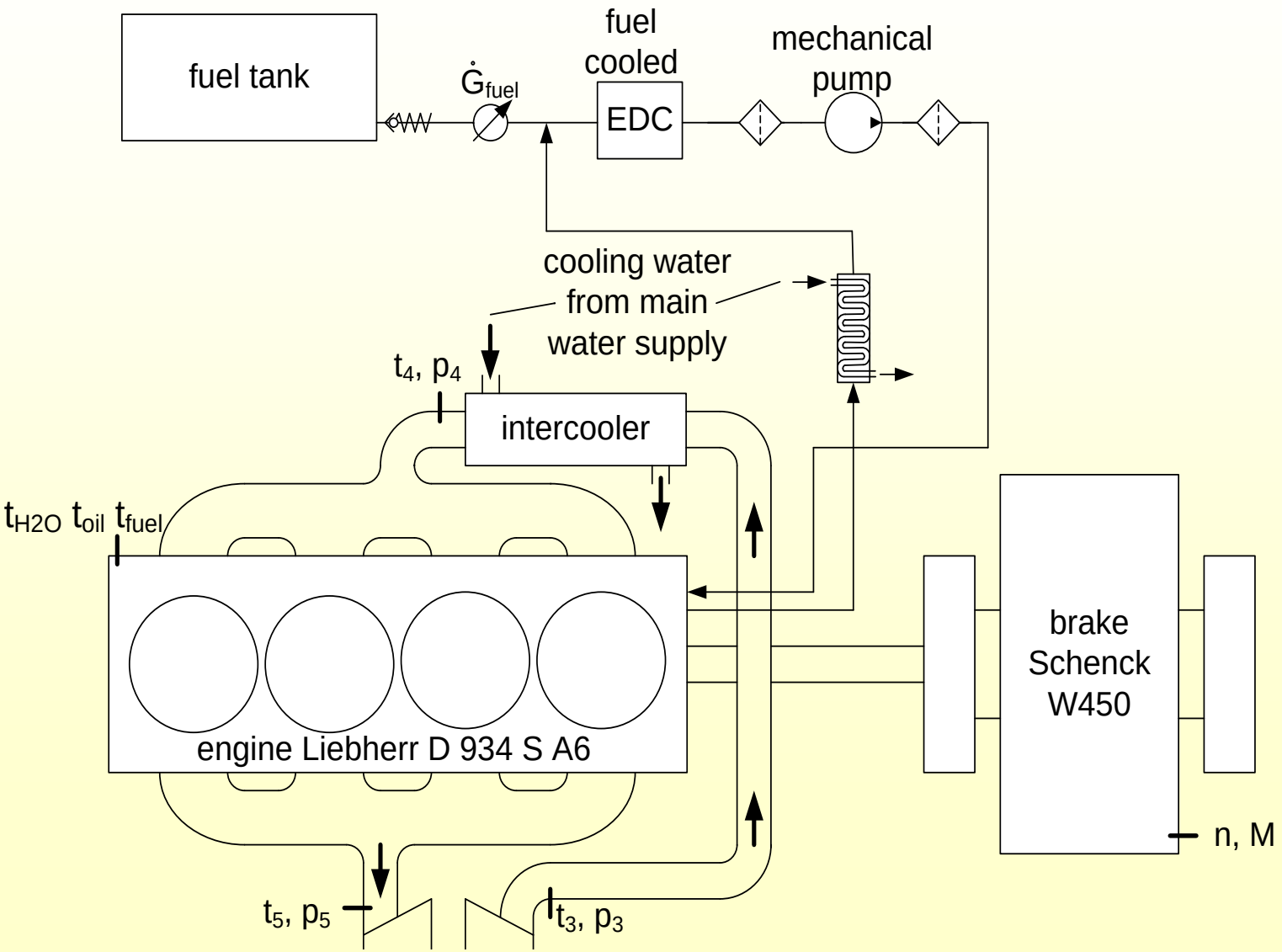
Manufacturer:	Liebherr Machines Bulle S.A., Bulle/Fribourg
Type:	D934 S
Cylinder volume:	6.36 Liters
Rated RPM:	2000 min^{-1}
Rated power:	111 kW
Model:	4 cylinder in-line
Combustion process:	direct injection
Injection pump:	Bosch unit pumps
Supercharging:	Turbocharger with intercooling
Emission control:	none (exhaust gas aftertreatment according to the requirements)
Development period:	2005



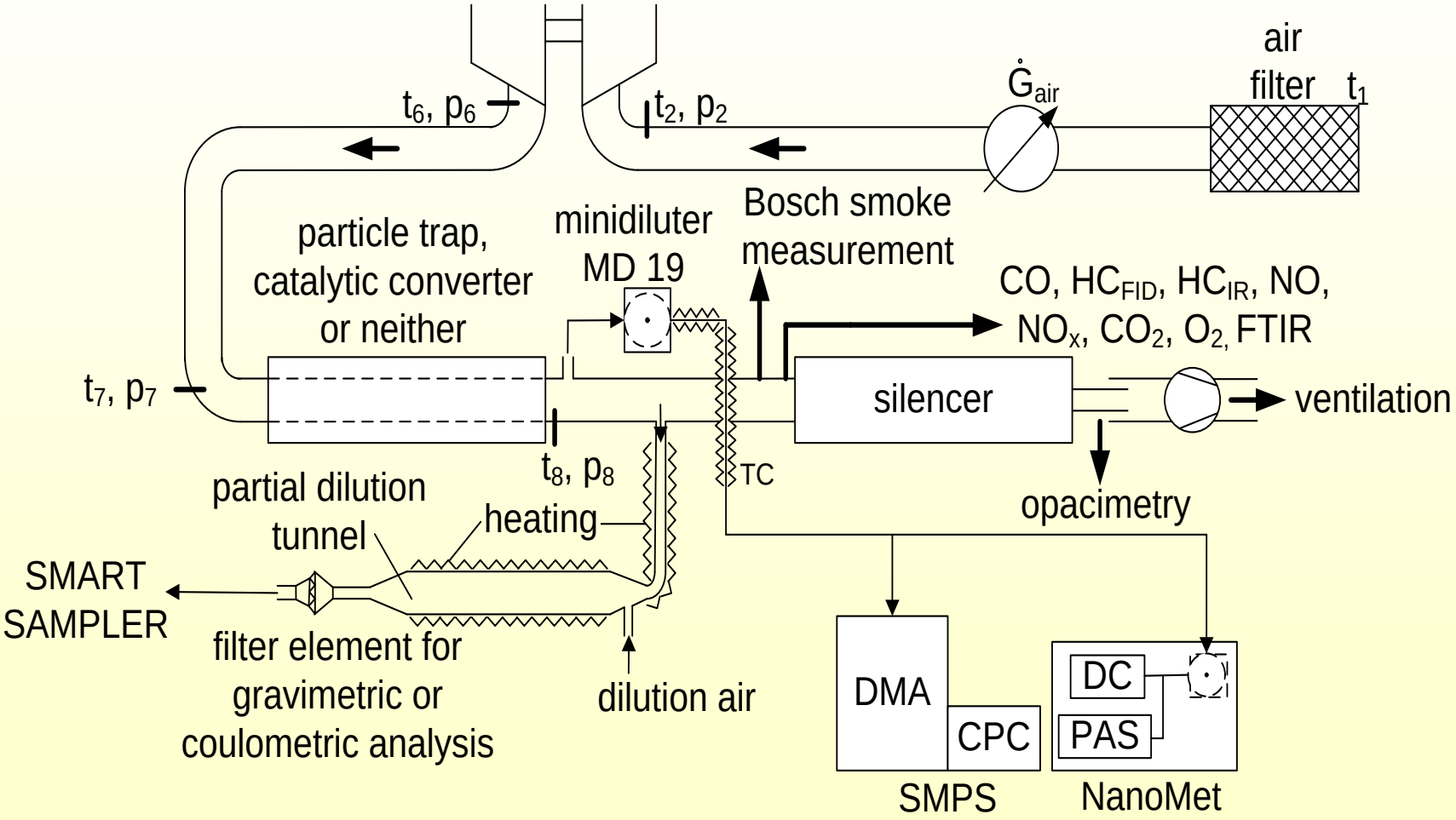


Equipment for nanoparticle measurements in the engine room

Measuring set-up (1)



Measuring set-up (2)



Investigated Fuels

	ρ(20°C) [kg/dm³]	Hu [MJ / kg]	Air min [kg A / kg F]
Diesel	0.832	42.70	14.52
RME 20	0.842	41.55	14.10
RME 100	0.880	37.20	12.49

Investigated DPF-Systems

Investigated DPF-Systems

HUG DOC + CSF
HUG mobiclean R5
DOC - Pt coating 2g/l, CSF - V coating 14g/l

HUG CSF
HUG mobiclean R5 basic
CSF – V coating 16g/l

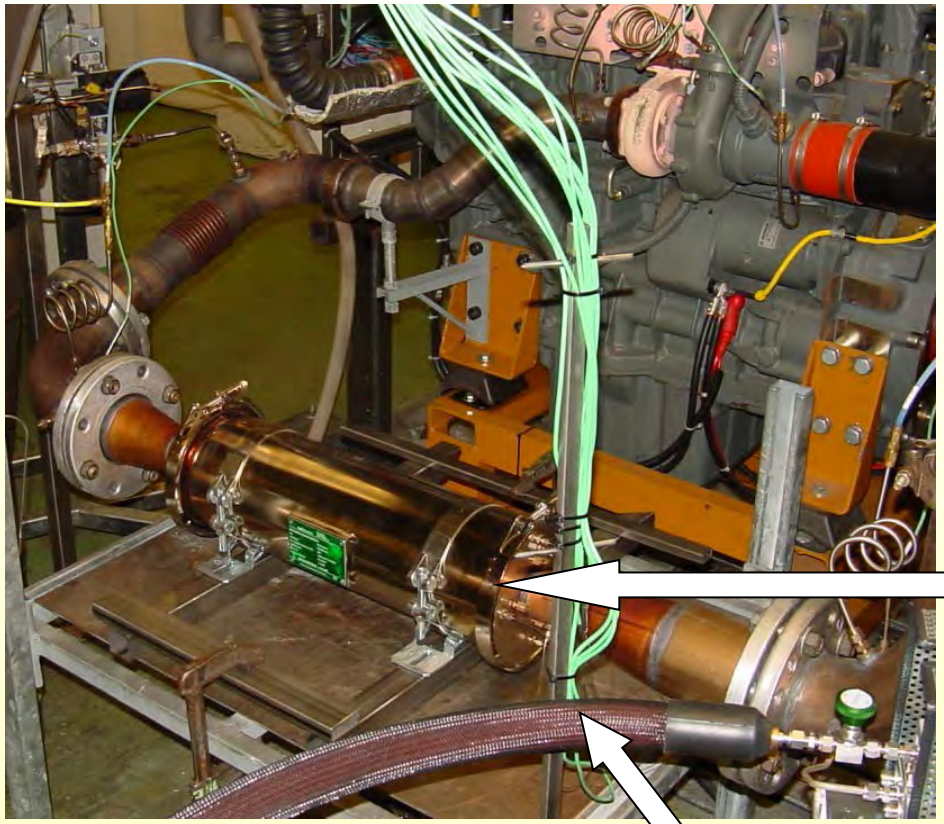
passive regenerations

HUSS MK system
with standstill burner regeneration

HUSS MD system
fuel injection + DOC

active regenerations

DPF-Systems HUG on the engine test bench

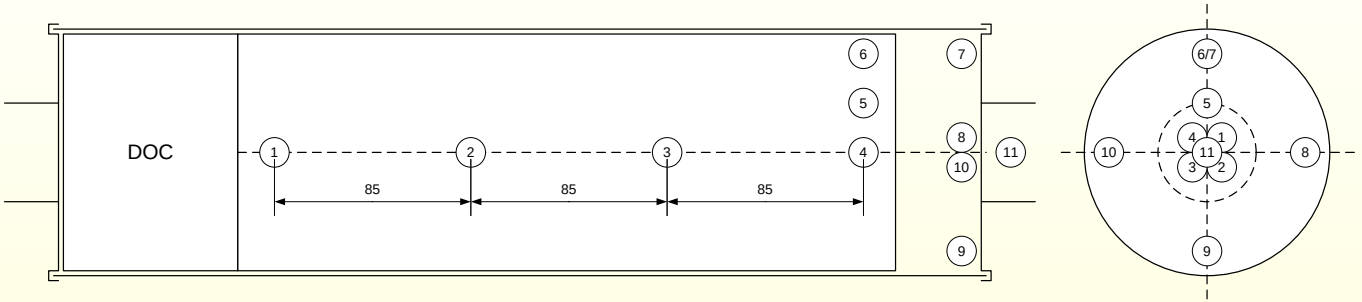


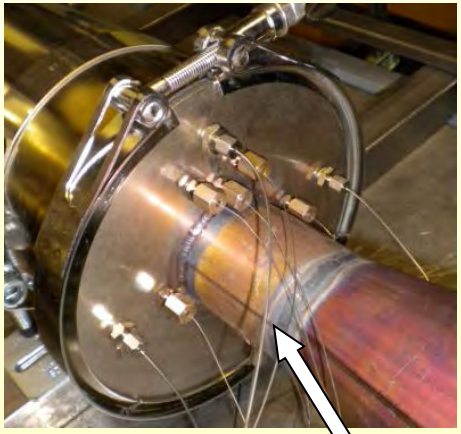
DPF installed in the exhaust line

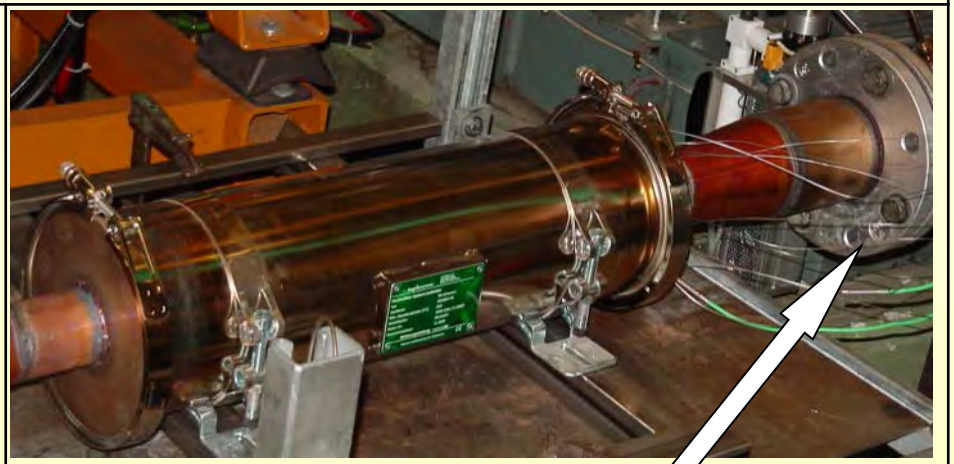
Heated sampling line for exhaust gas analysis

Thermocouples for Research of regeneration progress

University of Applied Sciences
Biel-Bienne, Switzerland
IC-Engines and Exhaust Gas Control



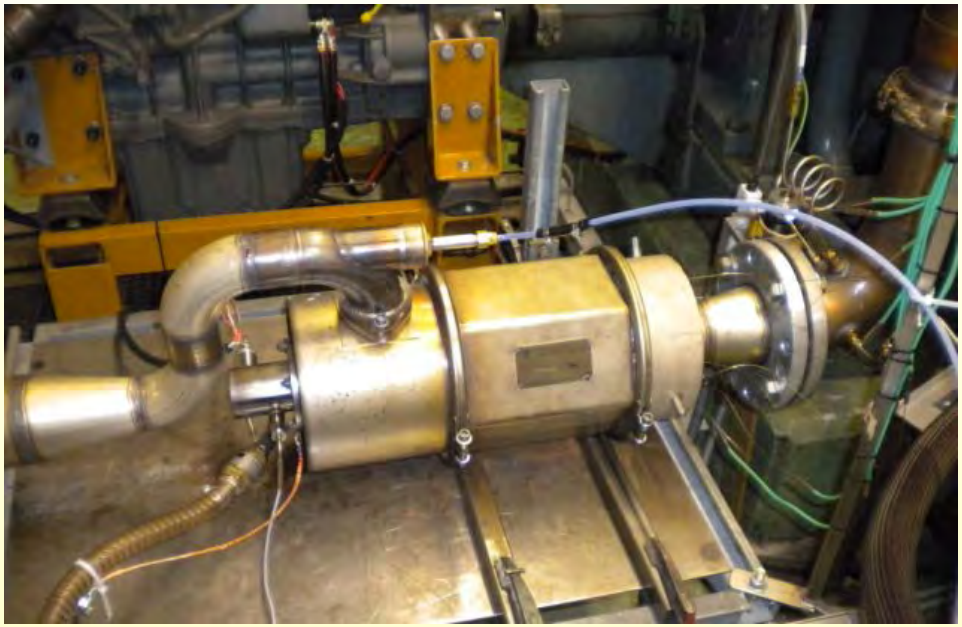


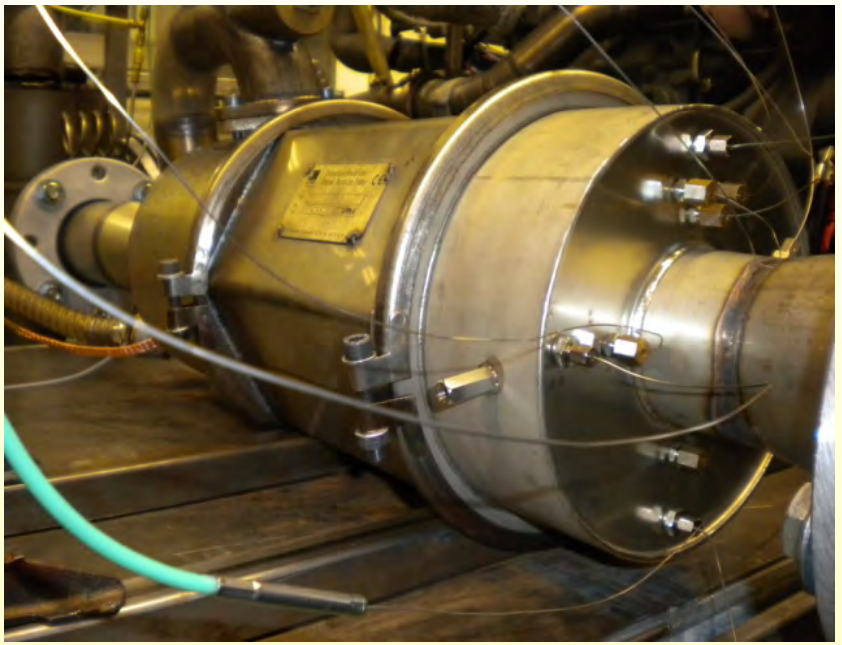


Thermocouples for research of regeneration progress

DPF-System HUSS MK on the engine test bench

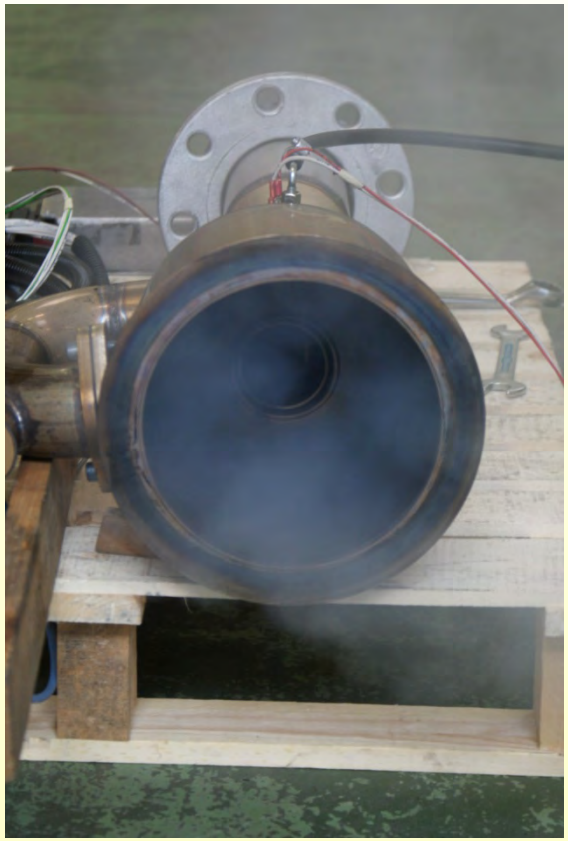
University of Applied Sciences
Biel-Bienne, Switzerland
IC-Engines and Exhaust Gas Control



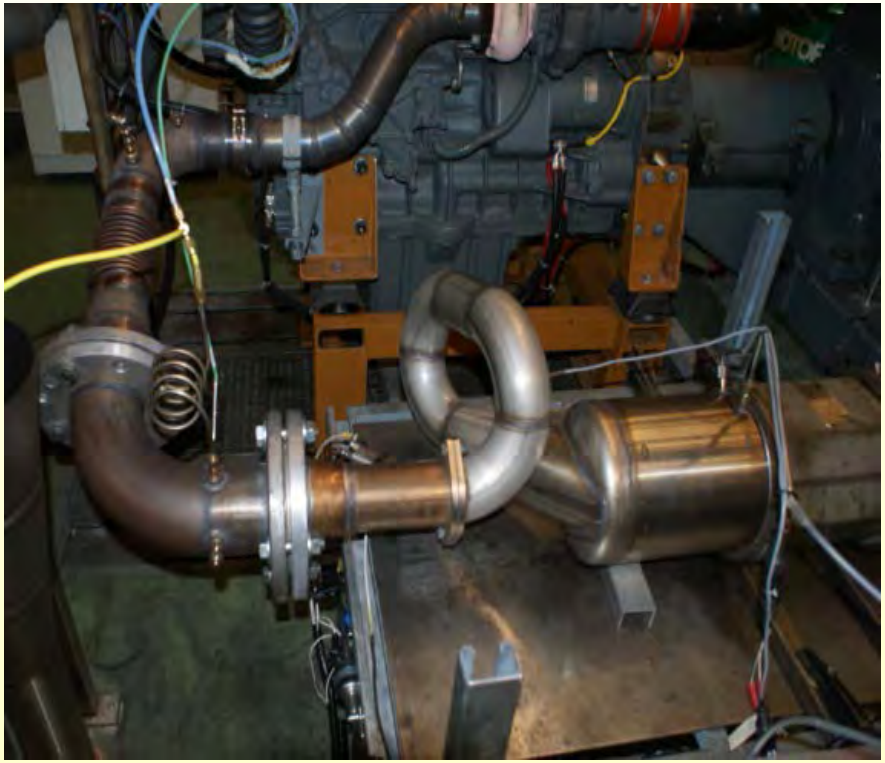


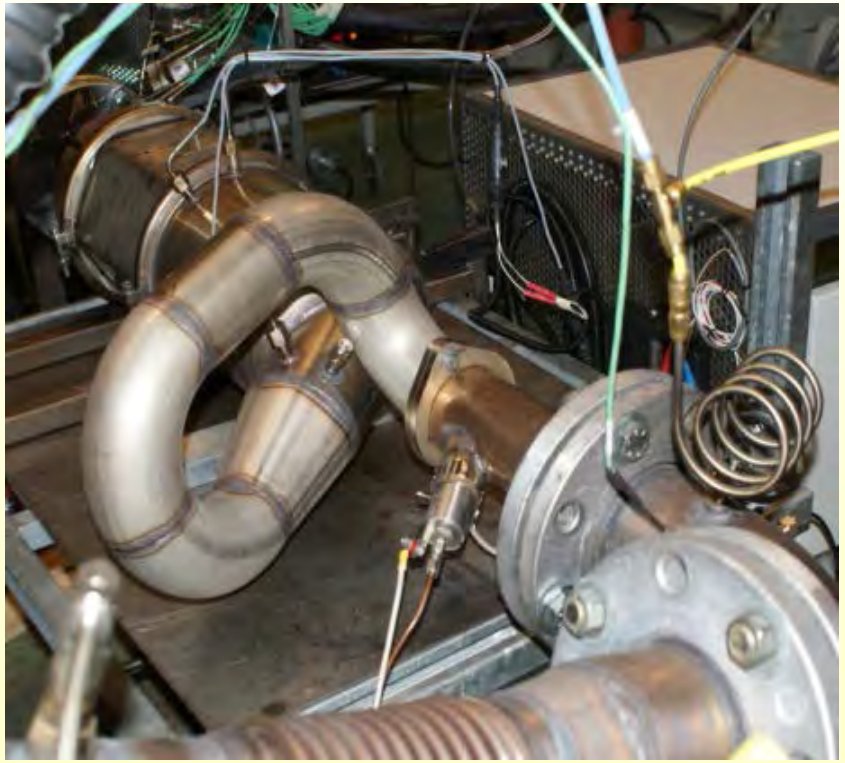
DPF-System HUSS MK external test of the standstill burner

University of Applied Sciences
Biel-Bienne, Switzerland
IC-Engines and Exhaust Gas Control



DPF System HUSS MD on the Engine Test Bench

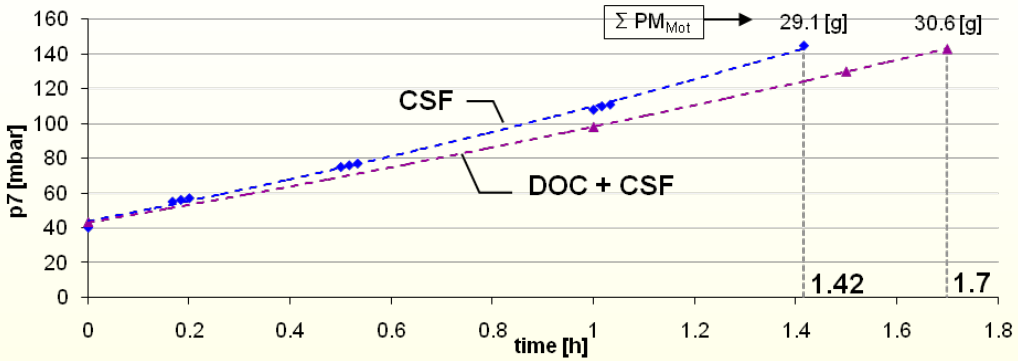




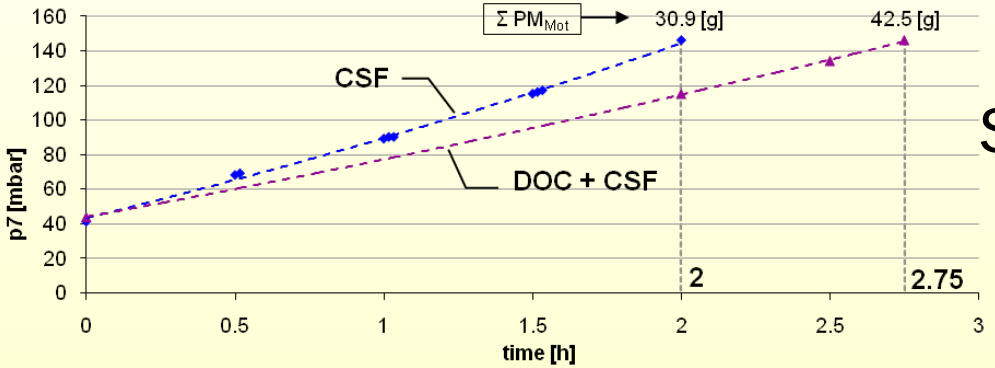
Results

Soot Loading

Backpressure during soot loading CSF vs DOC + CSF

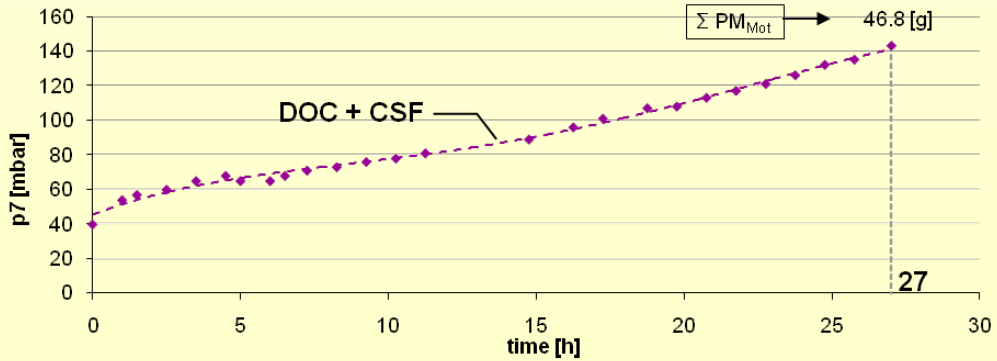


Soot loading Diesel (B0)



Soot loading B20

Soot loading B100

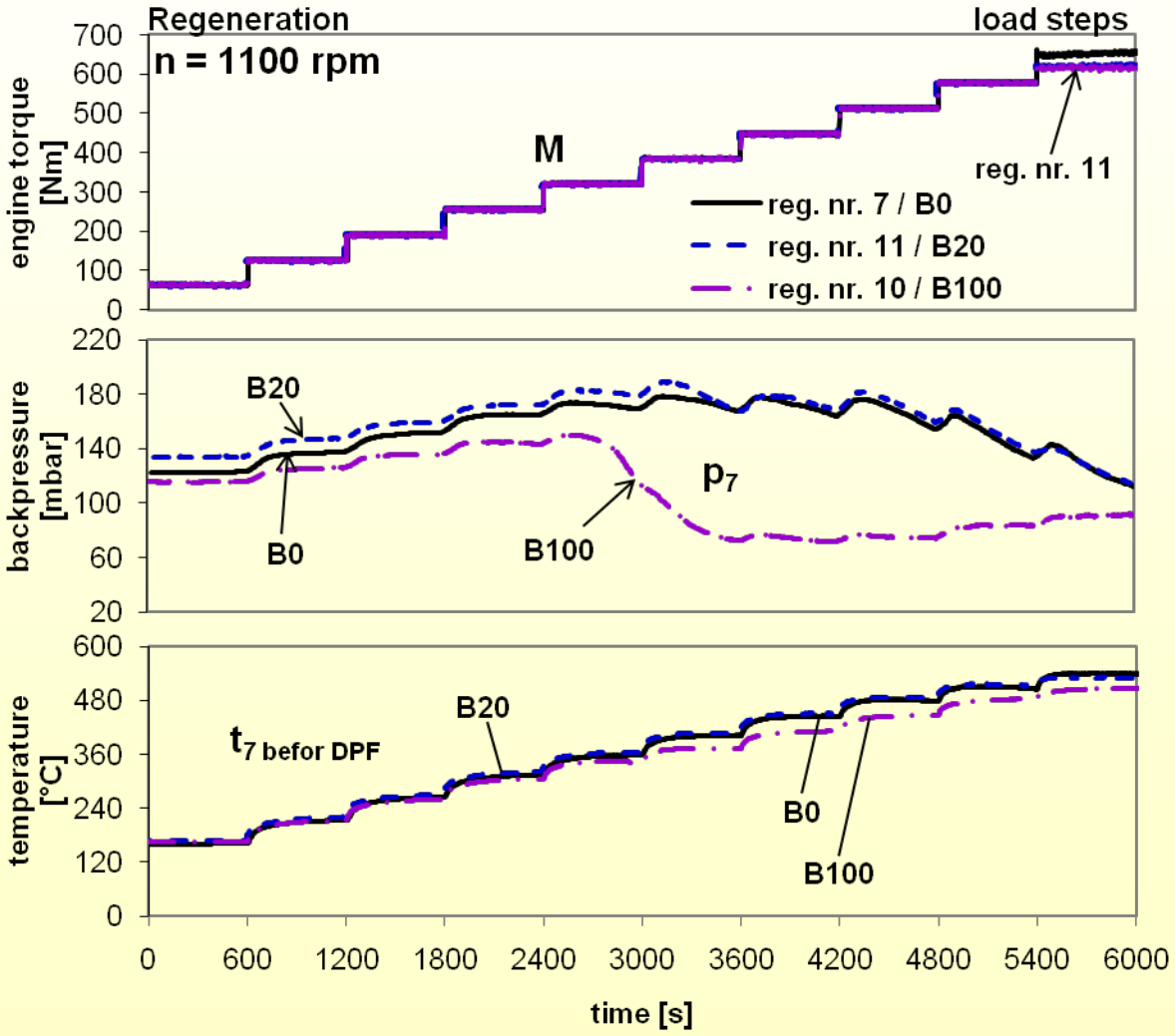


Regeneratins with

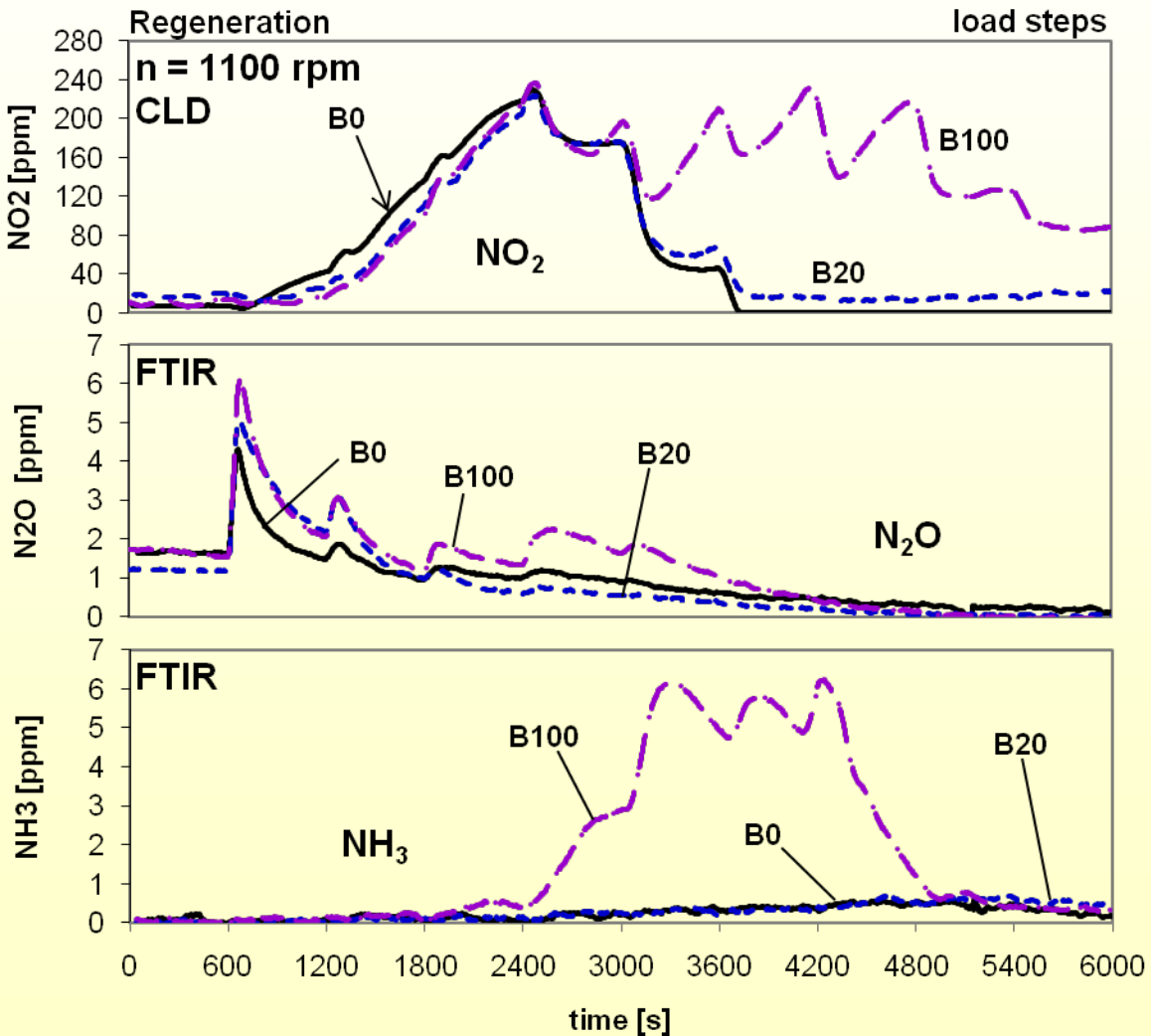
B0, B20 & B100

(DOC + CSF)

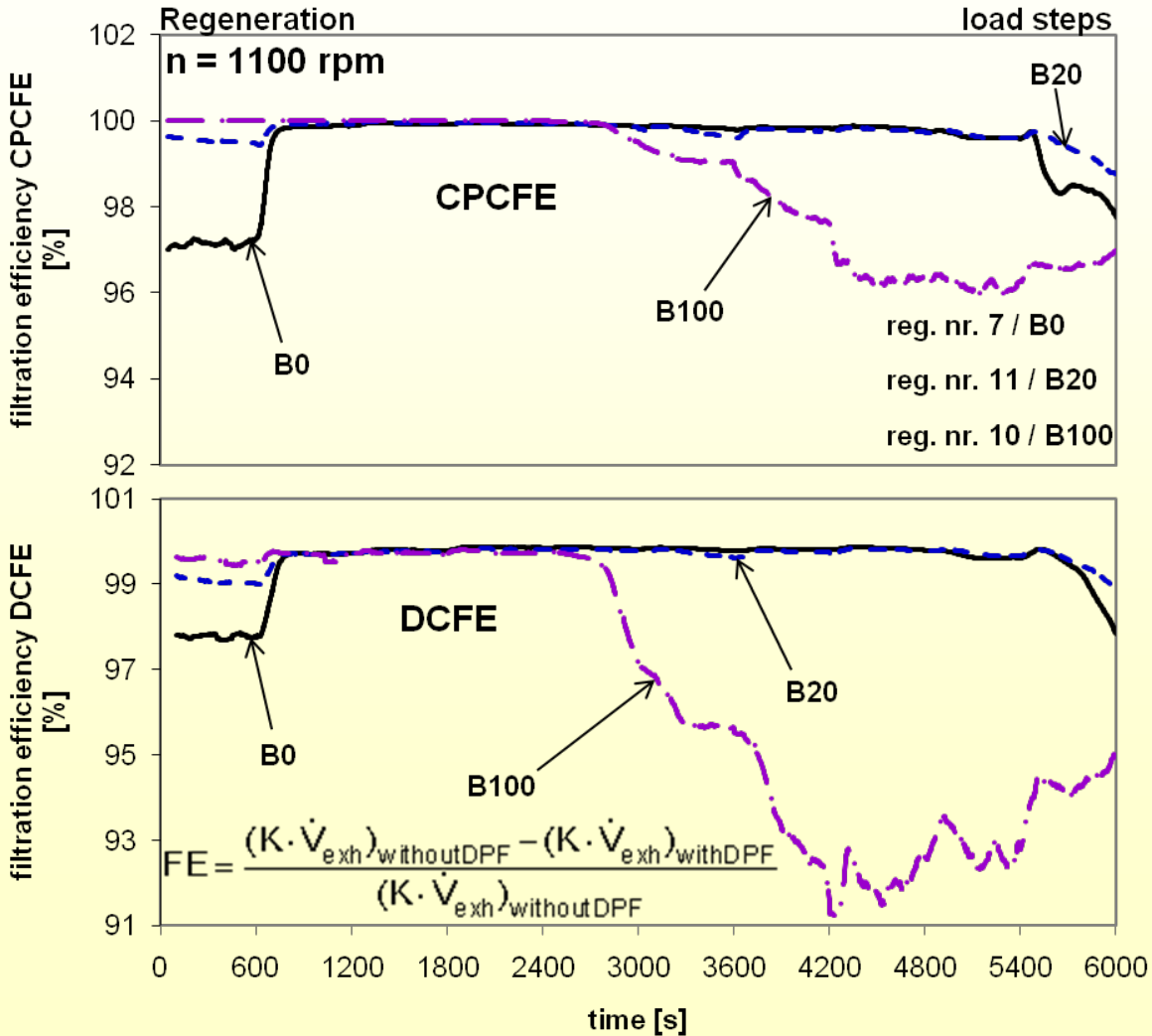
Regenerations with (DOC + CSF) & B0, B20, B100



Regenerations with (DOC + CSF) & B0, B20, B100



Instantaneous nanoparticle filtration efficiency during the regeneration procedures with (DOC + CSF) & B0, B20, B100

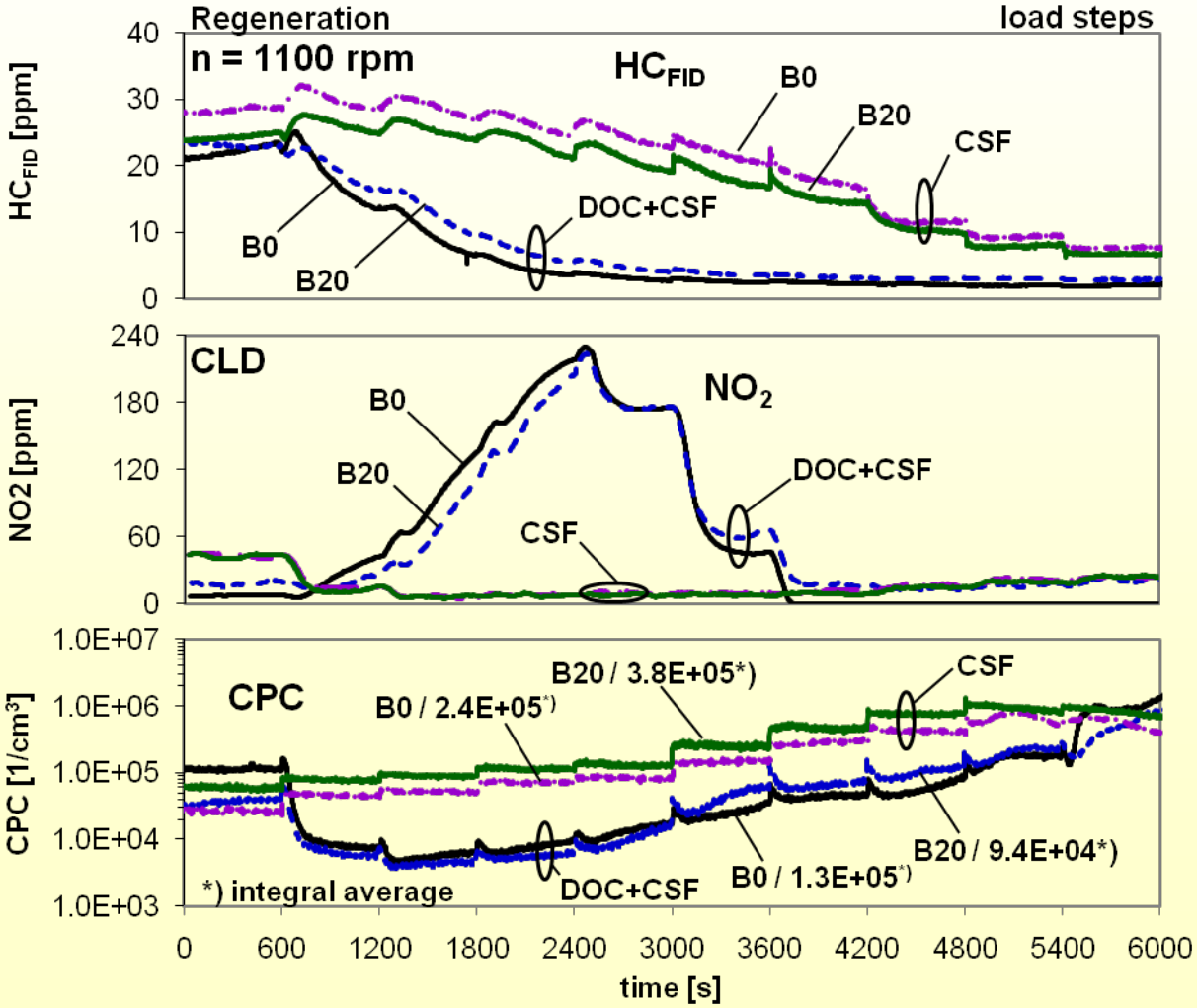


Regenerations with

(DOC + CSF) vs. (CSF)

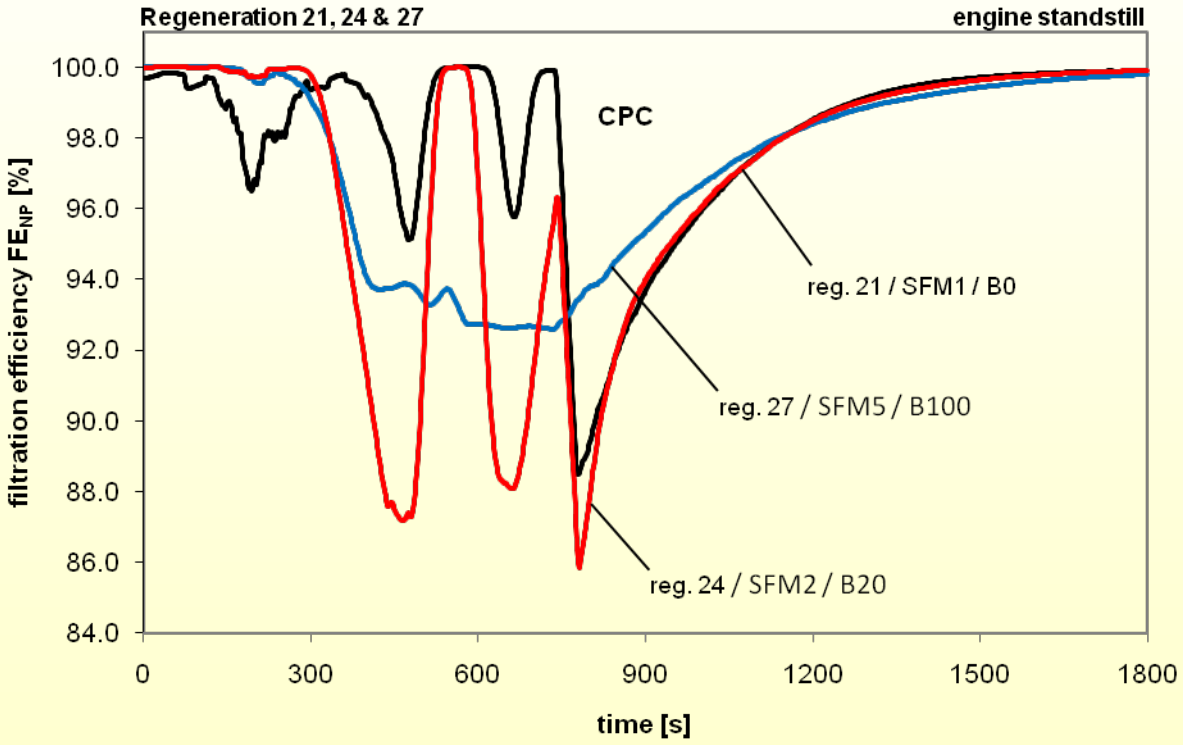
B0 & B20

Regeneration with (DOC + CSF) vs. (CSF) with B0 & B20



Nanoparticle Instantaneous Reduction Rate with Standstill Burner

Comparison of instantaneous filtration efficiecies during the standstill burner regeneration with different Bio-content (burner fuel B0 & B20)*)

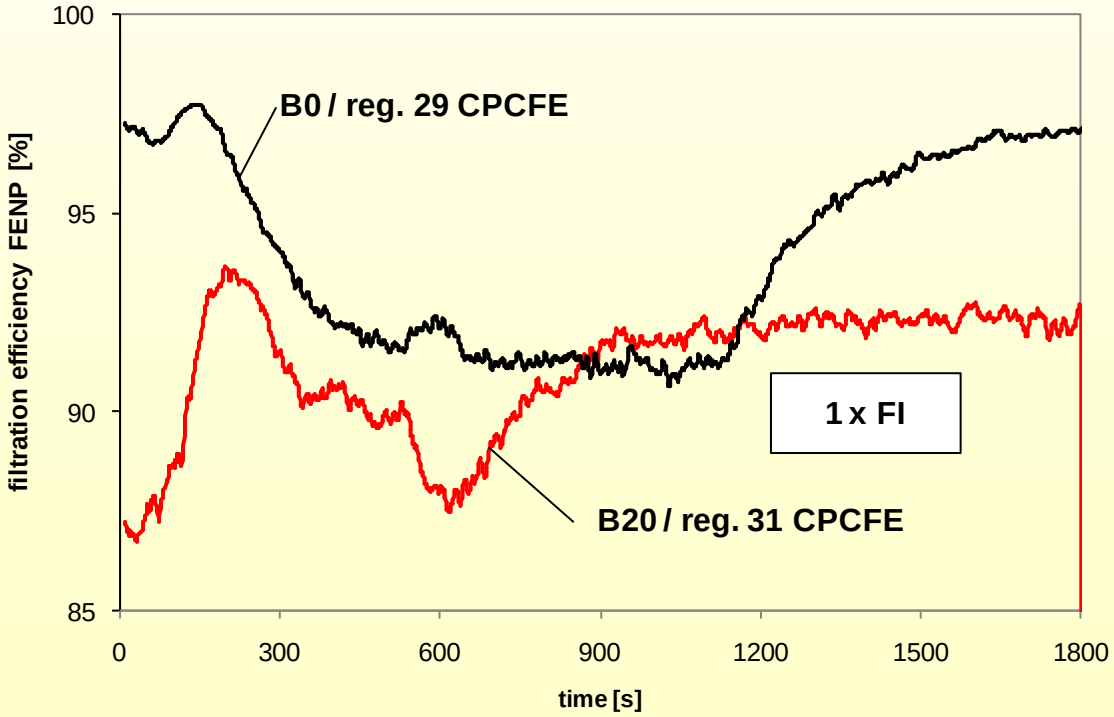


$$FE_{NP} = \frac{(K)_{withoutDPF} - (K)_{withDPF}}{(K)_{withoutDPF}}$$

*) all reg. with burner fuel B0 except reg. 24 with B20

Nanoparticle Filtration Efficiency with Fuel Injection + DOC

CPC Filtration Efficiency during Regeneration with B0 & B20



Fazit Passive Systeme

Fazit Passive Systeme (1)

Durch die Erhöhung vom B-Gehalt entsteht eine längere Beladungszeit weil:

- geringere PM-Emission (engine-out)
- stärkere Reaktion der PM → Oxidation in DOC
- intensive NO_2-Bildung durch den DOC

Fazit Passive Systeme (2)

- Die Regenerationintensität ist mit B100 am höchsten
- Sehr gute Wiederholbarkeit der Regeneration
- Bedingt durch die unterschiedlichen Beladungszustände ist in der ersten Stufe eine Abweichung des Gegendruckes ersichtlich

Fazit Passive Systeme (3)

- Abgastemperatur beim Erreichen des Balancepunktes:

DOC + CSF			**CSF**	
B0	B20	B100	B0	B20
362°C	360°C	342°C	460°C	450°C
at step 5	at step 5	at step 5	at step 7	at step 7

- Keine NO_2-Entstehung mit CSF

Fazit Aktive Systeme

Fazit standstill burner regeneration

- Die Temperatur- und Emissionenverläufe sind vom Regenerationsverfahren abhängig
- Die Nanopartikelkonzentration ist während der Flammperiode verstärkt, der Abscheidegrad ist niedriger
- Die Biokomponenten erhöhen die NO_x - & NO_2 - Werte, sowie die NP-Emissionen während der Flammperiode

Fazit FI + DOC

- Durch die längere Einspritzdauer (doppelte Einspritzung) wird das hohe Temperaturniveau, welches für die Regeneration benötigt wird, verlängert
- Bei Lasterhöhung der Regeneration ist eine Zunahme der Temperatur und der NO_x feststellbar
- Nach dem Ende der Einspritzung ist eine intensive Erhöhung der NO_2-Konzentration erkennbar. Dieses Phänomen ist bedingt durch das Sinken der Abgastemperatur in den Bereich der maximalen NO_2-Entstehung


Thank you
for your
attention !

ETH
Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo

BfE Verbrennungsforschungstagung 28th Oct. 2011

Multiplecycle-LES Simulation of an 1.4L DI gas engine

M. Schmitt, Y.M. Wright, C.E. Frouzakis and K. Boulouchos

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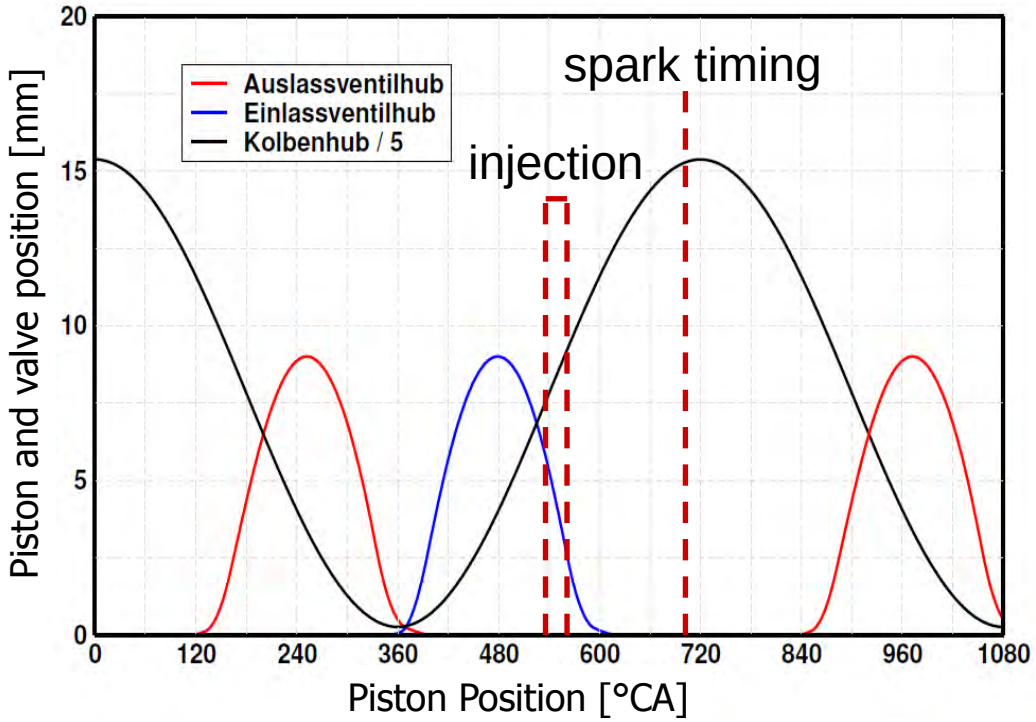
ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory, Switzerland

Outline

- **Experimental configuration and conditions**
- **Numerical setup**
- **Simulation matrix**
- **Single cycle calculations**
  - Wall heat losses
  - Combustion with G-equation
- **Multiple cycle calculations**
  - Setup
  - Results
- **Discussion / open questions**

Engine specifications and operating condition

- **Four-stroke, turbo-charged passenger car engine**
- **1.4 litres total displacement, four cylinders**
- **Direct injected gasoline, retrofitted to CH_4 direct injection**



Engine parameters:

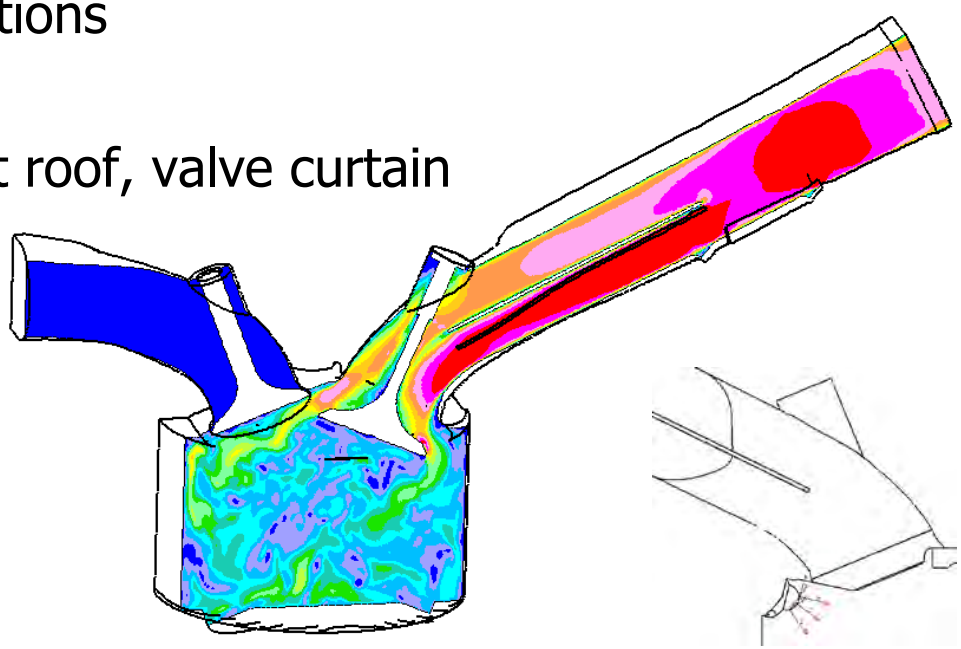
Bore	76.5 mm
Stroke	75.6 mm
Epsilon	9.6
Fuel	CH_4

Operating point :

Speed	2000 U/min
p_{mi}	2 bar
SOI	540 °CA
Spark timing	700 °CA

Simulation Setup

- **Half domain discretized**
- **Finite volume solver STAR-CD v4.14**
  - arbitrary cell shapes, fully unstructured grids
  - Compressible formulation, choked flows during scavenging
  - High performance computing w/message passing interface (clusters)
  - wide variety of user coding options
- **Mesh motion plug-in es-ICE**
  - Piston- and valve motion (pent roof, valve curtain regions overlap)
- **Models:**
  - turbulence: LES k-l
  - combustion: G-equation
  - Lagrangian-Eulerian approach for fuel injection



Grid resolutions employed

Coarse mesh (Δ = 0.65mm)

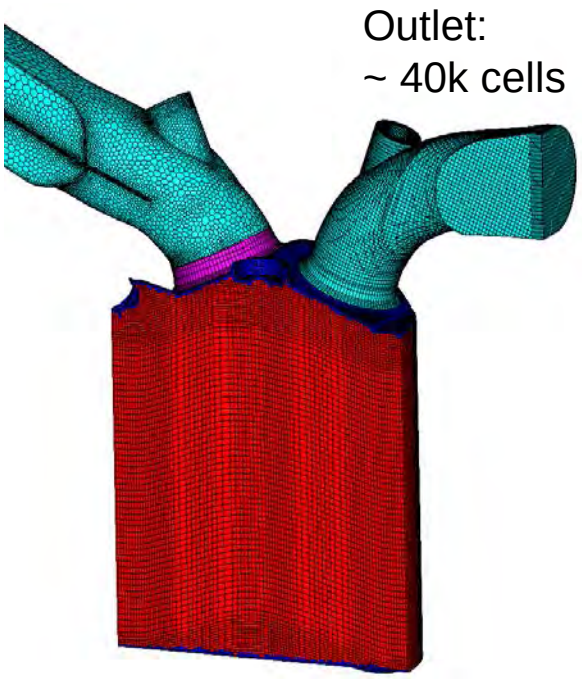
ca. 411k Cells BTC
ca. 156k Cells TDC

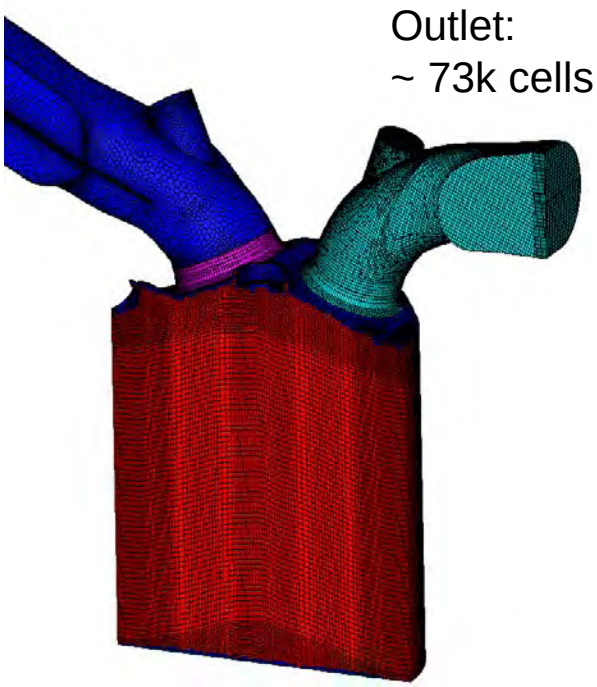
middle mesh (Δ = 0.55mm)

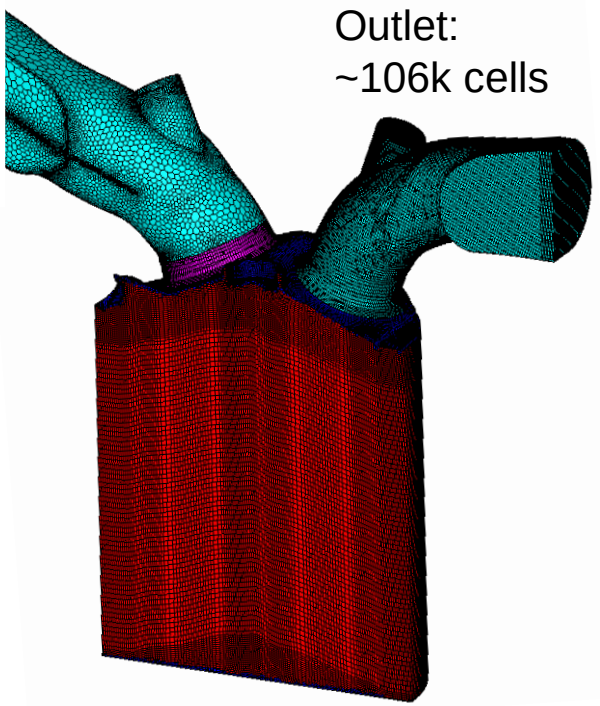
ca. 738k Cells BTC
ca. 283k Cells TDC

fine Mesh (Δ = 0.45mm)

ca. 1.196 Mio Cells BTC
ca. 412k Cells TDC







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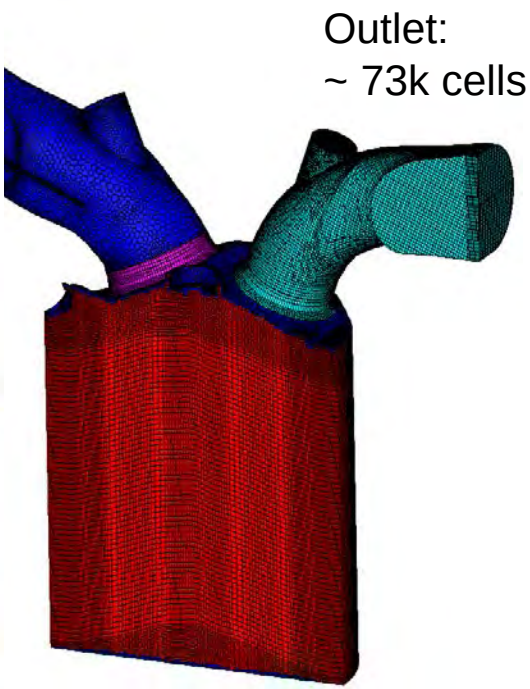
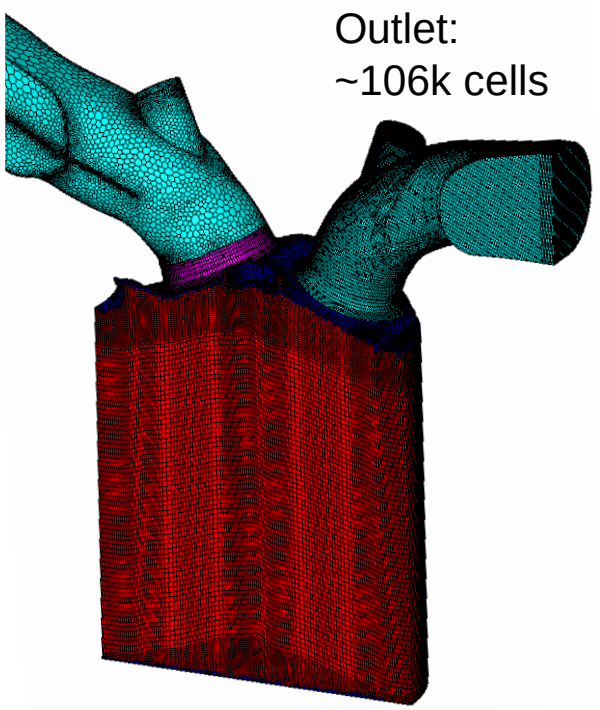
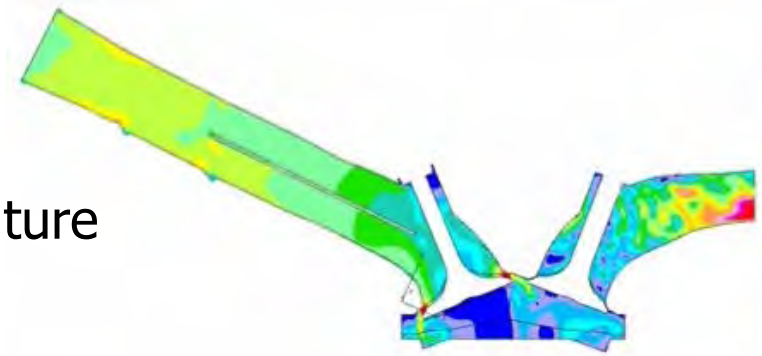




Inlet: 198k cells (polyhedral) employs stubs for simple replacement (tumble flap in intake runner)

Initial and boundary conditions

- **Simulation starts just prior to exhaust valve closure**
- **Initial conditions:**
  - Intake manifold: pure air
  - Chamber and exhaust: fully burnt products (λ=1)
- **BCs**
  - Walls: non-adiabatic, fixed temperature
  - Intake: tabulated pressure and temperature from separate stand-alone process calculation (GT-Power)
  - Exhaust: tabulated pressure, zero gradient for scalars and temperature



Simulation matrix

single cycle simulations:

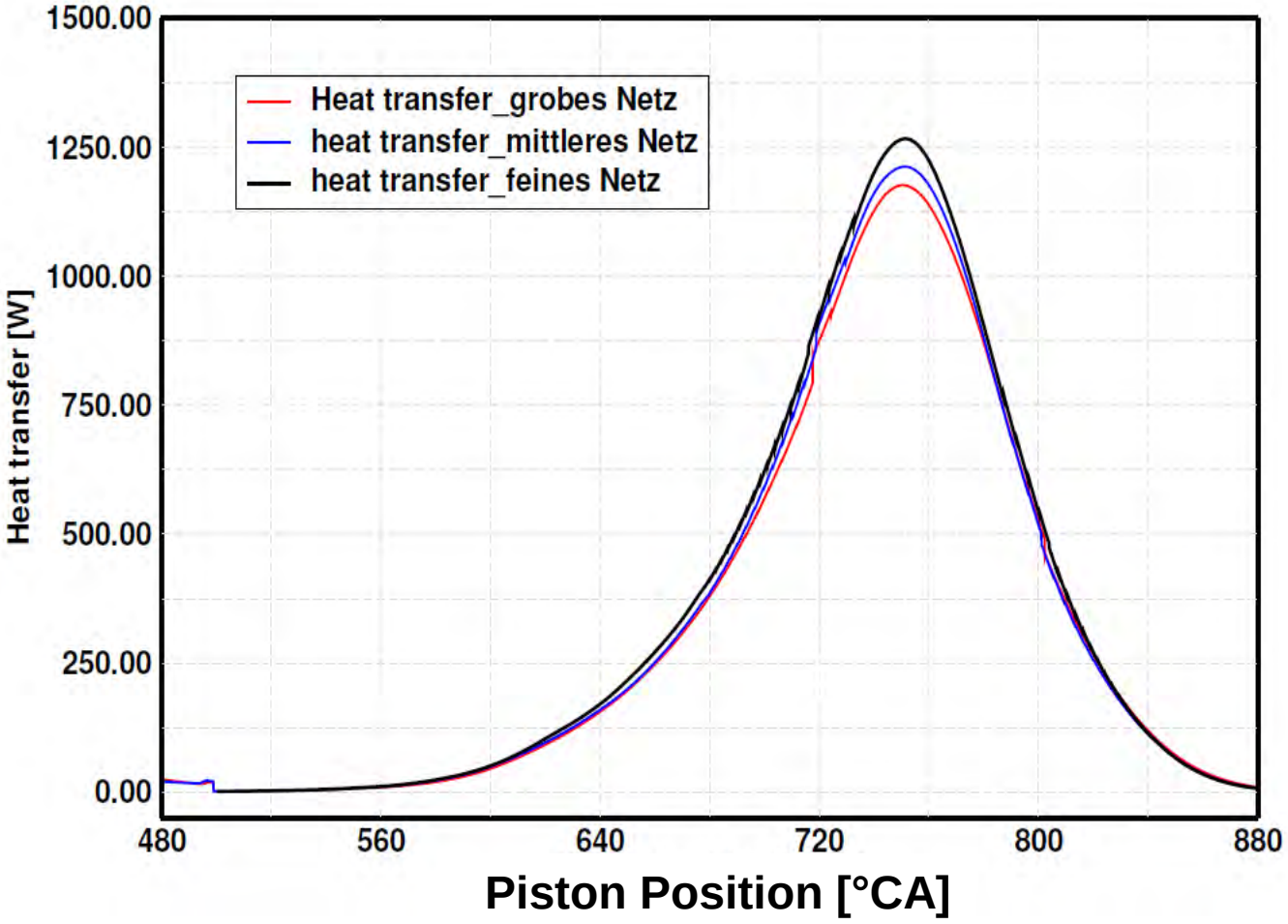
Mesh	coarse	middle	fine
Cold Flow All 2nd order	RANS LES	LES	LES
Combustion 2nd order mom./turb. 1st order temperature	RANS → LES	LES	LES

- Differences of RANS und LES calculations in engine simulations
- Change in the turbulence modeling with increasing cell number
- Differences due to the order of the numerical method for the turbulence and energy equation

Outline

- Experimental configuration and conditions
- Numerical setup
- Simulation matrix
- **Single cycle calculations**
  - Wall heat losses
  - Combustion with G-equation
- Multiple cycle calculations
  - Setup
  - Results
- Discussion / open questions

Wall heat transfer – resolution influence



maximum values:

Fine	1267 W
Middle	1212 W
Coarse	1176 W

⇒ differences:

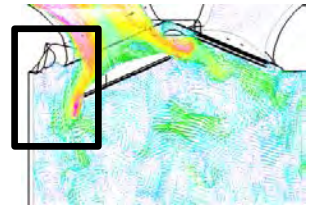
middle – fine 4.5%
coarse – fine 7.7%

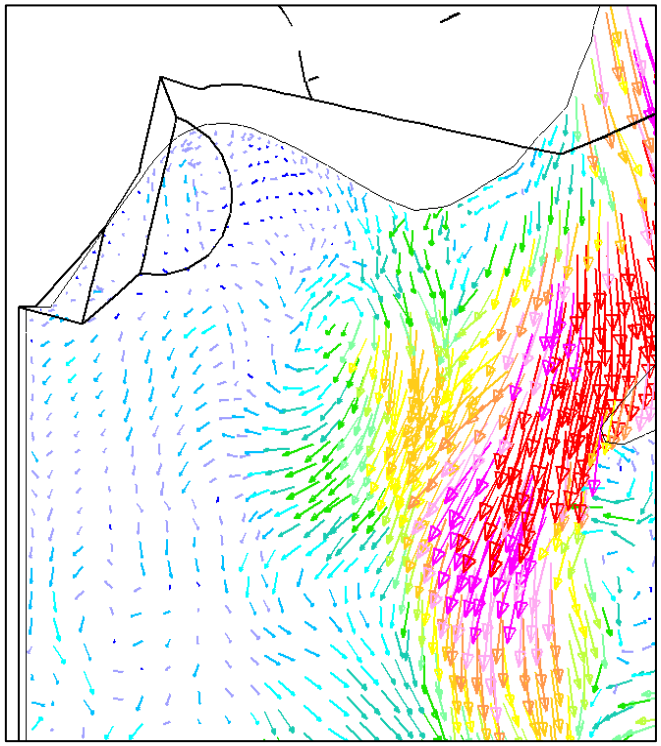
with combustion effect is more pronounced !

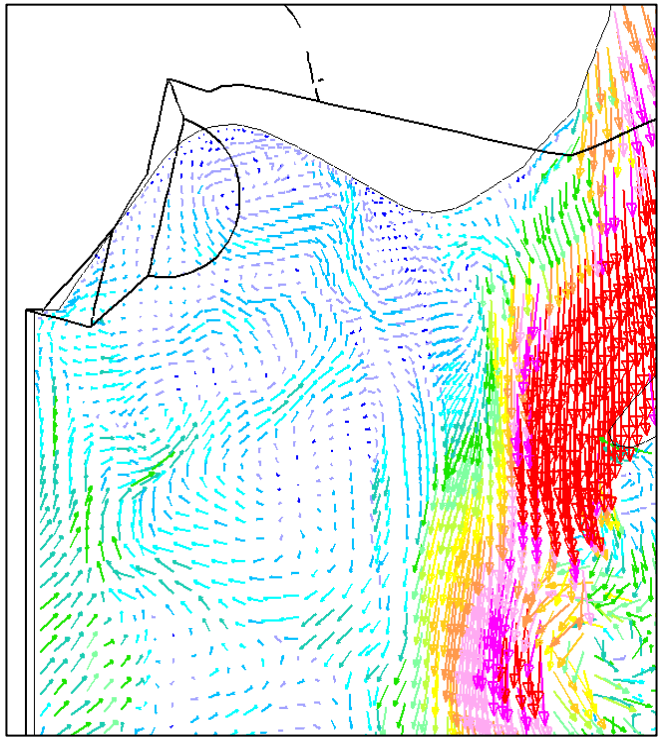
Wall heat transfer – resolution influence

coarse mesh

fine mesh







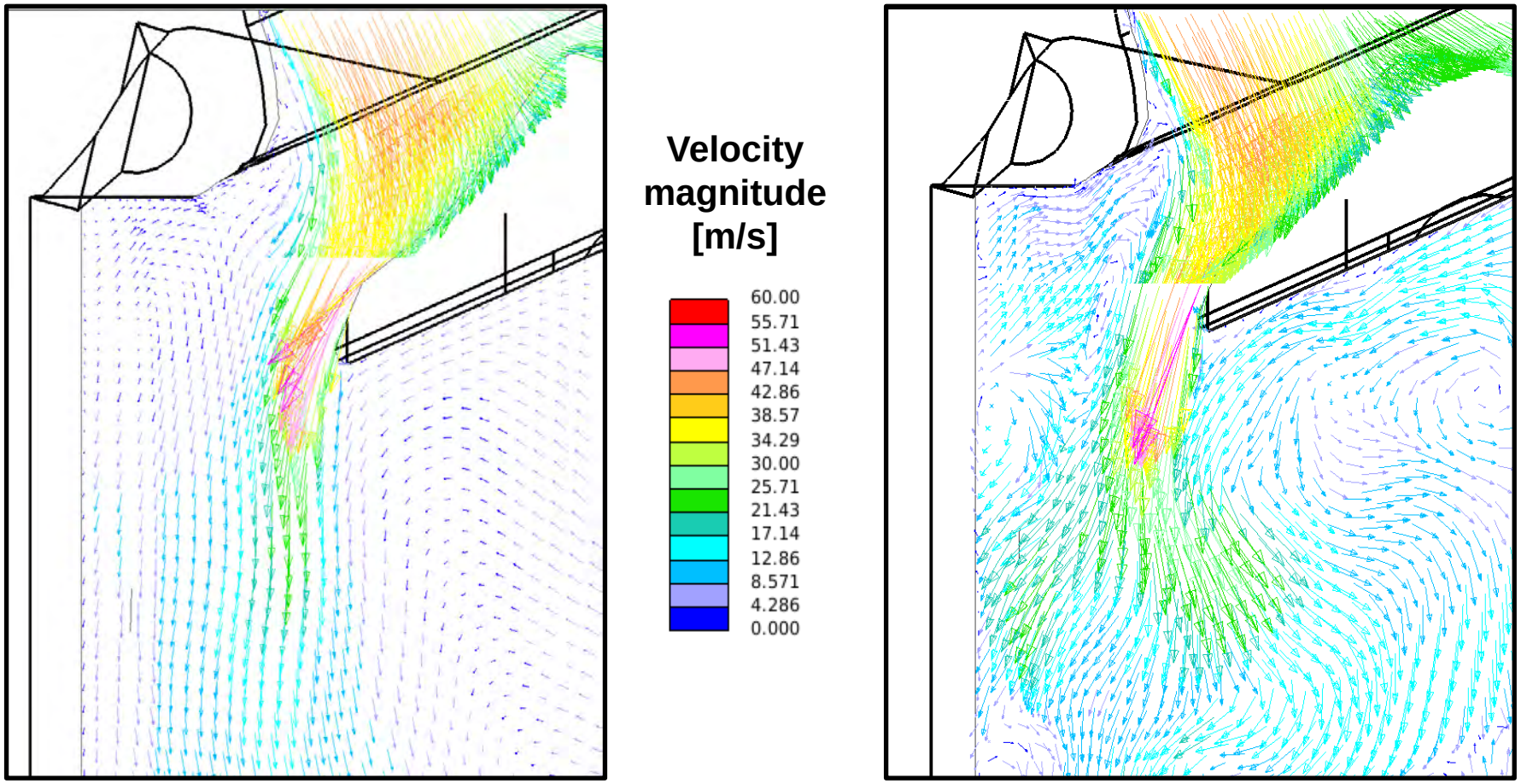
Velocity magnitude [m/s]

40.00
37.14
34.29
31.43
28.57
25.71
22.86
20.00
17.14
14.29
11.43
8.571
5.714
2.857
0.000

Wall heat Losses – potential of LES

RANS: Very low velocities at the wall

LES: Small eddies with higher velocities at the wall



G-equation model – governing equation

- **Level set approach**

$$\frac{\partial}{\partial t}\rho G + \frac{\partial}{\partial x_i}\rho u_i G = \rho s_T \left|\nabla G\right|$$

$$\frac{\partial}{\partial t}\rho G' + \frac{\partial}{\partial x_i}\rho u_i G' - \frac{\rho s_T \nabla G \cdot \nabla G'}{\left|\nabla G\right|} = 2\frac{\mu_T}{\sigma_T}\left[\frac{\partial G}{\partial x_i}\frac{\partial G}{\partial x_i}\right] - c_S \rho \frac{\varepsilon}{k} G'$$

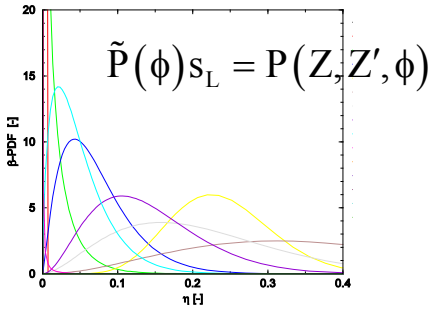
- **Need the turbulent flame speed**

$$s_T = s_L \cdot \left[1 + A \cdot \left(\frac{\sqrt{2/3\,k}}{s_L}\right)^{\frac{5}{6}}\right] \qquad s_L = \int s_{L_0}(\phi)\,\tilde{P}(\phi)\,d\phi \qquad s_{L_0} = f(\Phi)\cdot\left(\frac{T_u}{T_0}\right)^{\alpha}\cdot\left(\frac{p}{p_0}\right)^{\beta}\cdot\left(1 - f(\chi_{EGR})\right)$$

- **Account for partial premixing (mixture fraction + variance)**

$$\frac{\partial}{\partial t}\rho Z + \frac{\partial}{\partial x_i}\rho u_i Z - \frac{\partial}{\partial x_i}\left[\left(D_Z + \frac{\mu_T}{\sigma_T}\right)\frac{\partial Z}{\partial x_i}\right] = \dot{s}_d$$

$$\frac{\partial}{\partial t}\rho Z' + \frac{\partial}{\partial x_i}\rho u_i Z' - \frac{\partial}{\partial x_i}\left[\left(D_{Z'} + \frac{\mu_T}{\sigma_T}\right)\frac{\partial Z'}{\partial x_i}\right] = 2\frac{\mu_T}{\sigma_T}\left[\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}\right] - c_S \rho \frac{\varepsilon}{k} Z'$$

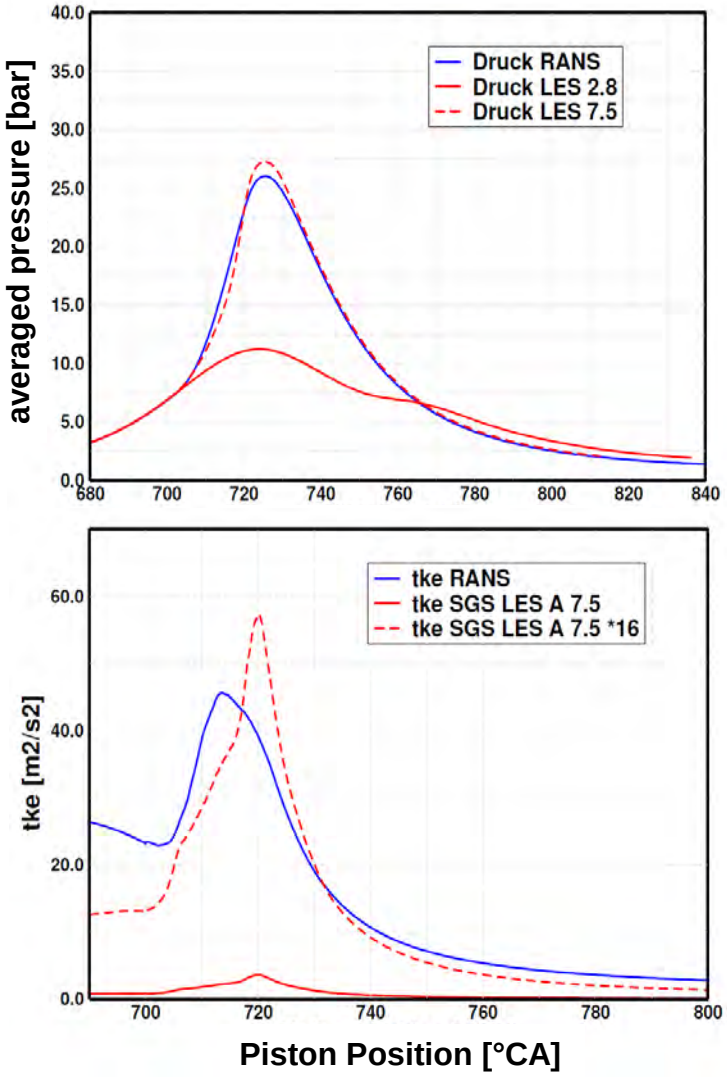


G-equation – «let's just run it and see»

- **Use coarse grid**
- **Flame area multiplier A=2.8 value from previous RANS calculations**

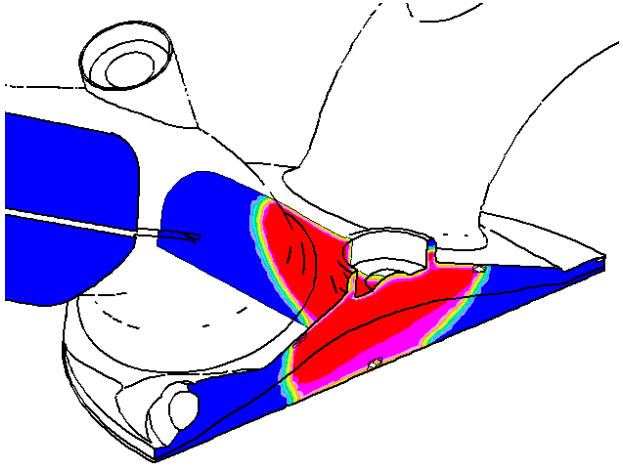
$$s_T = s_L \cdot \left[1 + A \cdot \left(\frac{\sqrt{\frac{2}{3} k}}{s_L} \right)^{\frac{5}{6}} \right]$$

  - Use in LES unchanged
  - Re-tune for LES (A=7.5)
  - $A_{LES} / A_{RANS} = 2.68$
- **s_T depends on turbulent kinetic energy**
  - $k_{SGS.LES}$ diminshes the more we resolve
  - Good agreement of $k_{SGS.LES}$*16 and k_{RANS}
  - $k_{SGS,LES}$ is scaled with 16 for s_T calculation
  - A_{LES} / A_{RANS} can also be theoretically derived from the ratio of the turb. kinetic energies

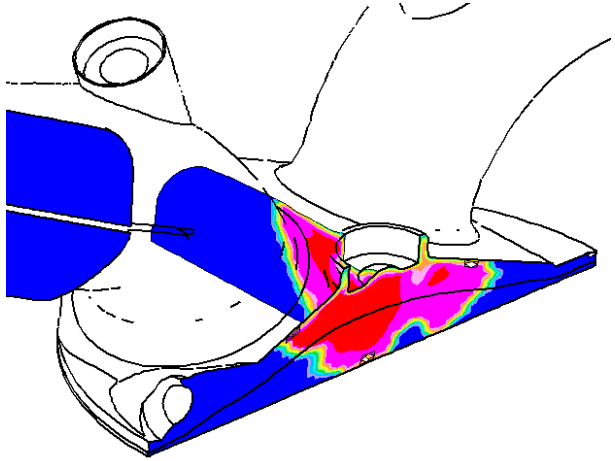


Flame area – grid resolution influence

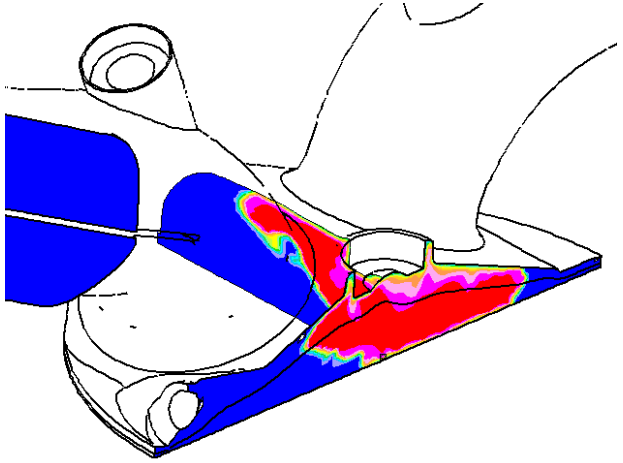
RANS coarse mesh

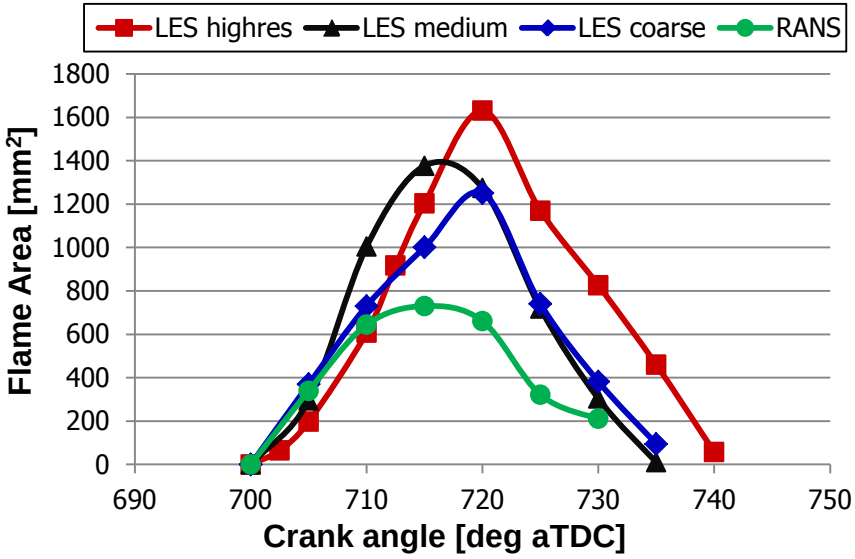


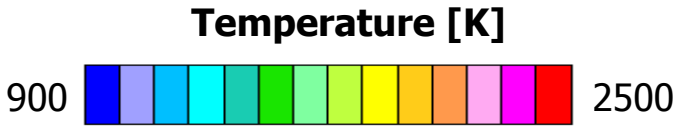
LES coarse mesh



LES fine mesh







Conclusion/discussion combustion

- When using G-equation with LES, the Damköhler coefficient (A) is a function of the mesh resolution (A = f(Δ))
- A finer mesh has two competing effects on flame propagation

  1) $\Delta \downarrow$ => $k_{SGS} \downarrow$ => A $\uparrow$
  2) $\Delta \downarrow$ => Flamearea $\uparrow$ => A $\downarrow$

- A priory estimates for A difficult

- Based on these findings, may be possible to create a model which accounts for these effects (user code s_T, additional terms)

- Idea = keep the volume expansion (s_T * A_{flame}) konstant

Overview

- Experimental configuration and conditions
- Numerical setup
- Simulation matrix
- Single cycle calculations
  - Wall heat losses
  - Combustion with G-equation
- **Multiple cycle calculations**
  - Setup
  - Results
- Discussion / open questions
- Outlook

Multiple Cycle – calculation setup

- **A simulation setup to run multiple cycle calculations with G-equation is available**

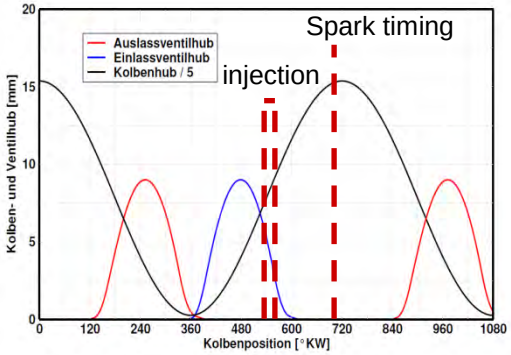
⇒ **usercoding was necessary to reset the combustion variables after one cycle. With the default esice/starcd settings it is not currently possible:**

For the combustion reset:

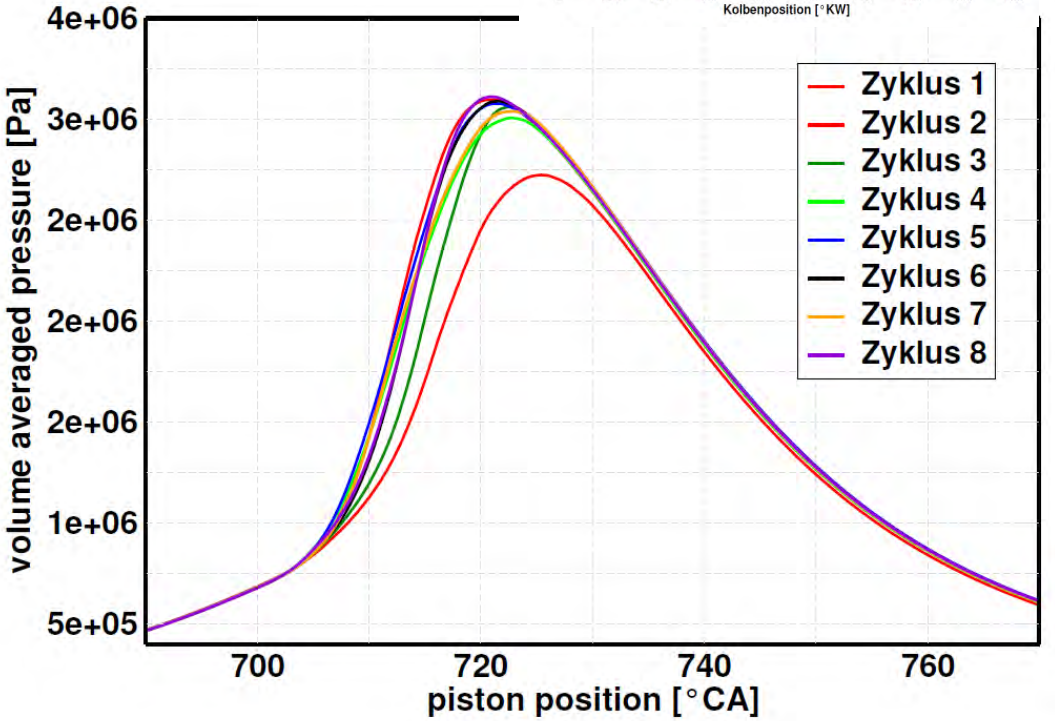
- Put the species into the EGR scalars
- Reset G to unburnt
- Reset Mixture Fraction

Multiple cycle – combustion events

- **Run many cycles (sequentially)**

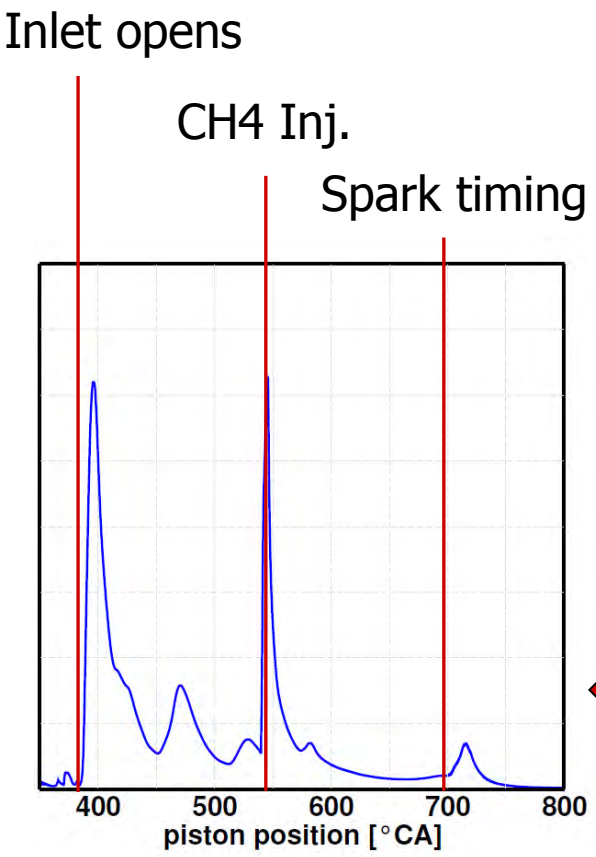


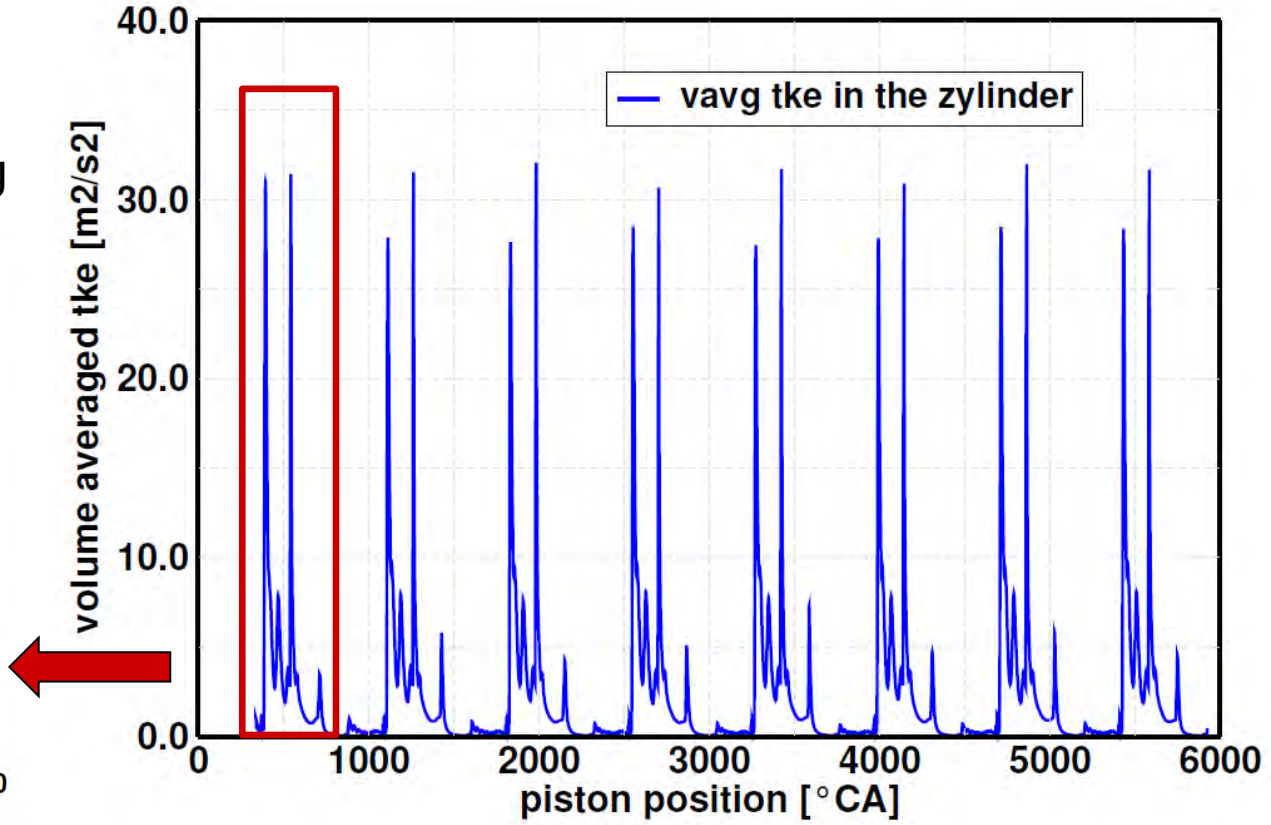
- **Initial conditions change from cycle to cycle**
  - Spread in phasing but similar peak pressure
  - Largest differences at initial flame kernel development
  - 1st cycle has pure air, all other cycles re-breathe gas from intake runner (higher λ)
  - Identical inlet/exhaust boundaries (tabulated)



- **Stochastic nature of turbulent inflow leads to different events**

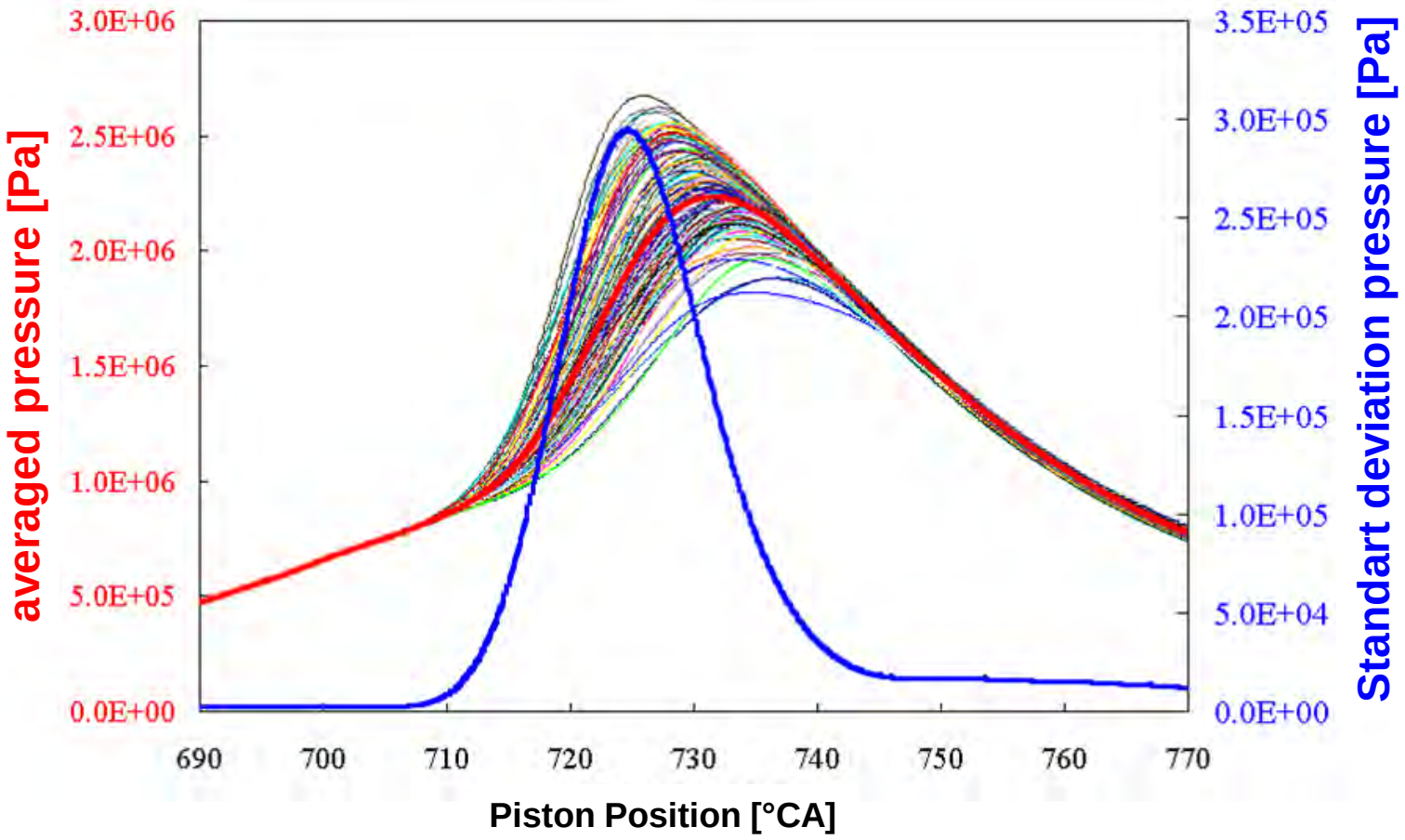
Multiple cycle – turbulence quantities





tke ign.	1	2	3	4	5	6	7	8
Spark plug	0.6	0.534	1.273	1.026	1.140	0.512	0.804	1.137
R=z=8 mm	0.8	0.698	1.007	0.966	1.095	0.55420	0.930	0.900

Experimental Data



Conclusions

- **Advantages RANS:**

- **Faster single cycle calculations of *AVERAGED* realisation**

- **Lower Calculation time**

- **Advantages LES:**

- **More realistic calculation of the physics**

  ⇒ **step towards predictive simulations:**

  - Calculation of multiple cycle fluctuations
  - Potential for more realistic calculation of wall heat losses
  - Impoved calculation of the turbulence – flame interaction

Outlook

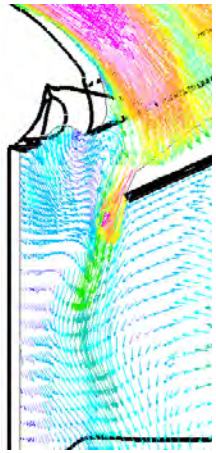
- **User code the turbulent flame speed: s_T**
  - add parameter as function of Δ
  - LES/level set approaches from literature (e.g. Pitsch et al., PCI 29, 2002)
- **Adapt an operating point to experimental data and reproduce multiple cycle fluctuations**
  - Use fully coupled simulation with GT-Power
  - Compare predictions of COV to experimental values
- **Resolve the boundary layers at the wall -> examine the heat losses**
- **Calculation of emissions**

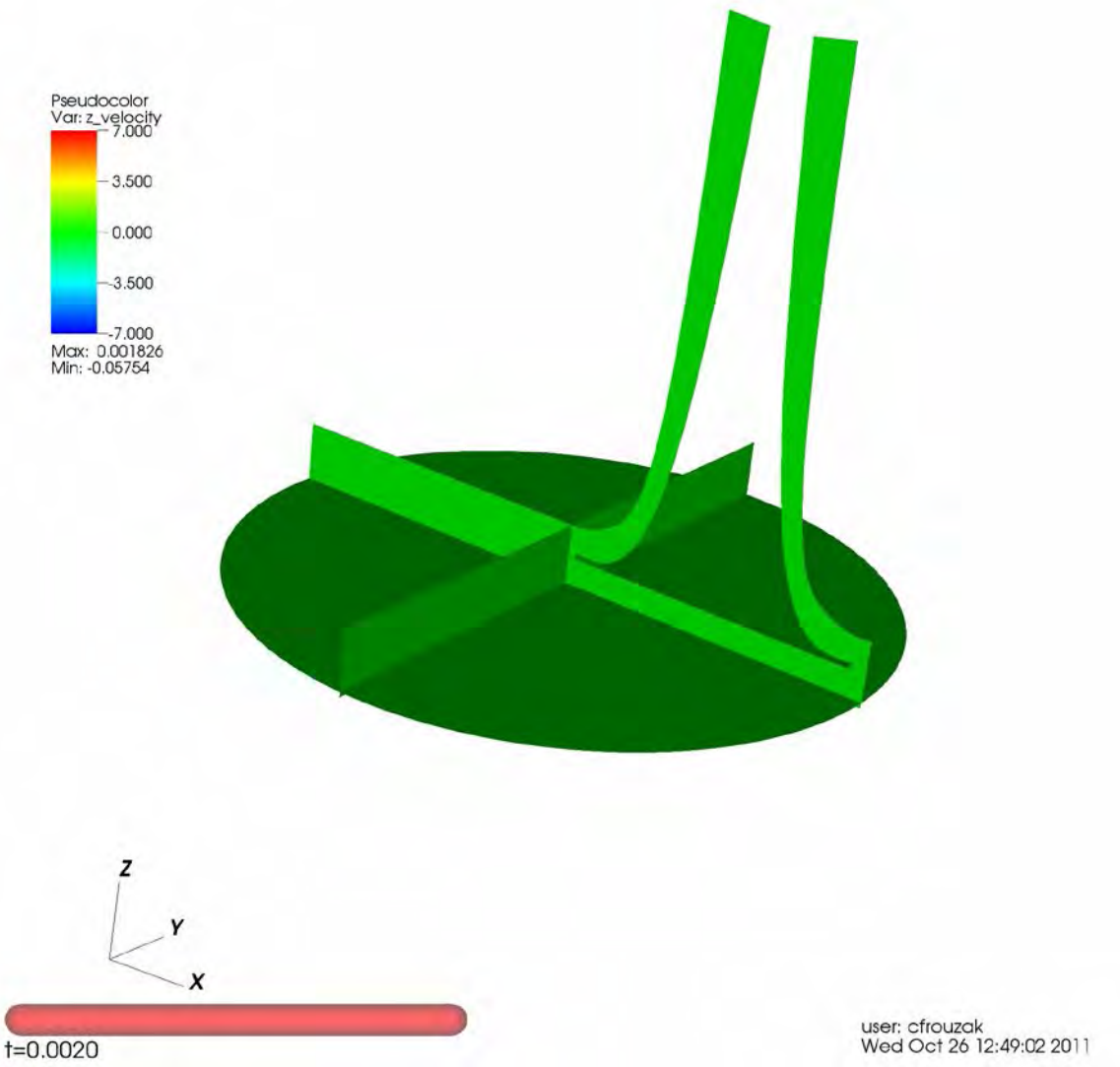
From RANS via LES to fully resolved DNS

RANS

- charac
- 0.35 M

use





The Grand Challange Reactive DNS ?

From RANS over LES to fully resolved DNS

Optimal design of thermoreactive energy converters
through DNS and High-Performance-Computing

	from state of the art →	to the future (~2020)
Flow Minimal scales	0.5 mm / 10 µs	25 µm / 100 ns
Chemistry Used species	1 – 10 species / reaction	10 – 100 species / reaction
Degress of freedom / Data per run	10^7 / 500 Giga Byte	at least 10^{10} / 1 Peta Byte
Codes / Plattforms	10^2 – 10^3 CPUs (partially) parallel	> 1 Mio. CPUs fully parallel

Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo

Funding from SFOE and SNF is gratefully acknowledged.

Thank you

M. Schmitt, Y.M. Wright, C.E. Frouzakis and K. Boulouchos

mailto:schmitt@lav.mavt.ethz.ch

ETH Zürich, Aerothermochemistry and Combustion Systems Laboratory, Switzerland

Katalytisch beschichtete Kolben im Benzin- und Erdgasmotor

Patrik Soltic

Tagung «Verbrennungsforschung in der Schweiz»

28.10.2011, ETH Zürich

EMPA

Materials Science & Technology

Inhalt

- Hintergrund / Motivation
- Kolbenbeschichtung
- Experimenteller Aufbau
- Resultate
- Diskussion / Ausblick

Hintergrund / Motivation (1)

- Methan is der stabilste Kohlenwasserstoff
  → katalytische Redultion im Katalysator ist sehr anspruchsvoll
- Die Methankatalyse zeigt ein seltsames Verhalten über Lambda
  (Detail: nächste Folie)
- Eine HC Reduktion im Brennraum würde helfen, den Katalysator zu entlasten (speziell bei Gasmotoren)

Hintergrund / Motivation (2)

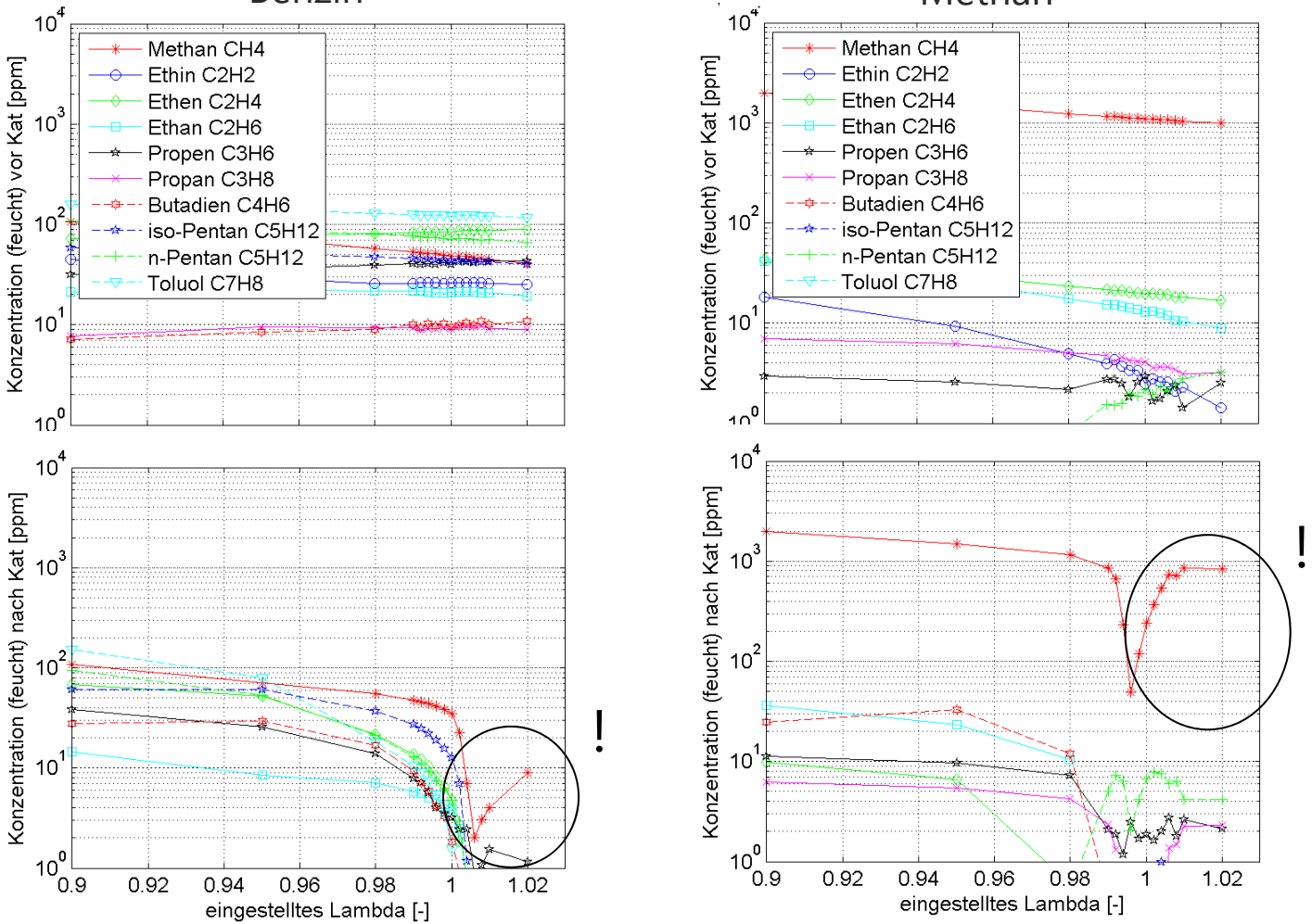
CH_4 Konversion an einem Pt/Pd/Rd Katalysator

Benzin

Methan

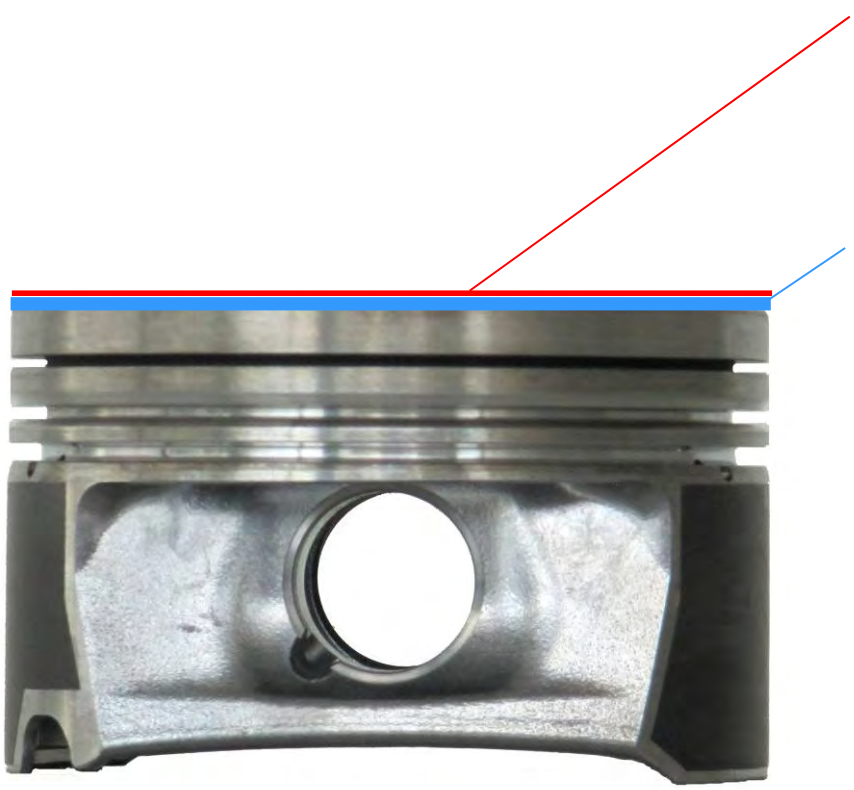
Roh

nach Kat



Hintergrund / Motivation (3)

Idee

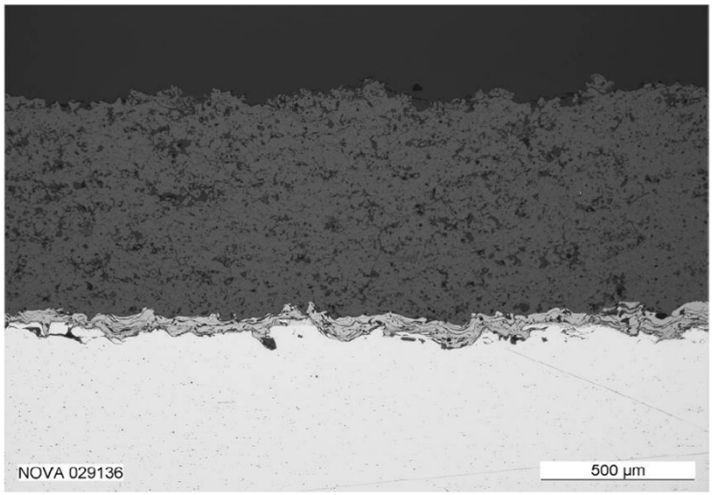


1. HC Reduktion im Brennraum:
   katalytische Kolbenbeschichtung
   (ca. 20 nm Platin)

2. Katalytische Aktivität durch die Erhöhung der Oberflächentemperatur sowie der Oberfläche fördern:
   Aufbringung einer porösen, isolierenden Schicht:
   “Themal Barrier Coating” (TBC)

Kolbenbeschichtung

TBC (thermisches Spritzen von Zirkonoxyd, Nova Swiss AG)



TBC (0.75mm)

Binding Coating (0.04mm)

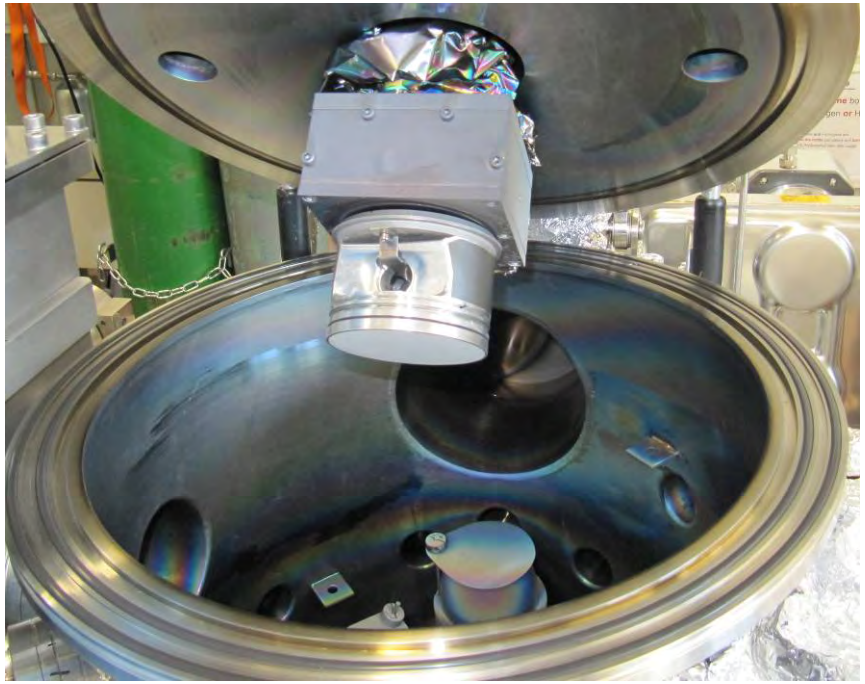
Aluminium

Kolbenbeschichtung

Schleifprozess: Reduktion TBC Dicke auf 0.6mm (Empa)

Kolbenbeschichtung

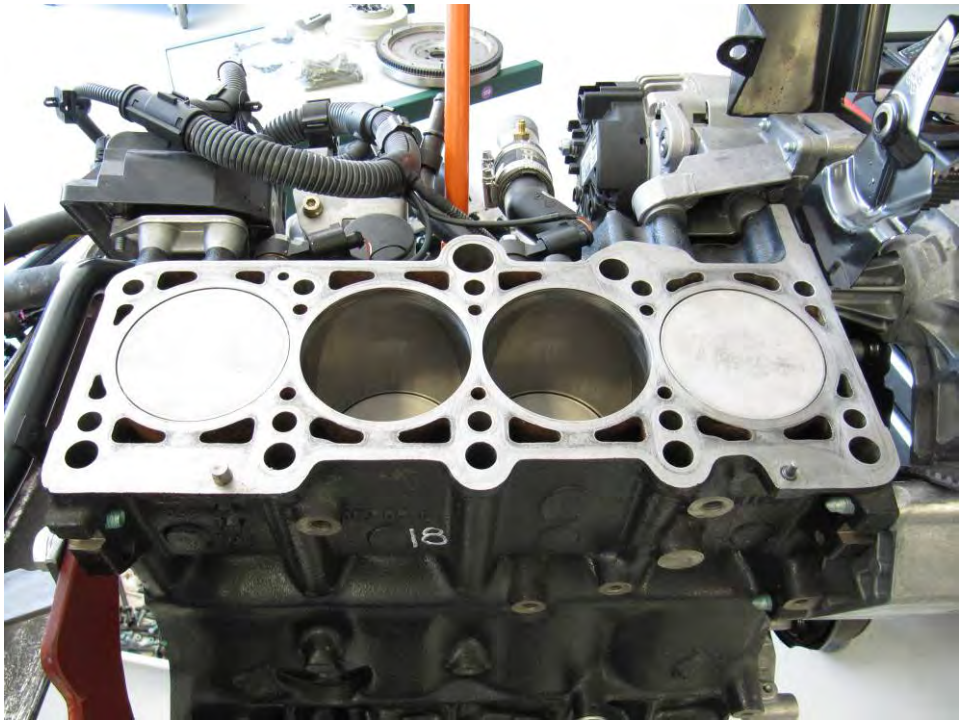
Platinbeschichtung (Sputtering im Vakuum): ca. 20nm (Empa)



Endresultat

Kolbenbeschichtung

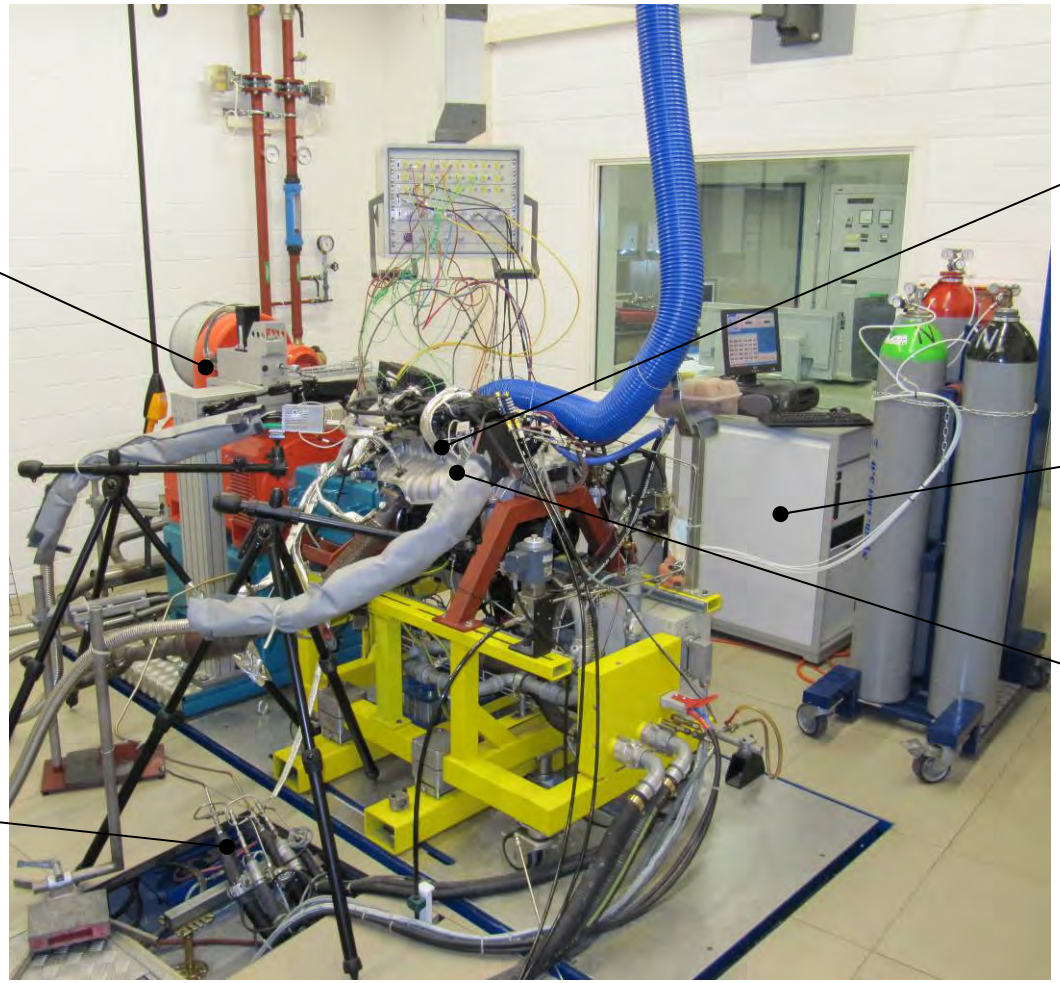
Montage



Experimenteller Aufbau

Verbrennungsluft konditioniert

Motorenprüfstand:
Schenck/Horiba
Dynas3 250LI



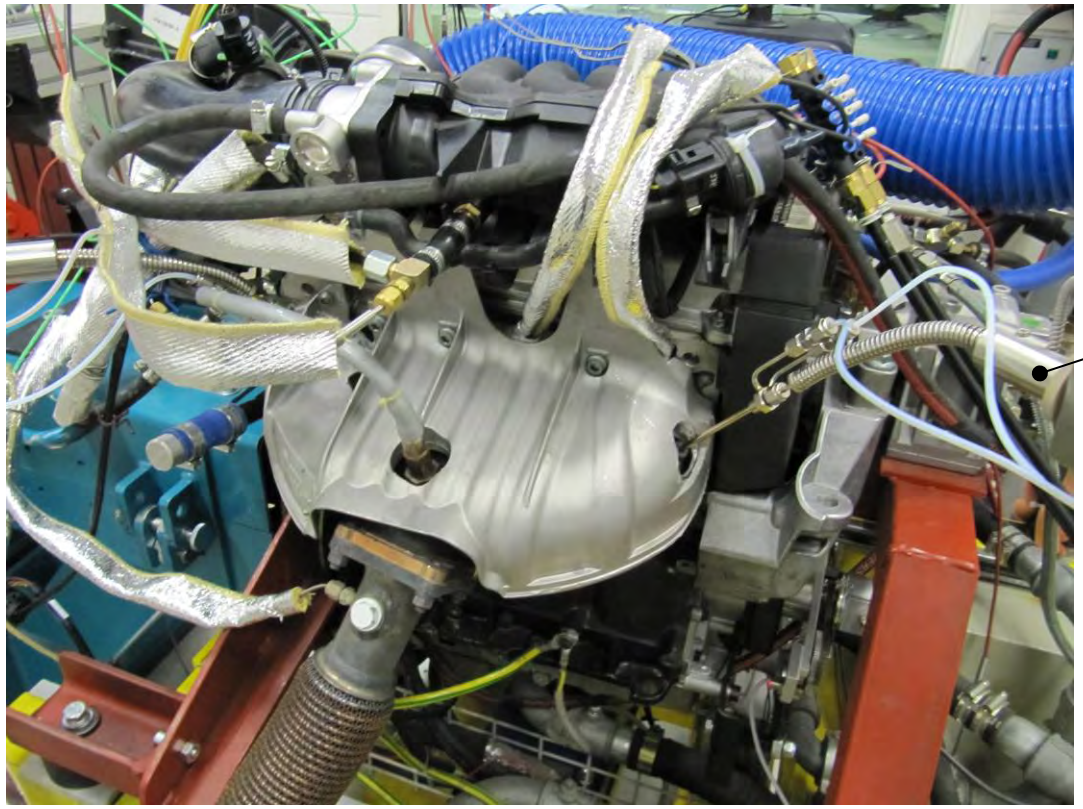
Motor:
2 l Hubraum
4 Zylinder
ε = 13.1
Saugrohr Benzinein-
spritzung und
Saugrohr Methan-
einblasung

Cambustion HFR500
Fast-FID Analysator

Zylinderdruckmessung
(Kistler 6061 Wasser-
gekühlt @ 50°C)

Horiba Mexa
9200D Abgas-
messanlage

Experimenteller Aufbau



Fast-FID: Probenahme in den Auslasskanälen der Zylinder 1 und 3

Experimenteller Aufbau

Traibstoffe / Motorbetrieb

- Treibstoffe
  1. Tankstellenbenzin ROZ 95 ($H:C|_{molar}$=1.78, H_I=43.05 MJ/kg)
  2. Reines Methan ($H:C|_{molar}$=4.00, H_I=50.0 MJ/kg)

- Motorbetrieb
  - Voll aufgewärmt, stationär
  - Verbrennungsluft: T = 24 (±1) °C, rH = 47 (±2) %
  - 2‘500 min^{-1} (mittl. Kolbengeschwindigkeit 7.7 m/s)
  - Effektiver Mitteldruck: 6 bar (Drehmoment 94.7 Nm)
  - Lambda Einstellung: 0.9, 1.0, 1.1, keine Zwangsamplitude
  - Zündwinkelvariation (durch Klopfen begrenzt)

Resultate

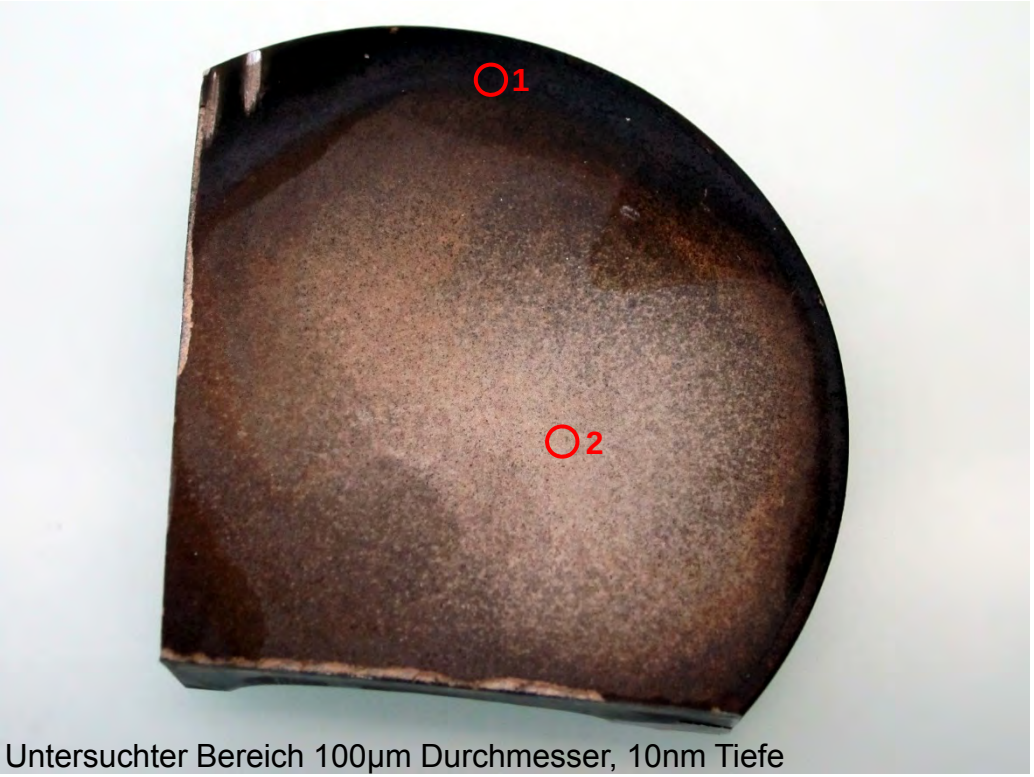
Nach ca. 28h Betrieb und ca. $1.75 \cdot 10^6$ Lastzyklen: Beschichtung einwandfrei

Nasse Bereche: Motorenöl (Demontage)

Schnitt durch den Kolben

Resultate

X-ray Photoelectron Spectroscopy (XPS)

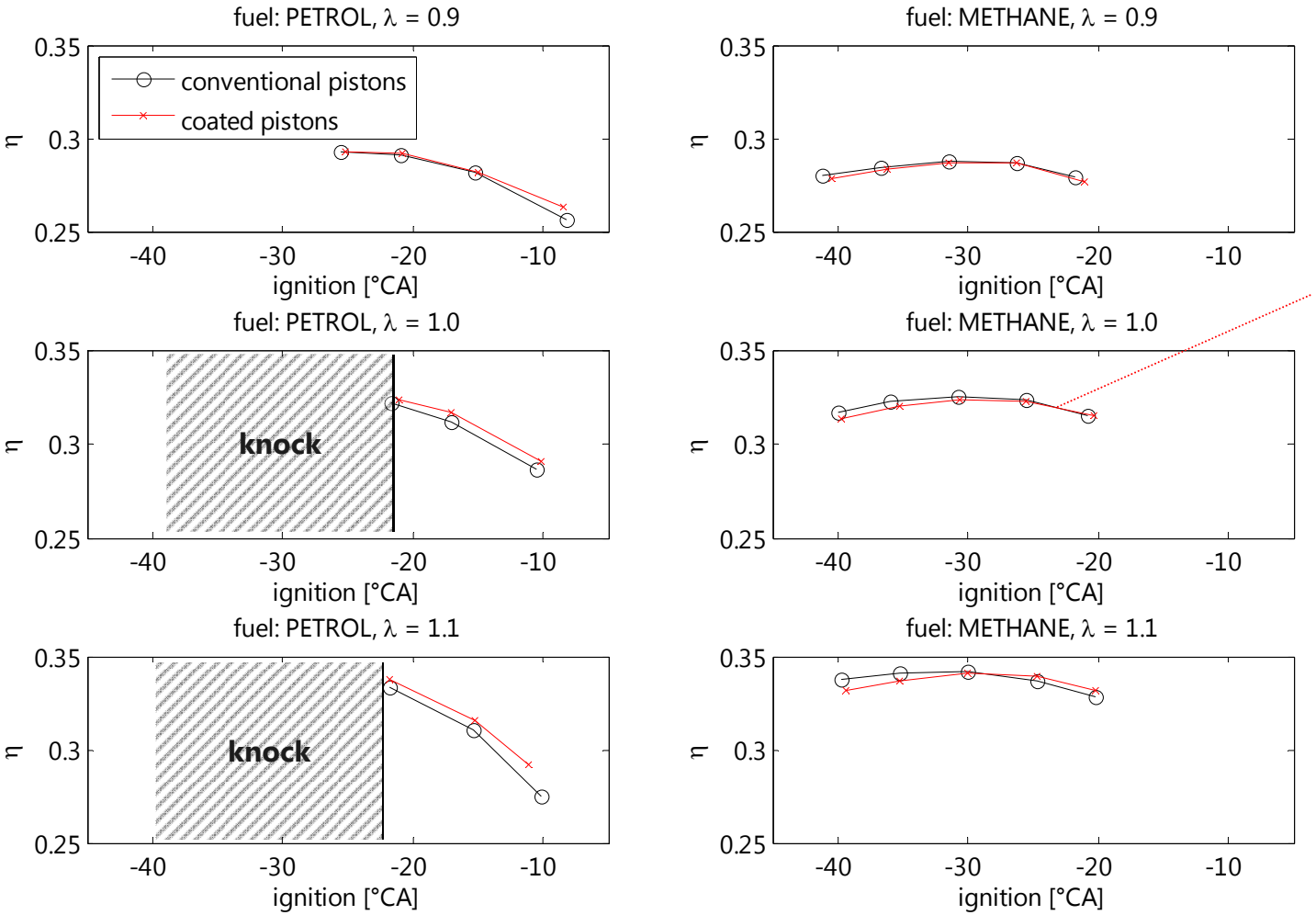


Untersuchter Bereich 100µm Durchmesser, 10nm Tiefe

- Bereich1: Viel Kohlenstoffablagerungen auf Platinlayer
- Bereich 2: Wenig Kohelnstoffablagerungen auf Platinlayer, Einige Ablagerungen von P, Zn, Ca (Quelle: Motorenöl)

Resultate

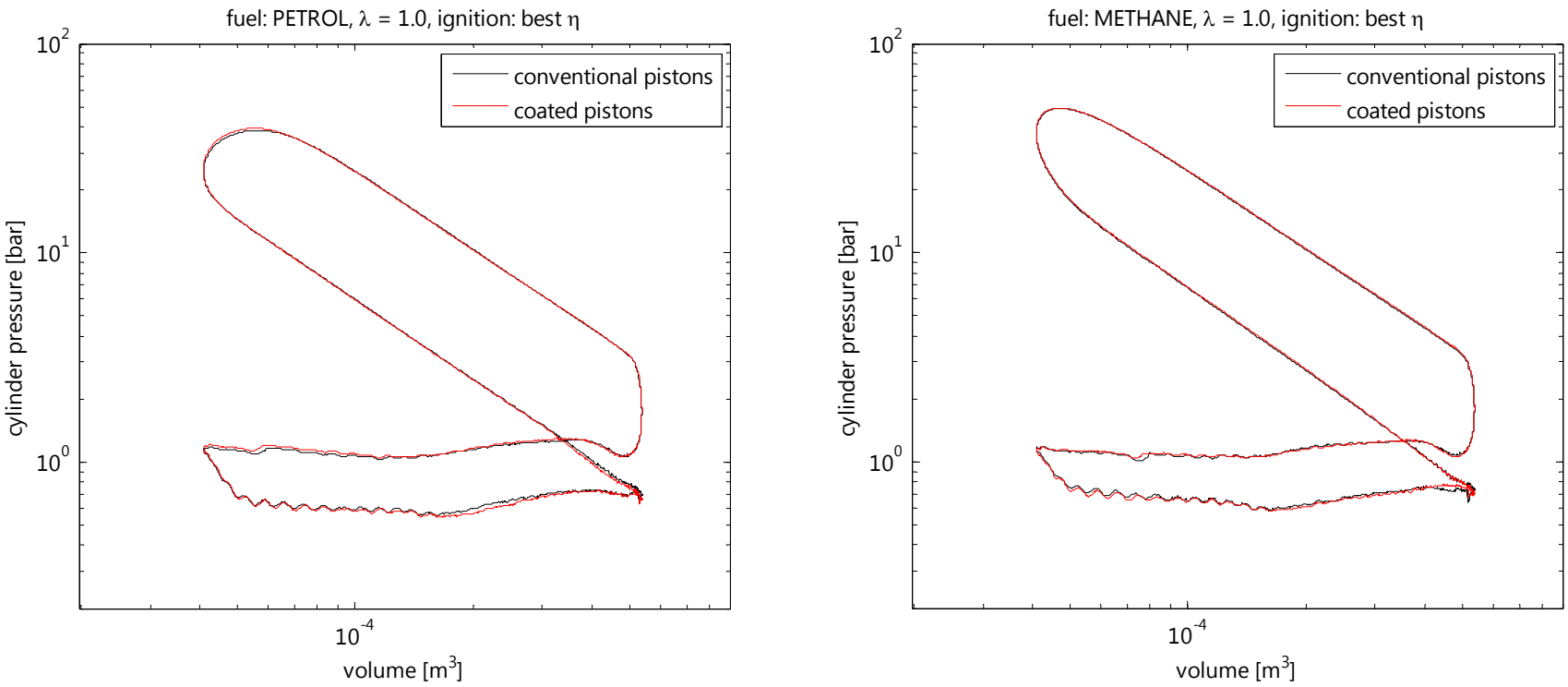
Wirkungsgrad: für Benzin etwas verbessert, keine Änderung für Methan



Beschichtete Kolben:
etwas spätere Zündung für besten Wirkungsgrad

Resultate

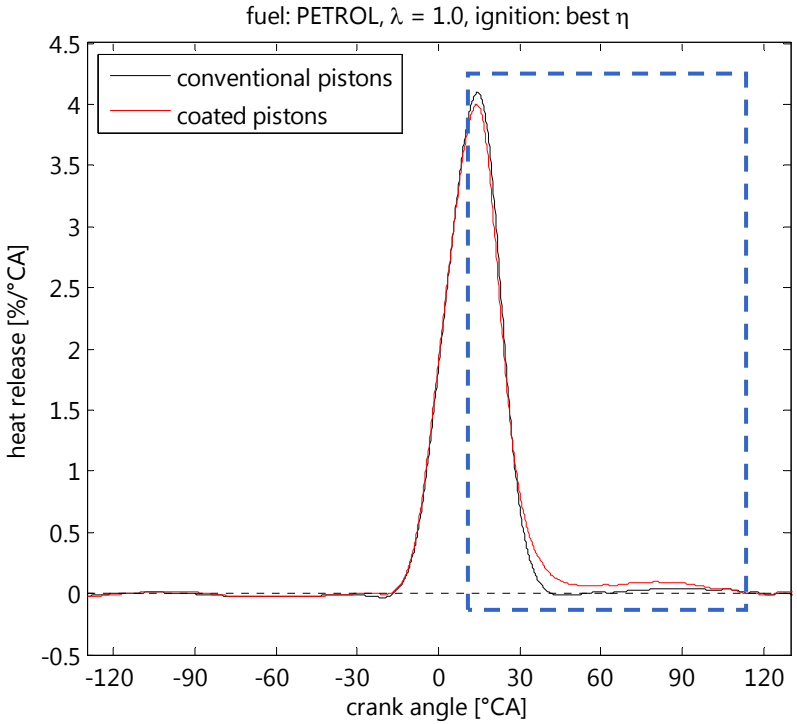
Zylinderdruckverläufe (λ=1, bester η): minimale Unterschiede

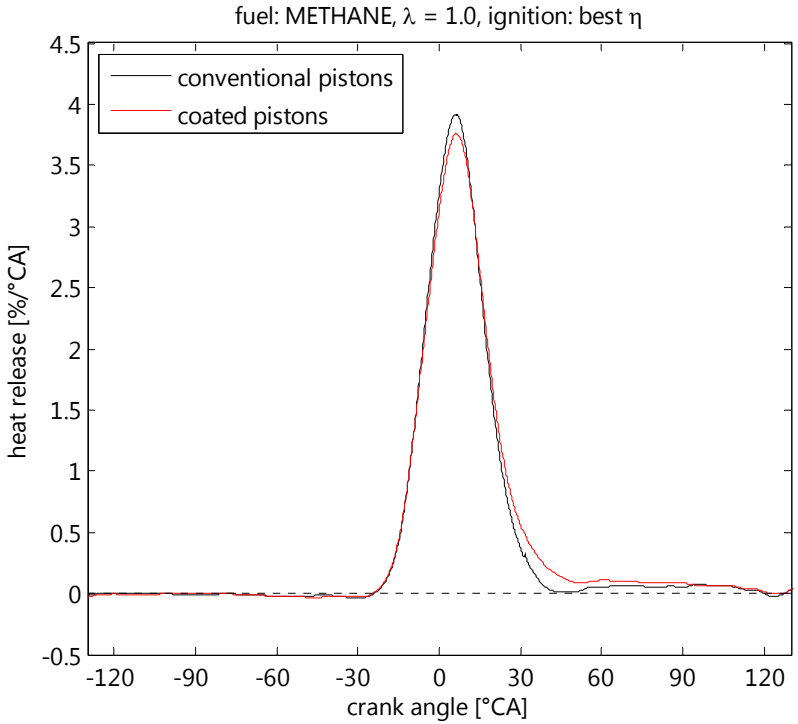


- No difference in the gas exchange process
- Coated pistons: slightly higher pressure in the high pressure part of the process for petrol (leads to better efficiency)

Resultate

Brennverläufe (λ=1, bester η): leichte Unterschiede beim Auftreffen der Flamme

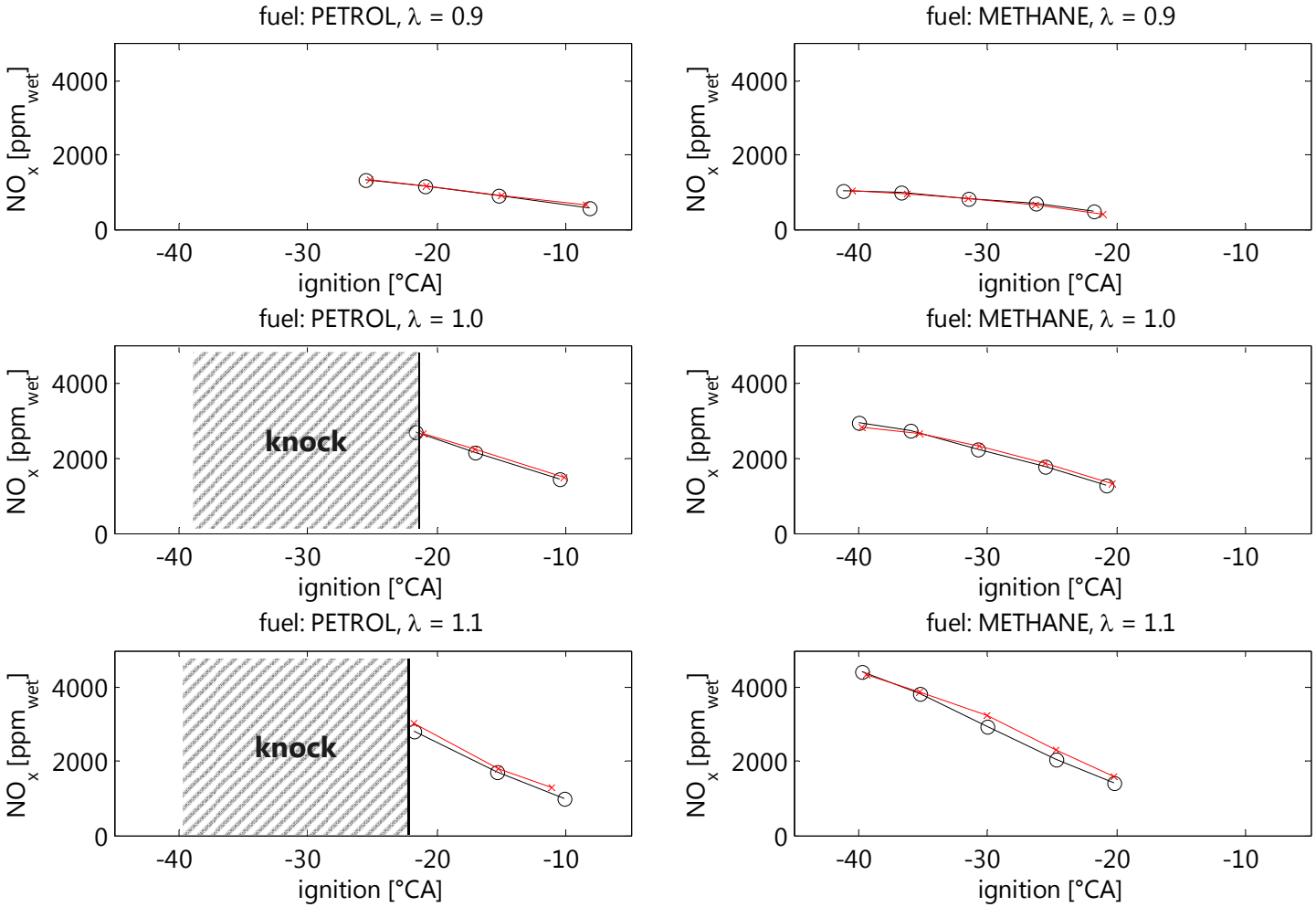




Brennverlaufsanalyse mittels WEG Software des LAV, ETH Zürich

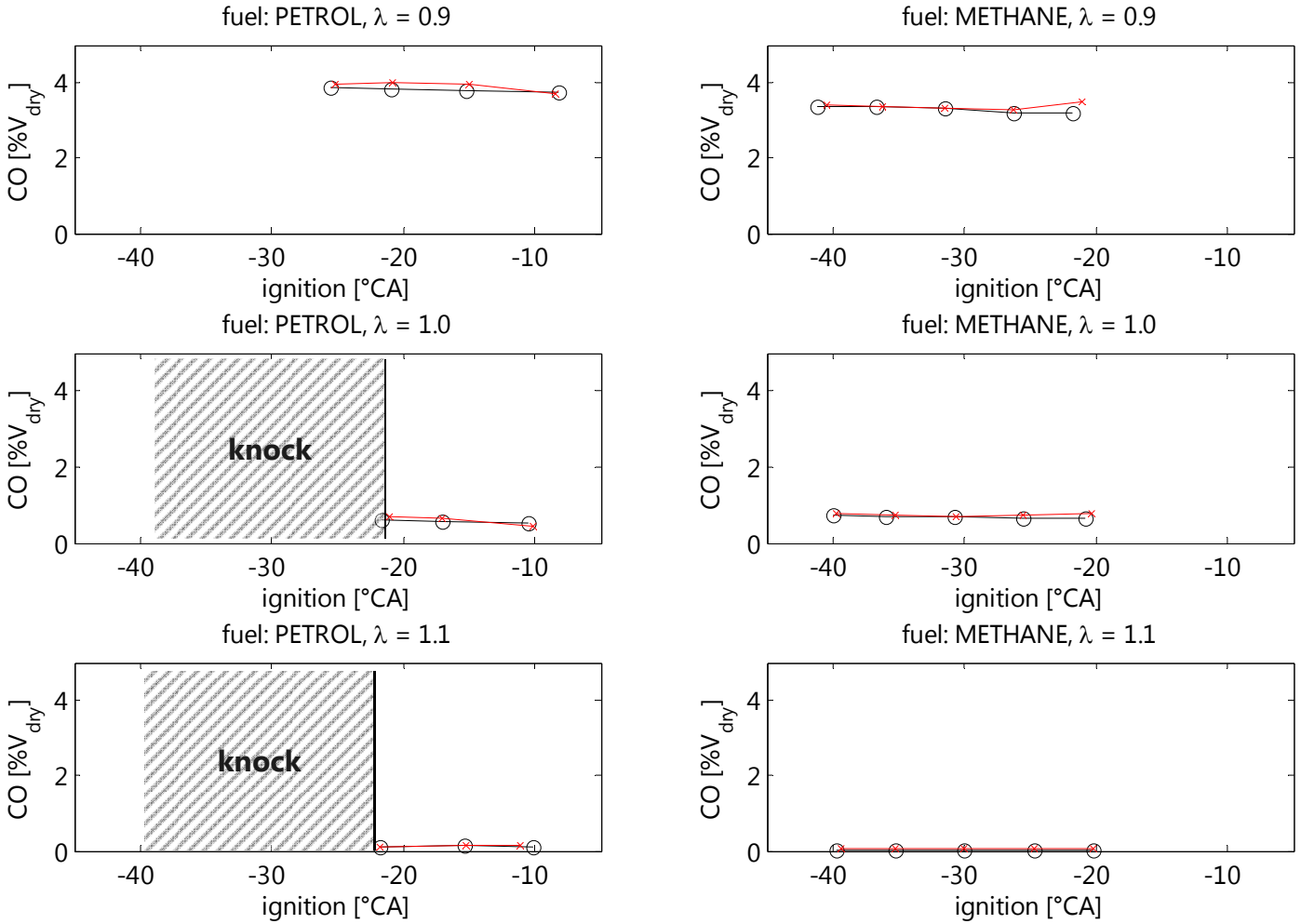
Resultate

NO_x Emissionen: Keine signifikante Veränderung



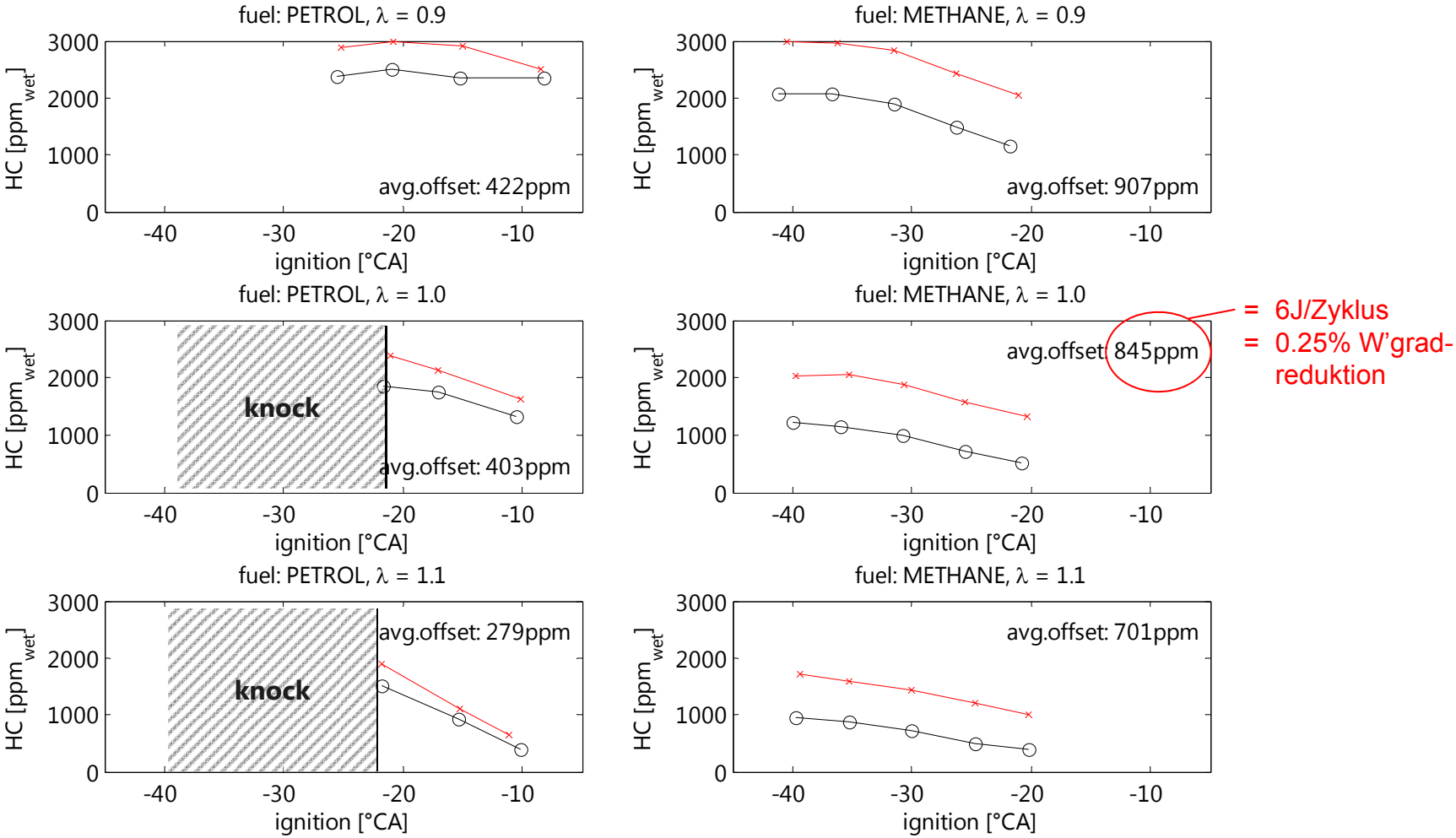
Resultate

CO Emissionen: Keine signifikante Veränderung



Resultate

HC Emissionen: Steigen durch die Beschichtung!

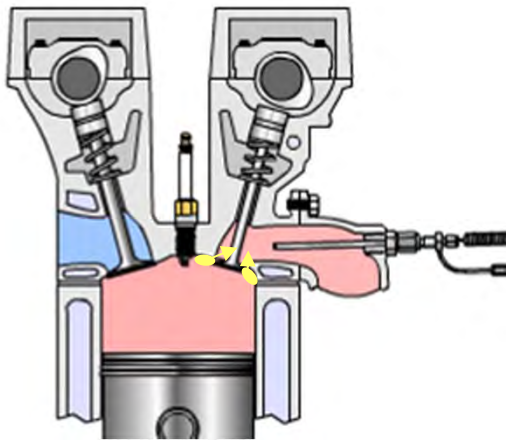


Bildquelle: www.cambustion.com (modifiziert)

Resultate

Fast-FID Messungen: Signalinterpretation während Auslassvorgang

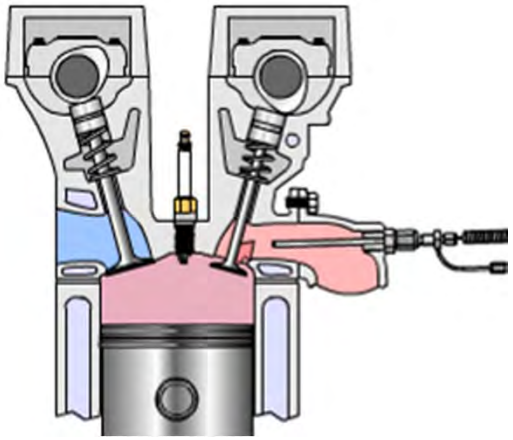
Phase 1: Auslassventil öffnet



HC Quellen: Ventilsitz-Spalte

HC Konzentration: hoch

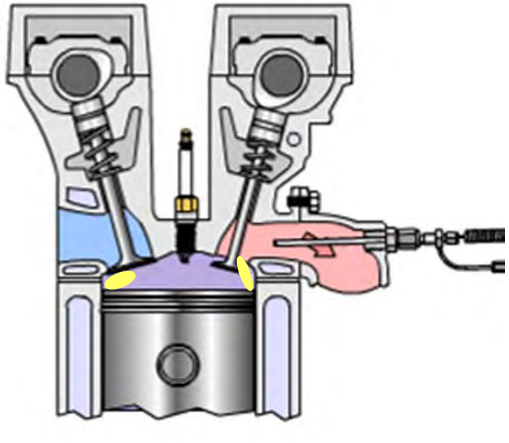
Phase 2: Bulk Flow



HC Quellen: gut durchmischte HCs von Flammlöschbereichen

HC Konzentration: tief

Phase 3: Auslassventil schliesst



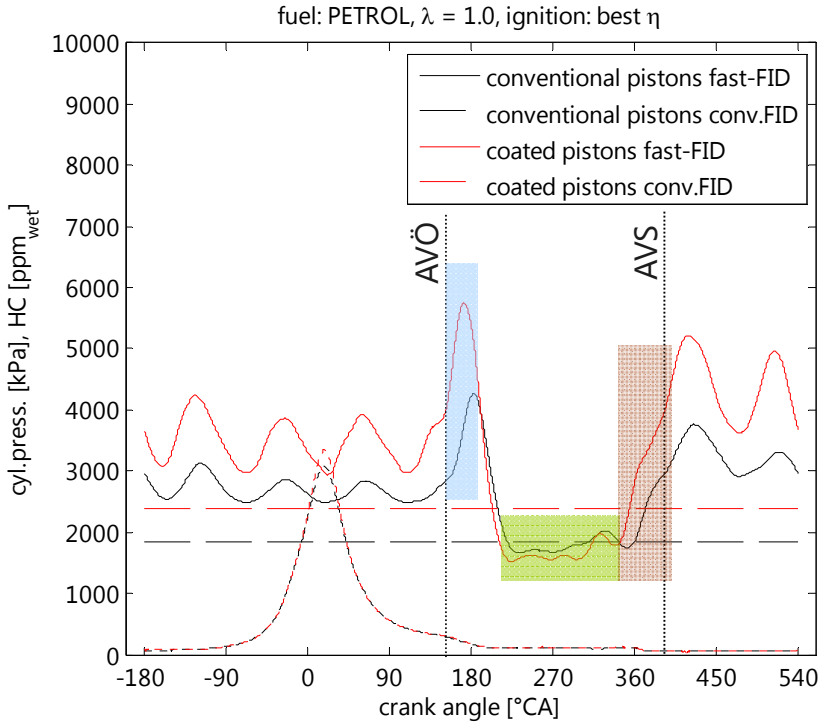
HC Quellen: Ringspaltbereich

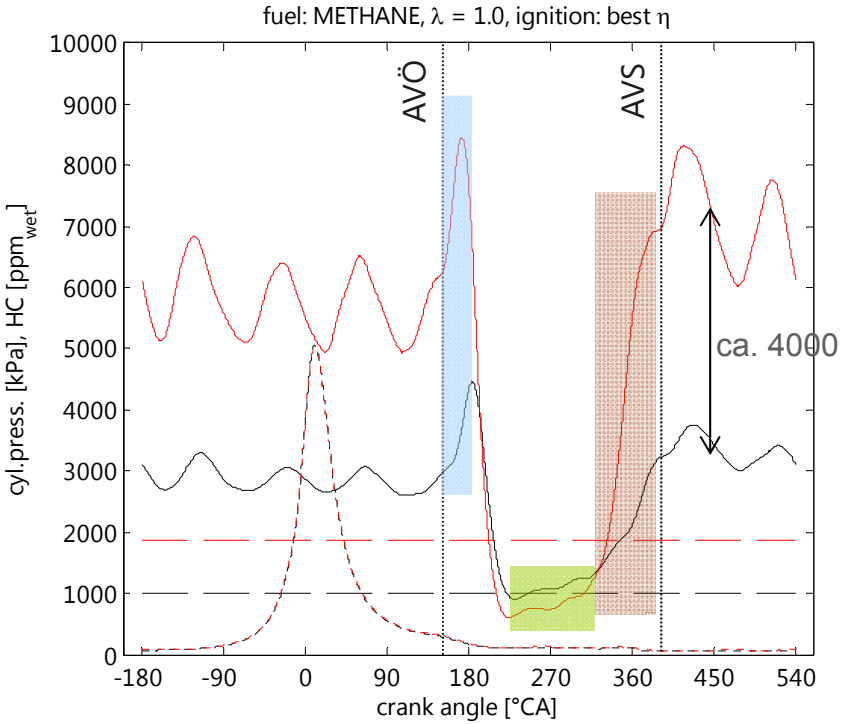
HC Konzentration: hoch

Resultate

HC Emissionen ca. 10cm nach Auslassventil (Fast-FID Messungen)

Gemittelt über 290 aufeinanderfolgende Zyklen





Phase 1 (Auslassventil öffnet): ähnliche HC Peaks unbeschichtet / beschichtet

Phase 2 (Bulk Flow): Tiefere HCs bei beschichteten Kolben

Phase 3 (Auslassventil schliess): höhere HC Peaks für beschichtete Kolben (viel höher bei Methan)

da muss ein methan-selektiver Prozess eine Rolle spielen

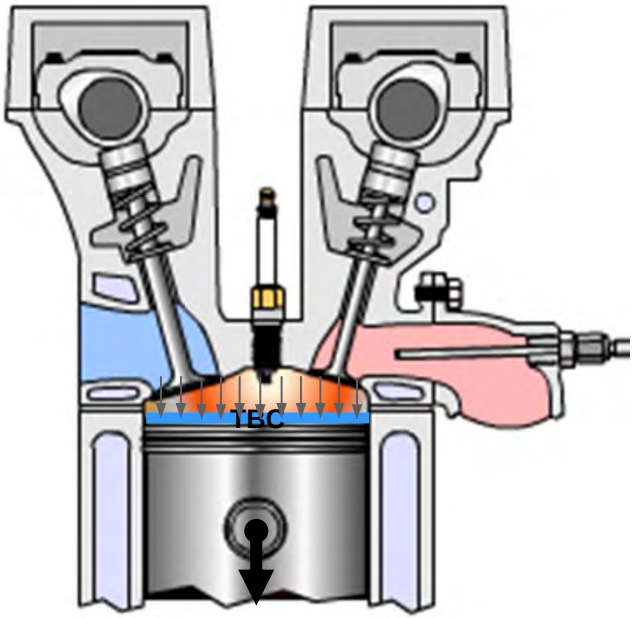
Picture source: www.cambustion.com (pictures modified)

Resultate

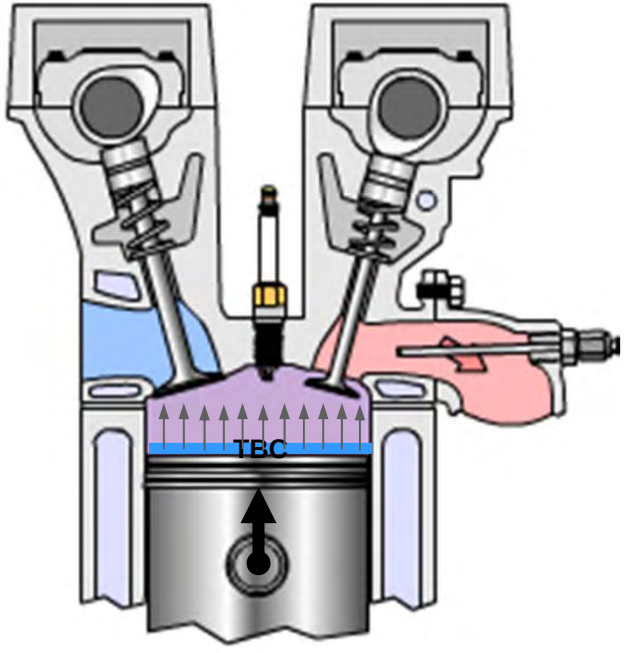
Methan-selektiver Prozess

- Hypothese: Methan Adsorpion / Desorption in der TBC Schicht

Verbrennung: hoher Druck



Ausstossen: tiefer Druck



Resultate

Methan Adsorption

TBC Sample der gelaufenen Kolben

Adsorptionsmessung
(Sorptionsisotherme, thermogravimetrische Analyse)

Methan-Adsorption bei 250 °C
- $1.74 \cdot 10^{-3}$ g pro Kolben
- Ergibt **$1.08 \cdot 10^{-4}$ mol CH_4 pro Kolben und Zyklus**

Abschätzung des Einflusses:

$$\frac{\text{adsorbiertes } CH_4}{\text{Gesamtzylinderladung}} = \frac{1.08 \cdot 10^{-4}}{2.186 \cdot 10^{-3}} \approx 5 \cdot 10^{-3} = 5000\,ppm$$

→ Eine bedeutende CH_4 – Menge kann im TBC Layer gespeichert werden

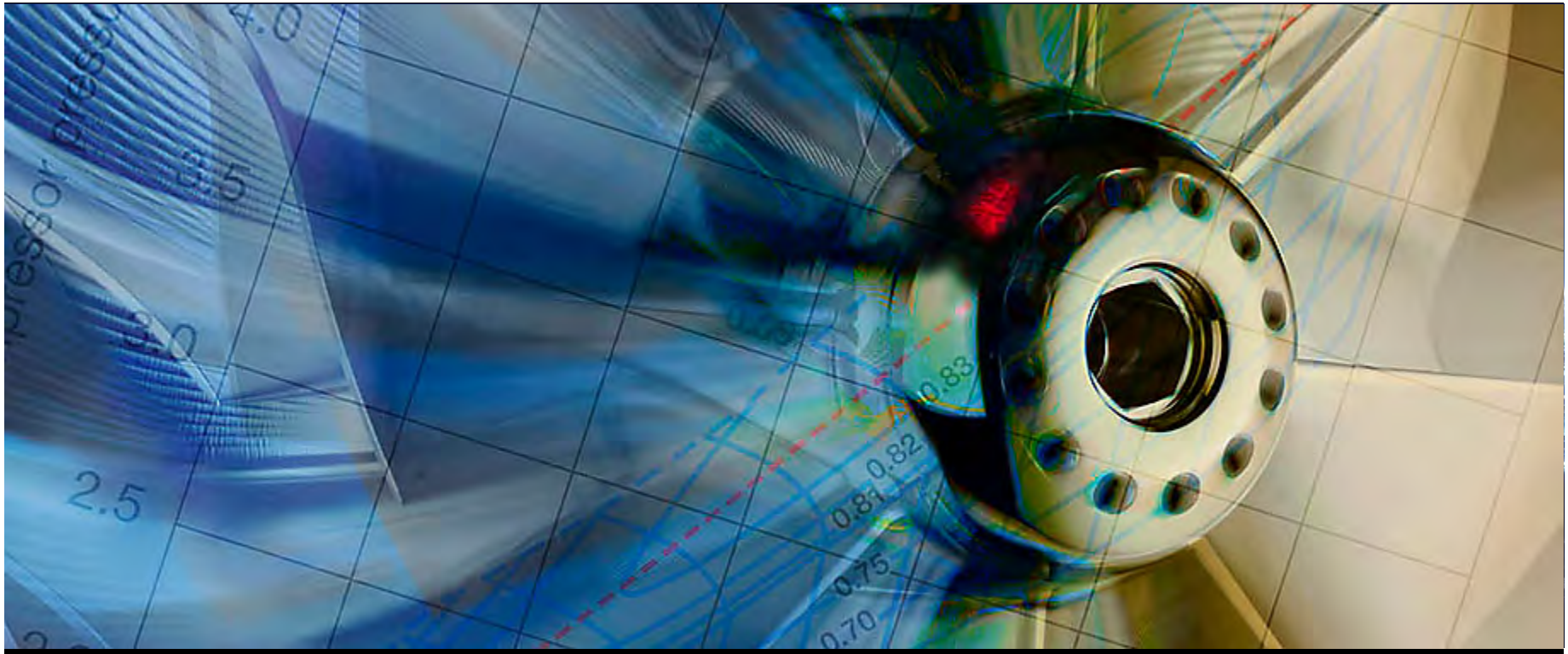
Diskussion / Ausblick

- TBC/Pt-beschichtete Kolben widerstehen der mechanischen und thermischen Belastung eines Ottomotors (getestet bis 3000 min^{-1} und einem Spitzendruck bis 70 bar)
- Die TBC/Pt Beschichtung erhöht im Benzinbetrieb den Wirkungsgrad im betrachteten Betriebspunkt leicht, im Methanbetrieb führen die erhöhten Methanemissionen nicht zu diesem Effekt
- HC Emissionen steigen mit der TBC/Pt Beschichtung deutlich, die anderen Schadstoffe werden davon nicht beeinflusst
- Die Betrachtung des HC-Verlaufes deutet darauf hin, dass die HC Emissionen der Zylinder-Hauptladung reduziert werden können
- Die Methanadsorption in der TBC Schicht erhöht die HC Emissionen schlussendlich
- Empfehlung: eine poröse Zirkonoxyd-Schicht ist nicht zielführend, eine alternative Isolationsschicht muss gefunden werden
- Bemerkung: Es gibt es theoretische Arbeiten welche vorhersagen, dass Zirkonoxyd im Brennraum eine katalytische Wirkung hat[1]. Adorptions-phänomene wurden dort nicht berücksichtigt.

[1] Nedunchezhian N, Dhandapani S, Study of flame quenching and near-wall combustion of lean burn air-fuel mixture in a catalytically activated spark-ignited lean burn engine, Combustion and Flame 144 (2006), 407-409

Danksagung

- **Bundesamt für Energie** für die Unterstützung
- **Nova Werke AG** für die TBC Beschichtung
- **Walter Brüllmann, Markus Hauser, Roland Graf, David Mauke** (Empa) für die Versuchsvorbereitungen
- **Alexander Winkler and Jacqueline Tschudin** (Empa) für die Probenpräparationen sowie für die XPS Analysen
- **Jörg Patscheider** (Empa) für das Pt-Sputtering
- **Paul Hug** (Empa) für die Wärmeduchgangsmessungen mitters Laser-Flash
- **Andreas Borgschulte** (Empa) für die thermogravimetrischen- und BET Messungen



Daniel Brand, Tagung Verbrennungsforschung, 28. Oktober 2011

Aufladung von Grossmotoren Forschungs- und Entwicklungsbedarf aus Sicht der ABB Turbo Systems AG

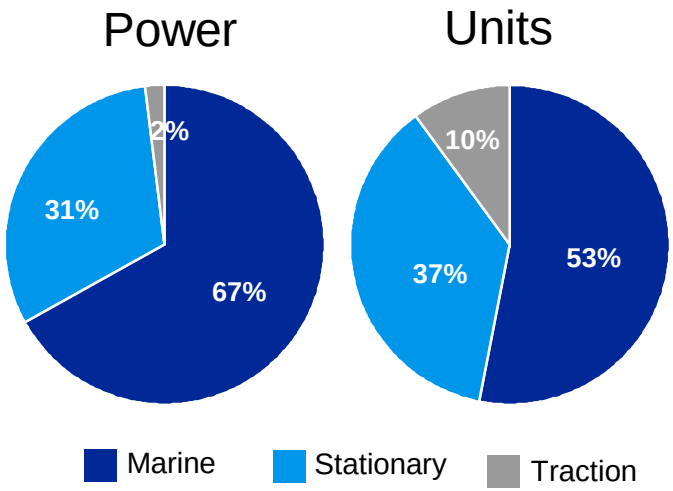
Übersicht

- ABB Turbo Systems AG
- Umfeld, Trends und Rahmenbedingungen
- Entwicklungsschwerpunkte bei den Grossmotoren
- Forschungs- & Entwicklungsaktivitäten
- Zusammenfassung und Ausblick

ABB Turbo Systems AG
Kerngeschäft: Turbolader für Motoren > 500 kW

- Turbolader für Motoren > 500 kW für die Segmente:
  - High Speed:
    4-Takt Gas- und Dieselmotoren
    1000 – 2000 rpm
  - Medium Speed:
    4-Takt Gas- und Dieselmotoren
    500 – 1000 rpm
  - Low Speed:
    2-Takt Dieselmotoren
    60 – 200 rpm
- Beratung der Motorenbauer und Verkauf von Neuladern (Baden, Japan, China, Korea, USA)
- Servicegeschäft (Baden, > 100 Servicestationen)
- Produktionsverbund (Schweiz, China, Indien, Lizenznehmer)

CH: ca 1000 MA
WW: > 2000 MA



Marktanteil > 30% → Marktführer

Anwendungen von Turboladern

Marine	Stationary	Traction
		
		

Umfeld, Trends, Rahmenbedingungen

ABB Turbo Systems AG Mission:
We multiply power of gas and diesel engines

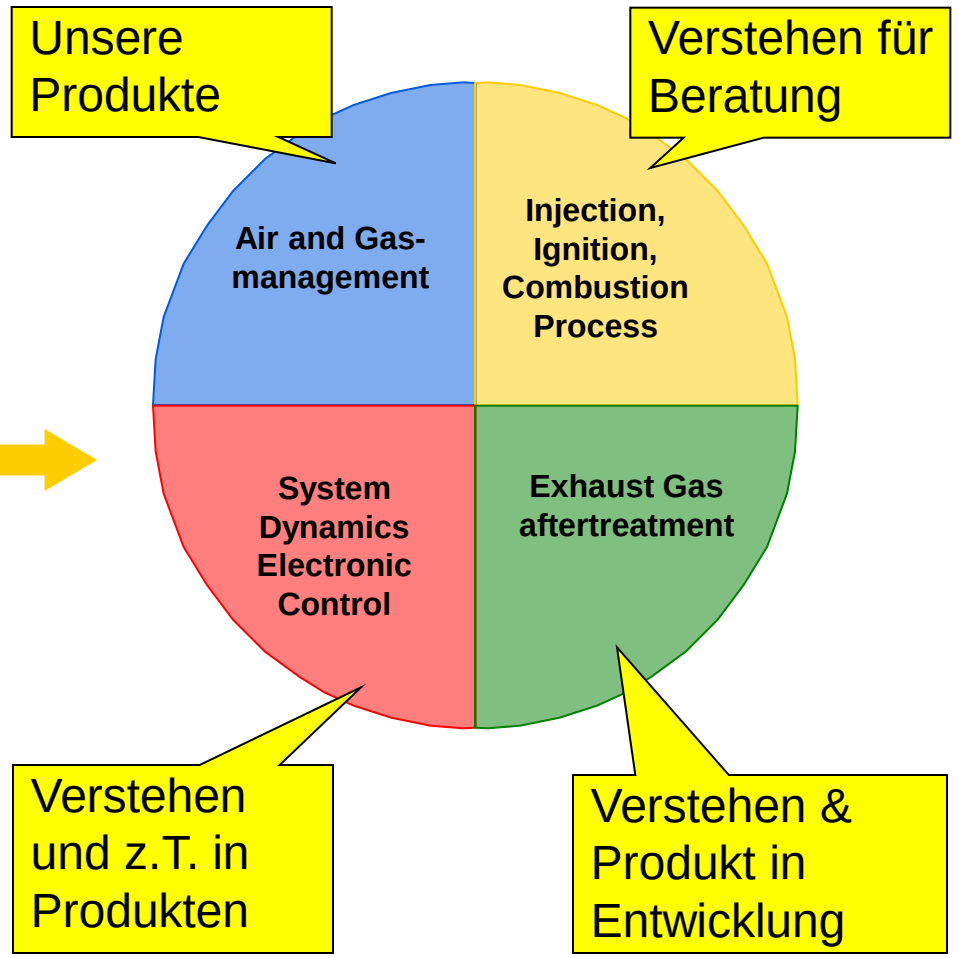
Trends:

Ressourcenknappheit
Bedarf an Transportkapazitäten ↑
Bedarf an Energie ↑
Reife Technologie

Identifikation von Innovationsfeldern Motoren

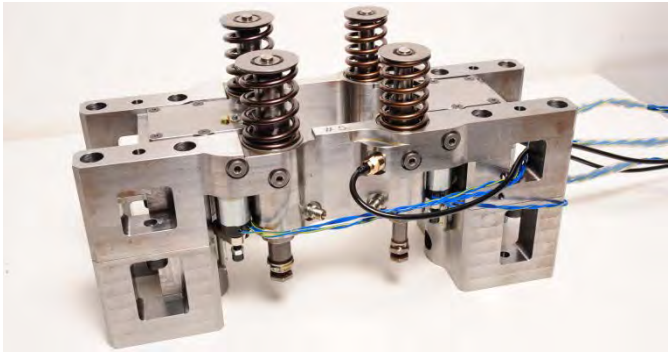
Rahmenbedingungen:

Emissionsrichtlinien
Verfügbarkeit von Treibstoffen,
…



Produkte, z.T. in Entwicklung

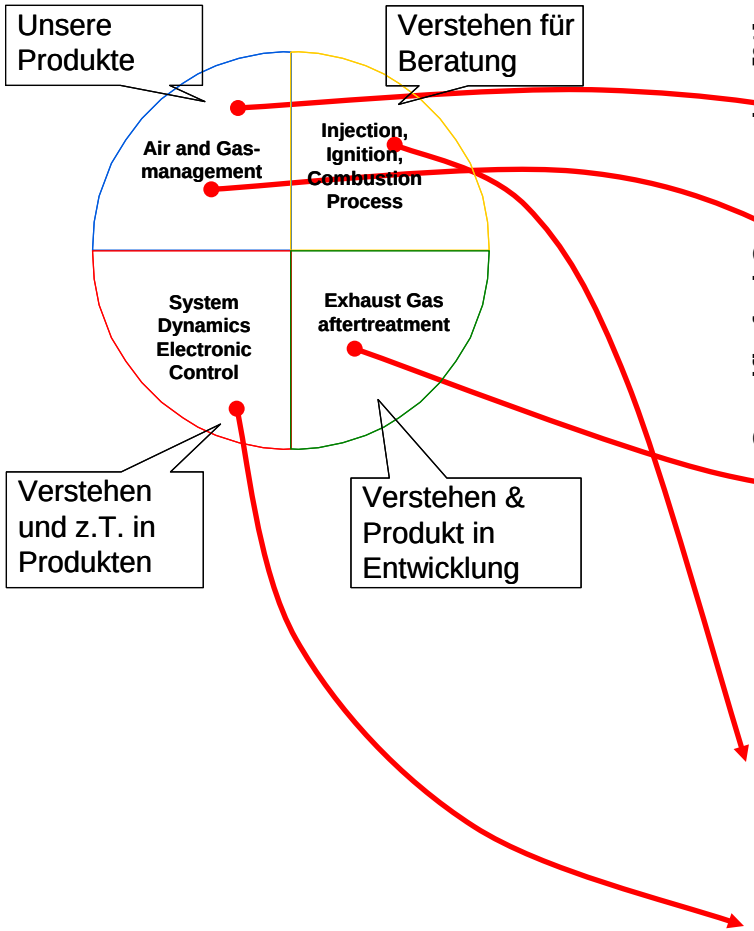
Turbolader
1-stufig oder 2-stufig mit Hoch- und Niederdruckstufe

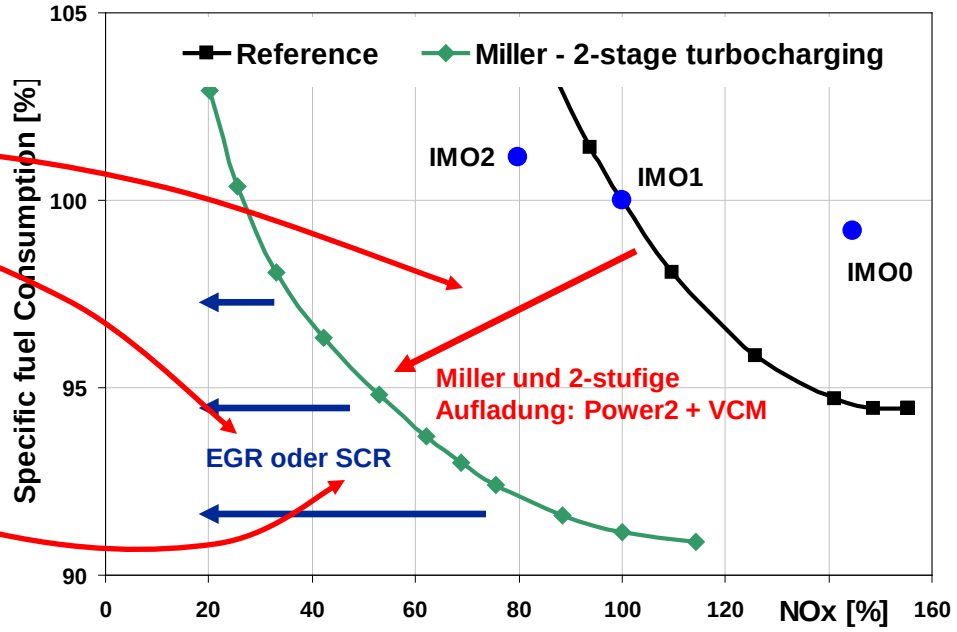


VCM
Valve Control Management

ITSCR
für 2-stufige Systeme, zwischen den Turbinen

Dieselmotor





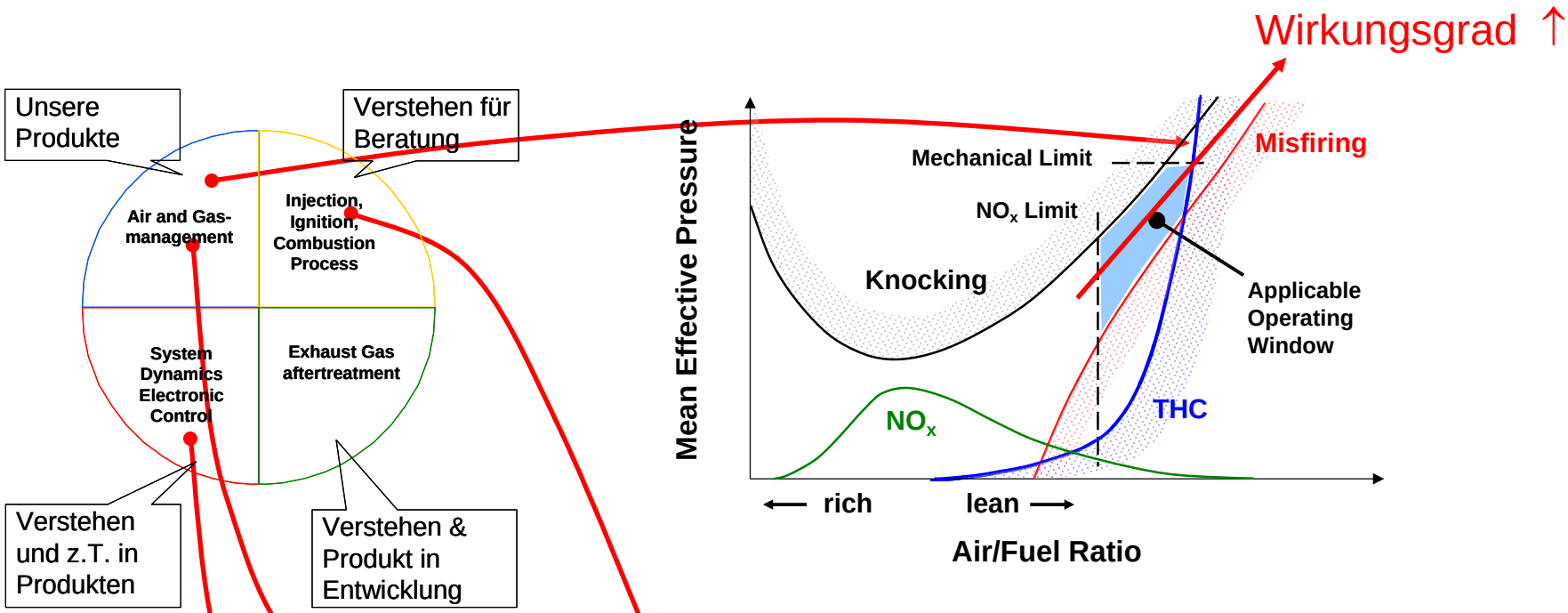
- Teillastverhalten mit SCR oder EGR
- Modellierung der Verbrennung, Emissionen
- Softwareentwicklung Simulation Gesamtsysteme inkl. innermotorischer Vorgänge

Entwicklungsschwerpunkte
Herausforderungen Diesel

- Miller-Prozess ist beschränkt durch Verbrennungsqualität
  - verbesserte Verfahren für stärkeren Miller entwickeln
    2-stufige Aufladung für noch höhere Ladedrücke
  - Variable Ventiltriebe: **VCM**
- Betriebstemperatur und Bauraum SCR → **ITSCR** zwischen Turbinen
  - kompaktes Design ↔ gute Homogenisierung Abgas/Reduktionsmittel ↔ wenig Druckverluste
- EGR: Ueberwindung Druckgefälle Luft – Abgas
  - **„EGR-Pumpe“**
  - EGR ein-/ausschalten
  - Regelung der EGR-Rate
- Dual-Fuel Motoren:
  - variable Kompression durch **VCM**
- Heavy Fuel Oil

Entwicklungsaktivitäten
ABB Turbo Systems AG

Gasmotor



- Modellierung der Verbrennung, Rohemissionen und Klopfverhalten
- Verbesserung Wirkungsgrad und Lastaufnahme
- Softwareentwicklung Simulation Gesamtsysteme inkl. innermotorischer Vorgänge

Entwicklungsschwerpunkte
Herausforderungen Gasmotoren

- Reduktion der Klopfneigung
  Magerbetrieb, **Miller und 2-stufige Aufladung**, EGR(?), Brennraumdesign
- Reduktion des Sicherheitsabstandes zur Klopfgrenze
  Regelung → **VCM**
- Verminderung der Zylinder-zu-Zylinder und Zyklus-zu-Zyklus Schwankungen
  Zylinderbalancing → **VCM**, Design Luft und Gaspfad, Zündung
- Verbesserte Lastaufschalte-Fähigkeit
  schnelle Aenderung der Zylinderfüllung → **VCM**
- Entdrosselung → **VCM**

Entwicklungsaktivitäten
ABB Turbo Systems AG

Forschungs- & Entwicklungsaktivitäten

- Produkte, z.T. in Entwicklung
  - Turbolader (1- und 2-stufig)
  - VCM, ITSCR, „EGR-Pumpe“
- Entwicklung von Grundlagen-Wissen:
  (Beratung unserer Kunden, Produktentwicklung, strategische Fragen)
  - Potential und Grenzen des Diesel-Verbrennungsprozesses (Millerprozess, EGR, Diesel-Wasser-Emulsion, Einspritzung)
  - Neue Möglichkeiten der Prozessführung für Gasmotoren oder Dual-Fuel Motoren
  - Modellierung / Simulation (inkl. Software) von Verbrennung, Aufladung, Motor, Antriebsstrang, Waste Heat Recovery, …
- Wir arbeiten zusammen mit
  - unseren Kunden, ETH, PSI, ZHAW, FVV, …

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for a better world™