

## COMBUSTION OF DIESEL SPRAY: LOW- AND HIGH-TEMPERATURE OXIDATION PROCESSES FOR FREE DIESEL INJECTION AND IN POROUS REACTORS

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### ABSTRACT

Heat release process in a free volume combustion chamber and in porous reactors has been analyzed in a wide range of initial pressures and temperatures under Diesel engine-like conditions. For investigating of this kind of reactions a special combustion chamber characterized by a constant volume and adiabatic conditions has been used as an engine simulator.

Diesel spray combustion is a very complex multi-step process. The physics of spray formation, penetration and mixture formation must be considered together with chemistry of low- and high-temperature oxidation.

The resulting pressure history in both porous reactors and in free volume significantly depends on the initial pressure and temperature. At lower initial temperatures the process in porous reactors is accelerated. There are five characteristic regions of the process characterized by different delay time, reaction rate and number of recognizable oxidation reactions. Combustion in porous reactor is characterized by heat accumulation in solid phase of porous structure and results in reduced pressure peaks and lowered combustion temperature. This depends on reactor heat capacity, pore density, specific surface area, pore structure and heat transport. Low- and high-temperature oxidation processes of Diesel sprays as performed in porous reactors are similar in nature to those in free volume combustion chamber.

### INTRODUCTION

Future internal combustion engine requires a clean homogenous combustion process. Such a process would result in simultaneous heat release characterized by a homogeneous temperature field in the combustion chamber. There are number of challenges in realizing of homogeneous combustion process in engine operating under variable load and speed conditions. Especially critical are: control of ignition timing, combustion duration, heat release rate and corresponding pressure gradient and pressure peak, control of combustion temperature for nearly zero- $\text{NO}_x$ -emissions, completeness of the process for low CO and HC emissions. There is no system known to the authors that can satisfy all conditions selected above, at least if variable load conditions are considered. Two of them are of special attention: control of ignition timing and lowering of combustion temperature below thermal  $\text{NO}_x$ -level. A novel kind of engine with combustion process in highly porous three-dimensional reactors that could satisfy above selected conditions has been proposed by Durst and Weclas [1,2]. This engine concept has great potential for high cycle efficiency and for a nearly-zero emissions level allowing combustion temperature control due to heat accumulation in reactor. During the time between fuel injection begins and the rapid pressure increase corresponding to the high-temperature heat release process (ignition delay) a number of complex chemical and physical processes must be performed. Physics of the process must consider fuel supply process (injection), spray distribution in space, spray atomization, fuel vaporization and mixing with air. These processes are of high

complexity in the case of Diesel engine-like conditions where the resulting mixture is highly non-homogeneous and time-space dependent. For future engines requiring clean combustion process (overall called as homogeneous combustion processes) the chemistry of the pre-ignition processes as well as controlled auto ignition are the key factors for process control under variable engine loads and rates. The low-temperature oxidation is usually treated as a two-stage process: cool- and blue flames are followed by a high temperature oxidation (depending on the initial temperature and pressure as well as on mixture composition). Additionally, development of high-temperature open cell and highly porous structures for application to internal combustion engines is necessary for development of this kind of combustion systems [3]. These processes can be divided into two groups: direct fuel injection into porous reactor (Diesel jet interaction with porous structure) and low- and high-temperature oxidation in the reactor. Thermal ignition and high-temperature oxidation (heat release) complete the investigated process [4-11]. There are almost no experimental data available in the literature on these processes. The paper describes selected aspects of these complex phenomena as performed in a free volume combustion chamber and in porous reactors under engine-like conditions. Heat release process in porous reactors having different structures and heat capacities is discussed in comparison to Diesel-like process (free volume combustion). In both cases a direct fuel injection using a common-rail diesel injection system into combustion chamber (free volume as well as porous reactor) is used.

## DIESEL SPRAY INTERACTION WITH POROUS STRUCTURE

Diesel jet may be considered as a free jet propagating in space outwards of the nozzle exit characterized by narrow angle, high penetration velocity, large penetration length and to some extent by atomization. For jet interaction with porous structure there is almost no information available in the literature describing this complex phenomenon. Mostly for modelling, the spray interaction with porous structure is substituted by mono-disperse droplets homogeneously distributed in the porous structure, e.g. see [12]. For combustion of a liquid fuels, the interaction between the fuel spray and a porous medium (PM) is very complex [13]. These authors say that this process could not be observed and measured with conventional experimental methods because the complexity of porous structure does not allow optical access into it. They suggested that numerical simulation offers the only way to perform the analysis. Contrary to that, the present authors [4-9] presented experimental data allowing first insight into the process of Diesel spray interaction with a three-dimensional porous structure. If free jet interacts with porous structure there are some characteristic phases of the process to be described in [5]. In a free space between nozzle outlet and porous structure the jet develops having diesel spray properties. The injection pressure defines the jet properties, especially propagation and then impingement velocity. Jet impingement process onto inner surface of the porous structure depends on a number of parameters, especially on spray properties and degree of its development. Jet penetrating into porous structure interacts with wall junctions and a wide radial spreading of the impinging jet with reduced penetration velocity occurs in PM volume according to a multi-jet splitting [4-8] - fig.1. If the porous structure is hot a superposition of fuel distribution (multi-jet splitting) and fuel vaporization is observed – fig.2.

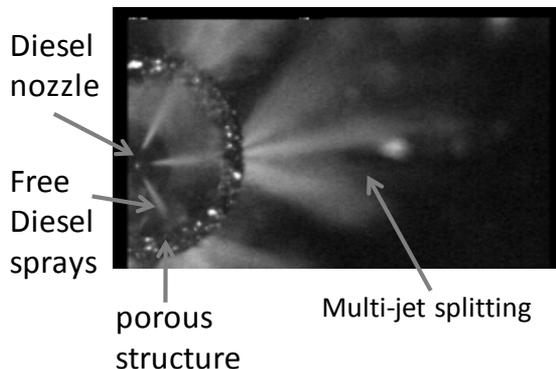


Figure 1: Multi-jet splitting by diesel jet interaction with porous structure

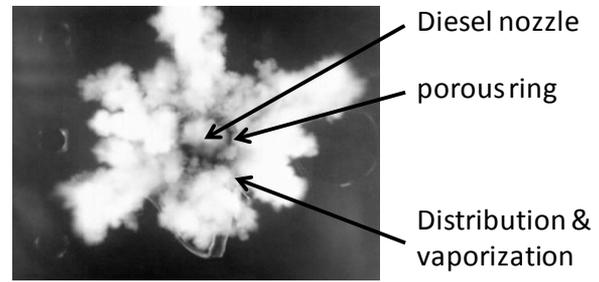


Figure 2: Diesel jet interaction with hot porous ring ( $T_{PM}=300^{\circ}\text{C}$ )

## SIMULATION OF ENGINE CONDITIONS FOR DIESEL SPRAY COMBUSTION IN FREE VOLUME AND IN POROUS REACTOR

Durst and Weclas [1,2] have proposed engine concept with mixture formation and combustion in a porous reactor. Application of a porous combustion reactor allows realization of homogeneous and flameless combustion process characterized by a near-zero emissions level. Heat recuperation in porous reactor may increase the engine-cycle efficiency resulting in reduction of  $\text{CO}_2$  emissions. Heat accumulation in porous reactor results in significantly lowered combustion temperature permitting near-zero  $\text{NO}_x$  level. This is the essential difference between the combustion process in conventional Diesel engine and in engine with combustion in PM (see fig.3 and 4). One of possible realization of real engine with combustion in porous reactor requires that the fuel must directly be injected into combustion reactor. This in consequence requires that the fuel must be distributed throughout the reactor volume together with vaporization and mixing with air. The hot reactor is used as a three-dimensional igniter and the heat release process must be performed in the reactor volume. The fuel should be injected in a short period of time close to the TDC of compression stroke. The reactor temperature (temperature of solid phase of the reactor and temperature of the gas trapped inside reactor volume) and homogeneity of mixture inside the reactor define the conditions for thermal ignition and following heat release process. This is because the reactor heat capacity and large specific surface area for inter-phase heat transfer inside the reactor volume change the thermodynamic conditions of the process [14].

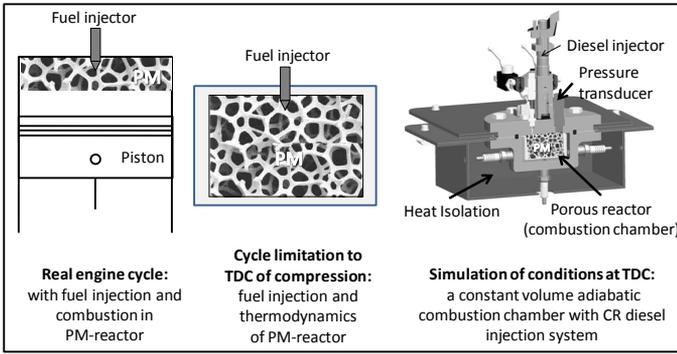


Figure 3: Simulation of real engine conditions in a special combustion chamber

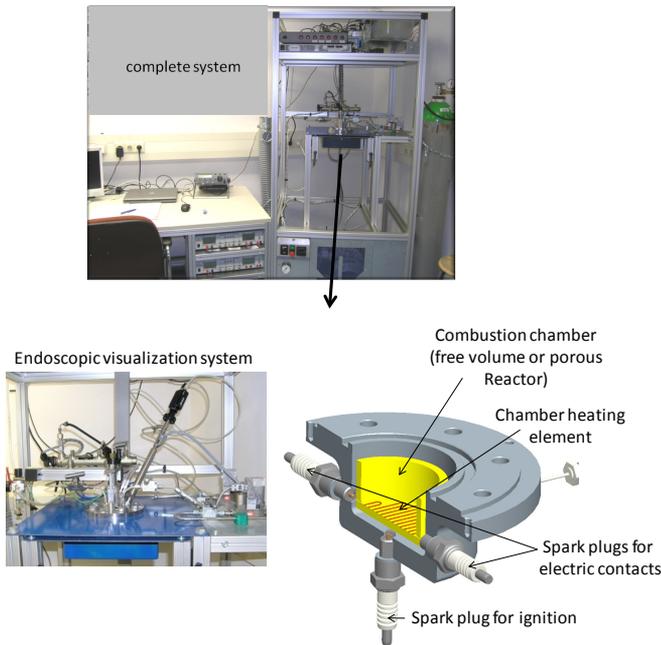


Figure 4: View of the combustion chamber

The whole process is analysed from time instance “zero” defined by the start of injection (“IB”). The procedure for setting of initial temperature  $T_{IB}=T_{PM}$  and initial pressure  $p_{IB}$  in the combustion chamber is shown in fig.5.

In a first step a given mass of synthetic dry air at certain pressure  $p_1$  is supplied to the chamber. After closing the system the air is trapped in chamber (or porous reactor) which is electrically heated up to required temperature  $T_{IB}$  corresponding to the porous reactor temperature  $T_{PM}$ . This also results in increasing chamber pressure achieving  $p_{IB}$ .

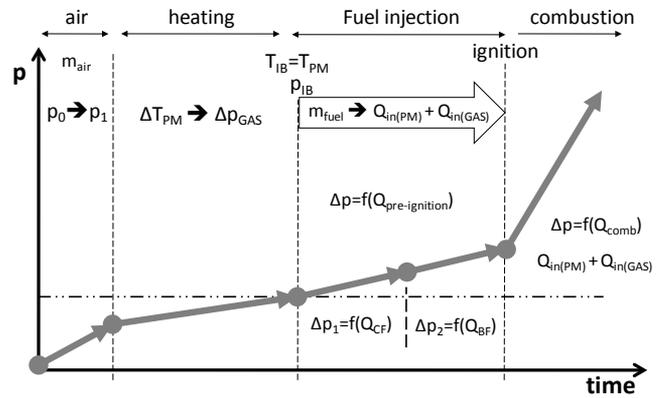


Figure 5: Measurement routing

Characteristic time  $t$  (delay time) of a particular process is analysed and measured starting at zero-time point (point IB)- see Fig.6. For analysis of the reaction rate a slope  $sl$  of the reaction curve corresponding to the particular oxidation process is described by average pressure changes in time [bar/ms].

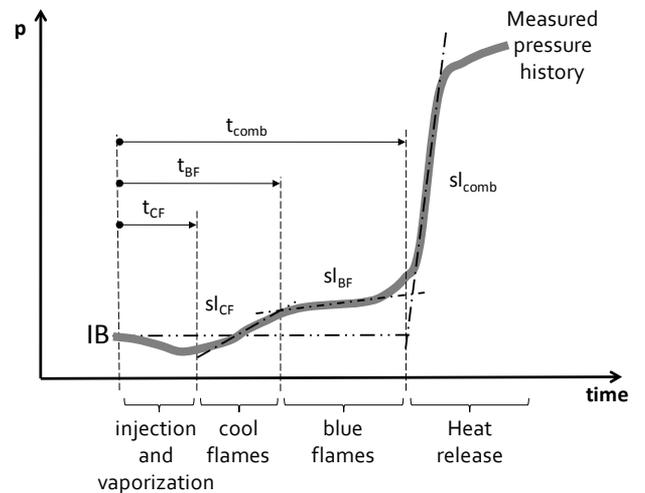


Figure 6: Definition of measured parameters on the pressure history

### OVERALL CHARACTERISTICS OF SPRAY COMBUSTION IN A FREE VOLUME UNDER DIESEL ENGINE-LIKE CONDITIONS

On the basis of performed investigations in a wide range of initial pressures and temperatures it is possible to construct fields representing characteristic combustion modes. These fields consider three kinds of parameters characterizing low- and high-temperature oxidation processes: characteristic reaction behavior represented by a single- or a multi-step oxidation, reaction rate and characteristic delay time. The data plotted have quantitative form, and only the shape of border lines among different combustion modes should be interpreted more qualitatively – see fig.7. On the left hand side of this figure characteristic modes are presented in  $p_{IB}-T_{IB}$  diagram. On the right hand side examples of pressure history in an initial part of the heat release process are plotted. There

are five characteristic modes of the process that have been selected:

Mode 1: Process at low initial pressures  $p_{IB}$  in a wide range of initial temperatures  $T_{IB}$  characterized by very long delay time ( $\sim 20$ ms), very low reaction rate ( $< 1$ bar/ms), and three slopes are recognizable.

Mode 2: Process at low initial temperatures  $T_{IB}$  in a wide range of initial pressures  $p_{IB}$  characterized by very long delay time ( $> 20$ ms), very low reaction rate ( $< 1$ bar/ms), and a single slope is recognizable.

Mode 3: Process at middle initial pressures  $p_{IB}$  and higher initial temperatures  $T_{IB}$  characterized by shorter delay time ( $< 10$ ms), middle reaction rate ( $\sim 5$ bar/ms), and three slopes are recognizable.

Mode 4: Process at middle initial temperatures  $T_{IB}$  and at higher initial pressures  $p_{IB}$  characterized by shorter delay time ( $< 10$ ms), middle reaction rate ( $< 10$ bar/ms), and two slopes are recognizable.

Mode 5: Process at high initial pressures  $p_{IB}$  and high initial temperatures  $T_{IB}$  characterized by short delay time ( $< 2$ ms), high reaction rate ( $> 20$ bar/ms), and two slopes are recognizable.

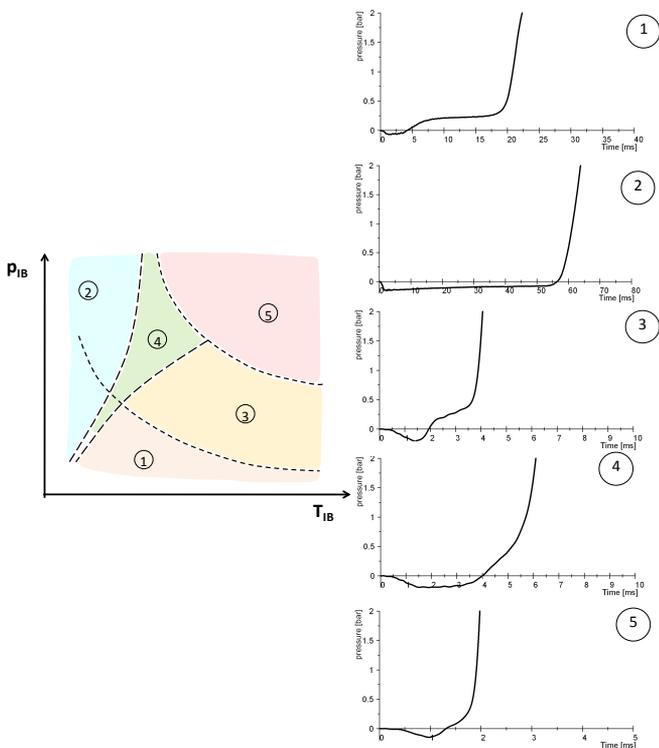


Figure 7: Characteristic modes of heat release process

In the range of low initial temperatures, mostly corresponding to cool flame reactions, a characteristic dependence of the delay time on the chamber pressure has been observed, as shown in fig.8. In a given range of pressures the delay time is the shortest and the corresponding reaction rates are the highest. This effect, in analogy to NTC (negative temperature coefficient), the authors have defined as a positive pressure coefficient PPC [11].

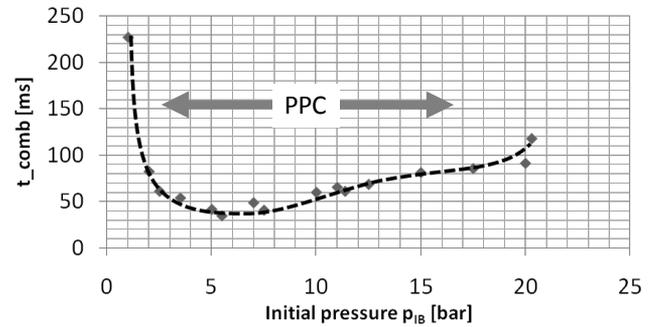


Figure 8: Range of positive pressure coefficient

An example of delay time distribution of characteristic reactions (top) as well as of reactions rate (bottom) is presented in fig.9. The data are plotted at constant air excess ratio ( $\lambda=1.5$ ).

## SPRAY COMBUSTION IN POROUS REACTORS UNDER DIESEL ENGINE-LIKE CONDITIONS

Application of highly porous three dimensional open cell structures to engines as well as to a combustion chamber significantly changes the conditions of mixture formation and combustion as compared to free volume combustion chamber:

- Large heat capacity of PM reactor (energy accumulation)
- Quite different conditions for spray development and its distribution in reactor volume
- Very effective and quick heat transport inside reactor
- Large specific surface area of PM reactor
- PM temperature dominates in the thermodynamics of the process (not gas temperature).

There are two types of reactor that have been considered: “ideal” porous reactor (IR) in which at any instant of time the gas temperature is equal to porous reactor temperature; “real” porous reactor (RR) in which at any instant of time after fuel injection starts the gas temperature is not equal to porous reactor temperature.

The thermodynamic analysis of the process in a free volume combustion chamber (FV) and in both considered porous reactors (IR and RR) allow formulating the following relations:

- Pressure change after fuel injection starts:

$$\Delta p_{G(FV)} > \Delta p_{G(RR)} \gg \Delta p_{G(IR)}$$

- Temperature change of gas after fuel injection starts:

$$\Delta T_{G(FV)} > \Delta T_{G(RR)} \gg \Delta T_{G(IR)}$$

The gas temperature change in a real reactor is a function of reactor temperature and can be expressed as [14]:

$$\Delta T_{G(RR)} = \Delta T_{G(FV)} - (K \cdot \Delta T_{PM})$$

where K is the factor characterizing reactor heat capacity and heat transfer conditions between gas and reactor solid phase.

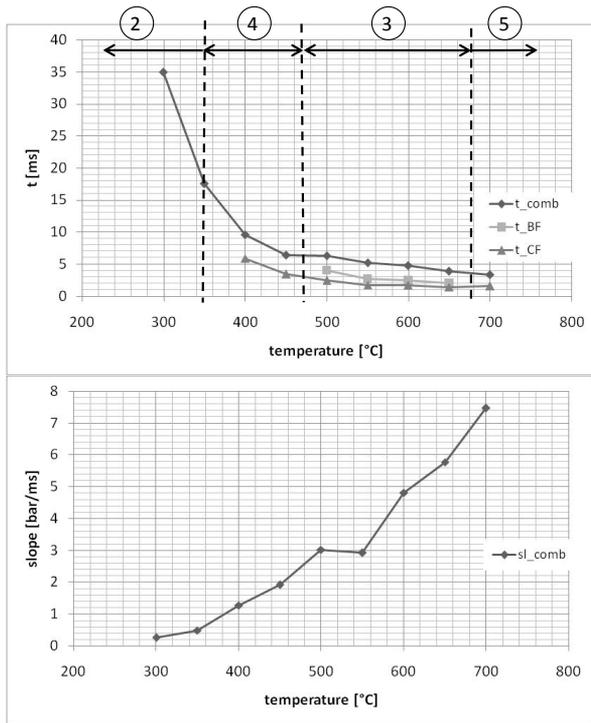


Figure 9: Distribution of delay times (top) and reaction rates (bottom) as a function of initial chamber temperature for a constant  $\lambda=1.5$

An example of heat release process in a porous reactor made of SiC foam structure (8ppi pore density) as compared to free volume combustion is shown in figure 10. Top diagram shows a pressure history as measured after start of fuel injection and the bottom picture shows the pressure gradients representing the heat release rate. The process in porous reactor is faster (delay time is shorter and the reaction rate is higher) and the resulting maximum pressure is lowered owing to the large heat capacity of the reactor. Pressure history corresponding to the heat release process as performed in a porous reactor has a similar character as observed for combustion in a free volume chamber.

The energy accumulated in the porous reactor lowers the combustion temperature keeping the reaction rate high. This temperature depends significantly on heat capacity of the combustion reactor. In figure 11 the heat release process in two SiC foam reactors having significantly different pore density (8ppi and 30ppi) is shown for different initial reactor temperatures.

Generally, the heat release process is more delayed with increasing pore density, i.e. with decreasing pore size (foam

structures). This effect is more visible at lower reactor temperatures. Also distribution of reaction rate indicates similar behaviour. The pressure peak level is pore density dependent and decreases with increasing pore density. This is mainly due to the heat capacity of reactor and heat transfer inside porous structure. The initial reactor temperature does not change this behaviour.

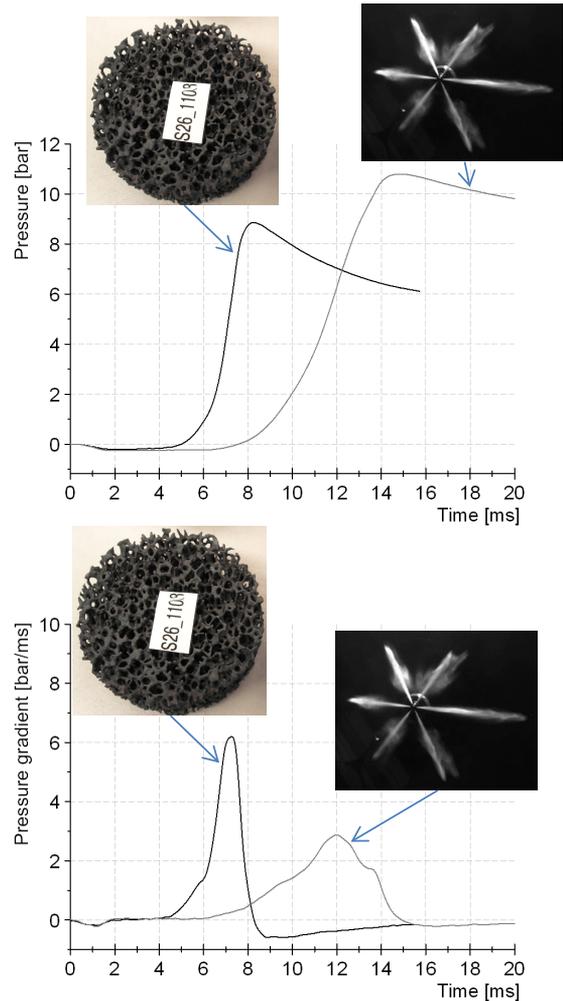


Figure 10: Heat release process in porous reactor (SiC foam structure, 8ppi) as compared to free volume process at  $p_{IB}=18\text{bar}$  and  $T_{IB}=400^\circ\text{C}$

The amount of heat accumulated in the porous reactor influences the maximum combustion temperature (real reactor conditions are considered). As shown in figure 12 the maximum combustion temperature for free volume combustion and for two different SiC foam reactors (8ppi and 30ppi) gradually increases with increasing initial temperature, and is significantly reduced in value for combustion reactors. This reduced temperature is a result of heat accumulation in a porous reactor and the maximum temperature reduces with increasing reactor heat capacity, pore density and specific surface area.

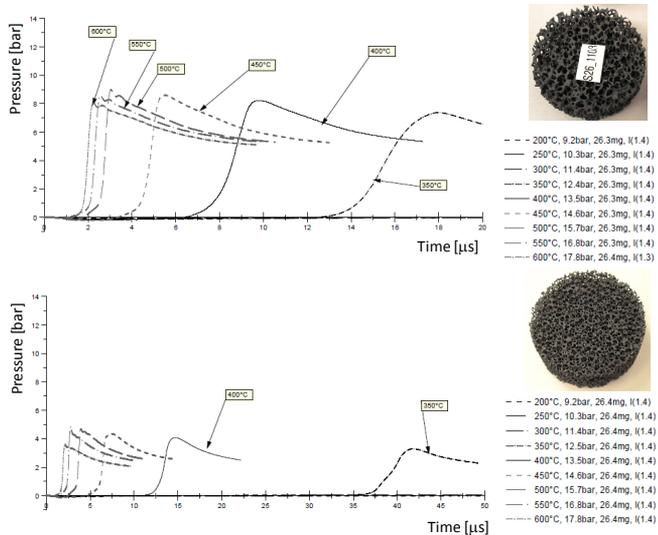


Figure 11: Comparison of pressure histories for heat release in different porous reactors after fuel injection starts at constant air access ratio  $\lambda$  (initial pressure, initial temperatures and mass of injected fuel are not constant)

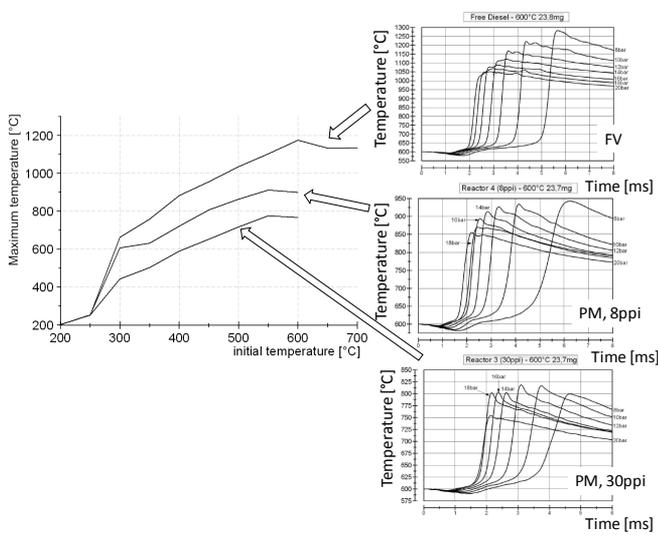


Figure 12: Distribution of maximum combustion temperature (left) versus initial temperature in free volume system and in two porous reactors (8ppi and 30ppi) for mass of injected fuel 23.8mg and a constant air excess ratio.

Characteristic features of heat release process can be constructed in two-dimensional fields representing characteristic combustion modes in porous reactors as compared to free Diesel injection conditions. There are two kinds of parameters to be considered: characteristic reaction behavior represented by a single- or a multi-step oxidation (fig.13) and distribution of characteristic delay time (fig.14). All these data are plotted in a two-dimensional field of initial chamber pressure and temperature. The data have been grouped according to pre-selected criteria, such as number of slopes in reaction curve and duration of delay time. The data plotted have quantitative character, and only the shape of

border lines among different combustion modes should be interpreted more qualitatively. The shape of border lines depends on the reactor heat capacity, pore density and pore structure.

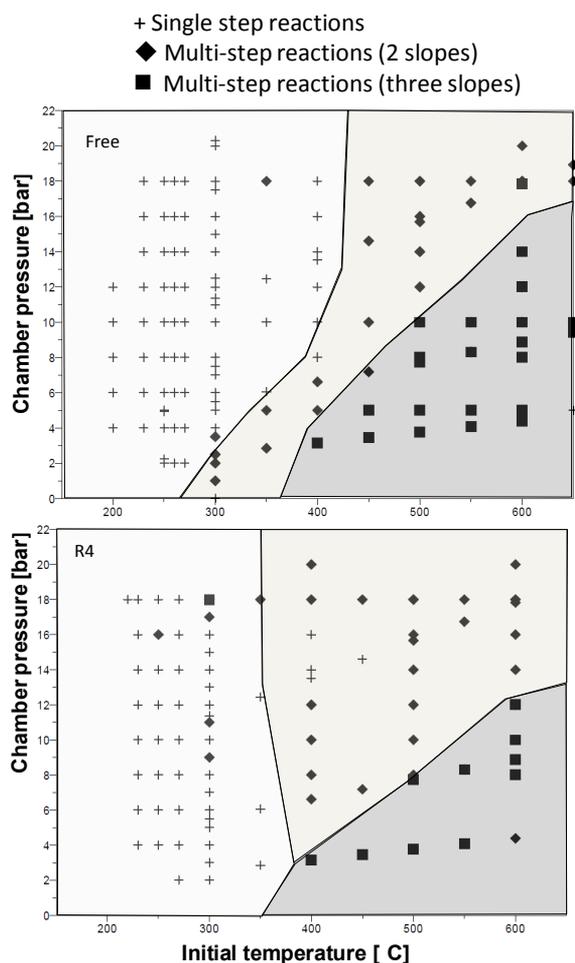


Figure 13: Fields representing characteristic combustion modes in SiC foam (8ppi) porous reactor as compared to free Diesel injection conditions

There are three characteristic regions selected in fig.13 representing three different characteristic modes of the oxidation process:

Region 1 is characterized by single-step reactions and is located at lower initial temperatures for all initial pressures.

Region 2 is characterized by multi-step reactions with two slopes recognizable in the reaction curve and is located in the range of middle-high initial temperatures at middle-high initial pressures.

Region 3 is characterized by multi-step reactions with three slopes recognizable in the reaction curve and is located in the range of higher initial temperatures at low-middle initial pressures.

In the case of reaction delay time the following regions are selected in fig.14:

Region A is characterized by delay times  $t > 20\text{ms}$  and is located at lower initial temperatures at all investigated initial pressures.

Region B is characterized by delay times  $10\text{ms} < t \leq 20\text{ms}$  and is located at higher initial temperatures and lower initial pressures as well as in a small region of high initial pressures.

Region C is characterized by delay times  $5\text{ms} < t \leq 10\text{ms}$  and is located at higher initial temperatures and lower-middle initial pressures as well as in a small region of high initial pressures.

Region D is characterized by delay times  $2\text{ms} < t \leq 5\text{ms}$  and is located at higher initial temperatures and middle to high initial pressures.

Region E is characterized by delay times  $t \leq 2\text{ms}$  and is located at high initial temperatures and high initial pressures.

Analysis of characteristic regions selected in figures 13 and 14 indicates qualitative similarity of heat release process as performed under Diesel-like conditions and in porous reactor. A quantitative influence of porous reactor features (reactor heat capacity, pore density, pore structure, specific surface area and fuel distribution in reactor volume) is clearly visible. This qualitative similarity of processes as performed in a free volume and in porous reactors indicates high probability for applicability of the concept with clean combustion in porous reactor to internal engine conditions. Quantitative influence of reactor conditions described by reactor heat capacity, pore density, pore structure, specific surface area, fuel distribution in reactor volume and heat transport indicates a large potential for system optimization for application to internal combustion engines.

### CONCLUDING REMARKS

1. Diesel spray combustion is a very complex multi-step process. The physics of spray formation, penetration and mixture formation must be considered together with chemistry of low- and high-temperature oxidation.
2. For investigating of this kind of reactions a special combustion chamber characterized by a constant volume and adiabatic conditions has been used as an engine simulator.
3. Positive Pressure Coefficient (PPC) indicates range of pressures  $p_{IB}$  where delay time of pre-ignition reactions is the shortest and the rate of these reactions is the highest (mostly corresponding to cool-flame reactions and transition to blue-flames).
4. Ignition delay time reduces with increasing chamber temperature and pressure: slow reactions are characterized by delay time of many tens to hundreds of milliseconds; fast reactions are characterized by delay time being less than one millisecond at high temperatures and high pressures.
5. Low- and high-temperature oxidation of Diesel sprays are significantly temperature and pressure dependent. There are five characteristic regions of the process characterized by different delay time, reaction rate and number of recognizable oxidation reactions.
6. Low- and high-temperature oxidation processes of Diesel sprays as performed in porous reactors are in nature similar to those in a free volume combustion chamber.
7. There are three main differences in the process conditions at similar thermodynamic conditions:
  - large heat capacity of the reactor influencing pressure peak level (heat supplied to the reactor)
  - large specific surface area of the reactor influencing heat transfer inside reactor volume
  - porous structure (pore size, density and structure) influencing the process of Diesel injection and fuel distribution in space as well as fuel vaporization and mixing with air.

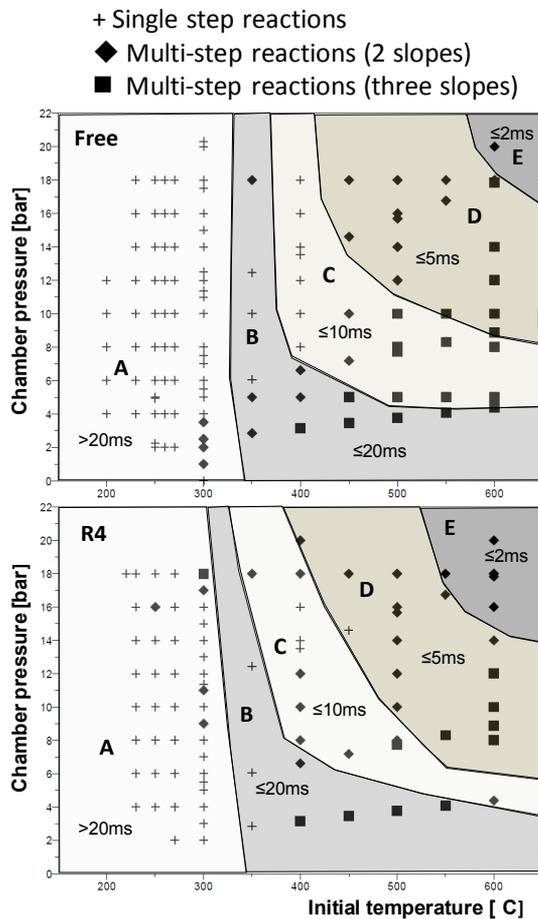


Figure 14: Fields representing characteristic combustion modes and delay times in SiC foam (8ppi) porous reactor as compared to free Diesel injection conditions

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