On Transient Temperature vs. Equivalence Ratio Emission Maps in Conjunction with 3D CFD Free Piston Engine Modeling

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ABSTRACT

In order to acquire knowledge about temperature vs. equivalence ratio, T-φ, conditions in which species are formed and destroyed during the combustion of diesel fuel, T-φ parametric maps were constructed for CO₂, CO, OH, soot and soot precursors (C₂H₂) as well as for nitrogen oxides (NO and NO₂). Each map was obtained by plotting data from a large number of simulations for various T-φ combinations in a zero-dimensional, 0D, closed Perfectly Stirred Reactor, PSR. Since both the elapsed time and pressure change in an engine cycle, the maps were constructed according to engine pressure traces obtained from the Computational Fluid Dynamics, CFD, simulations. Since the pressure is changing in elapsed time intervals, the maps are called transient. Correlations between the maps and the 3D engine simulation results were then examined by plotting the T-φ conditions in all computational cells of the CFD simulation on the maps. The map approach is a useful tool for visualizing the links between in-cylinder T-φ conditions and emission levels, and to identify conditions that promote efficient, low-emission engine operation. All engine simulations were made for a free piston engine, but conclusions can be valid for conventional engines as well. The effect of varying spray model parameters such as the initial sauter mean radius, droplet size distribution and the constants in the break-up model was studied.

INTRODUCTION

PREVIOUS STUDIES ON T-φ MAP ANALYSIS

Recently, great efforts have been made to develop new strategies for the reduction of soot and NOₓ emissions in diesel engines. As a tool to help understand the regions of emission formation, T-φ map analysis was first introduced by Kamimoto et al [1]. Later, Akihama et al. [2] applied the same approach, together with three dimensional, 3D, engine simulations to study Low Temperature Combustion, LTC, in a passenger car engine where high Exhaust Gas Recirculation, EGR, conditions were employed. Other applications of T-φ maps for combustion analysis can be found in [3,4,5]. However, in all these studies, only NOₓ, soot and soot precursors were the subject of investigation. Meanwhile, the maps are static in the sense that the pressure and elapsed time were kept constant during the engine cycle, i.e. only one map was used to analyze the whole engine cycle. In this study, which is a continuation of previous work presented in [6], transient T-φ maps were constructed according to the changes in pressure with time that occur during an engine cycle.

OBJECTIVE

Emission maps were constructed based on pressure traces from CFD simulations. Correlations between the maps and the engine simulation results were examined by plotting the T-φ conditions in all computational cells of the CFD simulation on the maps. The combustion chemistry incorporated into the CFD code is represented by the same detailed model as in the 0D code used to construct the T-φ maps. Hence, the formation and destruction of chemical species can be traced throughout the engine cycle, using the CFD code alone. Consequently, the T-φ maps were not used to determine the emissions in the T-φ regions of the CFD simulation results, which would have saved computational time, but to visualize and identify conditions that promote efficient, low-emission engine operation.

METHODOLOGY FOR THE CONSTRUCTION OF TRANSIENT EMISSION MAPS

Each map was derived from 720 simulations of different T-φ combinations in a 0D, closed Perfectly Stirred Reactor, PSR. The engine cycle was divided into ~20 steps of elapsed time and pressure, and for each step, a set of emission maps was constructed (see Figure 1), beginning at the time of the Start Of Injection, SOI. Input values for the next time/pressure step were acquired from the final mixture composition at each PSR point. Figure 2 represents an example of a soot - NO emission map, showing the location of various data on the map. The maps show mole fractions of the considered species in iso-lines. Circles, colored in accordance with the gas mass in each computational cell cluster, are plotted on the maps representing the T-φ conditions in the CFD engine simulation. The time since the start of the map simulation (reacting time) is chosen to correspond to the SOI in the CFD simulation. Some information obtained solely by the CFD engine simulation is also presented on the map (see Figure 2), including Mass Fraction Burnt,
MFB, mass fraction in T-φ cell clusters (circles plotted on the map) and spatially averaged species concentrations.

Figure 1. Elapsed time and pressure data acquired from an engine simulation and applied as initial conditions for the construction of T-φ maps

![Pressure, Mass Fraction in Burnt, Mass Fraction in T-φ bins](image)

![Time Since Start of Simulation](image)

![Spatially Averaged Species Concentrations](image)

**THE DIESEL OIL SURROGATE (DOS) MODEL**

Since the amounts of soot produced from n-heptane alone are considerably smaller than those produced from real Diesel oil, an aromatic fuel component, toluene, is included in the DOS model. The detailed oxidation paths of n-heptane, C_{14}H_{28}, and toluene, C_{7}H_{8}, found in the literature, were systematically reduced to contain 70 species participating in 305 reactions. N-heptane was chosen to be in excess, since its cetane number is 56, which is similar to the cetane number of real Diesel oil. Details on the mechanism construction can be found in [10].

Since the version of the KIVA-3V code used can only handle single-component fuels, and the DOS model consists of two components, a global reaction is introduced which decomposes the starting fuel, C_{14}H_{28}, into its constituent components; n-heptane, C_{7}H_{16}, and toluene, C_{7}H_{8}:

\[ 1.5C_{14}H_{28} + 0.5O_{2} \rightarrow 2C_{7}H_{16} + C_{7}H_{8} + H_{2}O \]

**SOOT FORMATION AND OXIDATION**

Since aromatic compounds are known to comprise about 10-30% of the constituents of Diesel oil, 33% toluene (by volume/mole) is present in the DOS model. Aliphatic compounds do not form soot at temperatures below 1800 K, but aromatics does [11]. The low temperature route goes through toluene oxidation, generating the phenyl radical, C_{6}H_{5}. A pathway is included from the phenyl radical to acenaphthylen, A2R5, via the HACA-mechanism (H-Abstraction-C_{2}H_{2}-Addition). In order to avoid having to continue to model the formation of the large polycyclic rings that coalesce to form soot, the elementary reactions stop at the formation of A2R5. The transformation from gaseous soot precursors to solid soot particles (nucleation) occurs via the global graphitization reactions:

\[ A2R5 \rightarrow 12C(s) + 4H_{2} \]
\[ C_{6}H_{2} \rightarrow 6C(s) + H_{2} \]

Oxidation of solid soot particles occurs via the four global reactions:

\[ C(s) + O_{2} \rightarrow O + CO \]
\[ C(s) + H_{2}O \rightarrow CO + H_{2} \]
\[ C(s) + OH \rightarrow CO + H \]
\[ C(s) + N_{2}O \rightarrow CO + N_{2} \]

**NO\textsubscript{x} FORMATION**

Thermal NO formation is accounted for by the extended Zeldovich mechanism (reactions 1-3 in Table 1). N_{2}O is formed (reactions 4-7 in Table 1), and can continue to form NO (reaction 8 in Table 1). The formation of NO\textsubscript{2}, which is known to be almost exclusively via the NO molecule by reaction number 9 in Table 1 [12], is also accounted for (reactions 9-12). The Fenimore mechanism, relevant to rich combustion, is not included.

**COMPUTATIONAL TOOLS**

The maps were constructed using the constant pressure, constant temperature option (TTIM) of the 0D SENKIN code of the Chemkin-2 package [7]. The CFD simulations were performed using a modified version of the KIVA-3V, rel. 2 code [8]. The models used in the CFD simulations at Chalmers University have been described in detail by various authors, e.g. [9]. The Diesel Oil Surrogate, DOS, model was implemented into both codes.
Table 1. Reactions of NO₂ (forward reaction rate: \( k = A_i T^\epsilon \exp(-E_i/RT) \) in cm\(^3\), mole, sec and cal units)

<table>
<thead>
<tr>
<th>( A_i )</th>
<th>( n_i )</th>
<th>( E_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. N + NO</td>
<td>N₂ + O</td>
<td>3.50E+13 0 330</td>
</tr>
<tr>
<td>2. N + O₂</td>
<td>NO + O</td>
<td>2.65E+12 0 6400</td>
</tr>
<tr>
<td>3. N + OH</td>
<td>NO + H</td>
<td>7.33E+13 0 1120</td>
</tr>
</tbody>
</table>

**N₂O formation and destruction**

| | |
| 4. N₂O + O | N₂ + O₂ | 1.40E+12 0 10810 |
| 5. N₂O + H | N₂ + OH | 4.40E+14 0 18880 |
| 6. N₂O + OH | N₂ + H₂O | 2.00E+12 0 21060 |
| 7. N₂O + M | N₂ + O + M | 1.30E+11 0 59620 |

**N₂O to NO** (low \( E_i \) i.e. at low temperatures)

| | |
| 8. N₂O + O | NO + NO | 2.90E+13 0 23150 |

**Main NO to N₂O branch [12]**

| | |
| 9. NO + H₂O | NO₂ + OH | 2.11E+12 0 -480 |
| 10. NO + O + M | NO₂ + M | 1.06E+20 -1.41 0 |
| 11. NO₂ + O | NO + O₂ | 3.90E+12 0 -240 |
| 12. NO₂ + H | NO + OH | 1.32E+14 0 360 |

**TURBULENCE CHEMISTRY INTERACTION**

The Partially Stirred Reactor (PaSR) model is used in order to predict the effect of sub-grid spatial mixing on the chemical source term. The change in concentration of species \( i \) due to one chemical reaction is:

\[
\frac{d[C_i]}{dt} = \tau_{\text{chem}} \left( \frac{d[C_i]}{dt} \right)_{\text{Arhenius}}
\]

The solution for the changes in the concentration of species \( i \) over all reactions is not coupled, but solved sequentially, although updating the species concentration after each reaction. The mixing time is calculated using the \( k - \delta \) turbulence model according to:

\[
\tau_{\text{mix}} = 0.015 \frac{k}{\delta}
\]

The shortest chemical time, \( \tau_{\text{chem}} \), is calculated using the Arrhenius reaction rate, \( k' f \), and the species in excess, \( C_i \), according to:

\[
\tau_{\text{chem}} = \frac{1}{k' f [C_i]}
\]

**BREAK-UP MODELING**

The Kelvin-Helmholtz, K-H, and Rayleigh-Taylor, R-T, models are implemented in a competing manner, i.e. the droplet breaks up by the mechanism that predicts the shortest break up time.

The K-H instabilities are due to turbulence within the fuel, leading to perturbations on the liquid / gas interface, whereas the R-T instabilities mainly occur as a result of deceleration of the droplets due to drag. The change in radius of the parent drop is given by:

\[
\frac{dr_o}{dt} = r_o - r_f
\]

Where \( r_f \) is the radius of the child drop and \( \tau \) is the break-up time. For the K-H instabilities the break-up time is:

\[
\tau_{\text{KH}} = \frac{3.726 B}{\Lambda \Omega}
\]

where \( \Lambda \) is the unstable wavelength on the liquid surface and \( \Omega \) is the frequency. A lower value of \( B \) represents more disturbances. Values of \( B \) in the literature range from 1.73 to 60 [13]. In this article values of 10 and 40 were examined. After wall impingement turbulence increases and \( B \) is switched to another value (1.73), since Reitz et al. found good agreement with the experimentally measured spray penetration for this value. Close to the orifice the R-T is usually the governing mechanism, whereas the K-H breakup becomes more dominant further downstream. In order to be able to reproduce experimentally obtained intact core or breakup lengths, e.g. given by the relation:

\[
L_{\text{bu}} = C \cdot \left( \frac{\rho_f}{\rho_g} \right)^{\frac{1}{3}} \cdot d_{\text{mic}}
\]

the R-T model that would predict extremely rapid breakup directly at the nozzle exit is “switched off” within this breakup length. The constant \( C \) usually ranges from 1 to 1.9 [14], in this study taken as 1.2.

**DEFINITIONS OF THE EQUIVALENCE RATIO**

**THE EQUIVALENCE RATIO BASED ON THE FUEL**

The fuel/oxidizer equivalence ratio is defined as:

\[
\phi = \left( \frac{m_f}{m_{\text{ox}}} \right) = \left( \frac{n_f MW_f}{n_{\text{ox}} MW_{\text{ox}}} \right) = \left( \frac{n_f}{n_{\text{ox}}} \right)
\]

where \( m_f \) and \( m_{\text{ox}} \), \( n_f \) and \( n_{\text{ox}} \), \( MW_f \) and \( MW_{\text{ox}} \) are the masses, number of moles and molecular weights of fuel and oxidizer in the mixture, respectively, and \( st \) denotes stoichiometry. The equivalence ratio will be zero even when only a single oxygen atom is attached to each of the original fuel molecules. However, sometimes it can be useful to have a measure of the mixing of C, H and O atoms during the entire engine cycle. In such cases, the calculation of the equivalence ratio needs to be based on the intermediate and product composition.
THE EQUIVALENCE RATIO BASED ON INTERMEDIATES AND PRODUCTS

If $n_i$ is kept at $n_{fr}$ for all equivalence ratios, i.e. only the amount of oxygen is varied, the above equation reduces to:

$$
\phi = \frac{n_{fr}}{n_{ox}} = \frac{n_{ox}}{n_{ox}} = \frac{O \text{ atoms required to fully oxidize } C + H}{\text{available O atoms}}
$$

The $\phi$ is now defined as the number of O atoms required to fully oxidize the available C and H atoms, divided by the number of available O atoms. Since two O atoms are required to fully oxidize one C atom to CO$_2$ and 0.5 O atoms to fully oxidize one H atom to H$_2$O:

$$
\phi = \frac{\sum_i 2n_{C_i}[C_i]}{\sum_i n_{O_i}[C_i]}
$$

where $n_{C_i}$, $n_{H_i}$ and $n_{O_i}$ are the numbers of C, H and O atoms, respectively, of the $i^{th}$ species and $[C_i]$ is the concentration of the $i^{th}$ species in moles/unit volume.

It is instructive to note that due to the mass conversion of O, H and C atoms, the global equivalence ratio will be constant from the end of the fuel injection until Exhaust Valve Opening, EVO.

THE OXYGEN EQUIVALENCE RATIO

The oxygen equivalence ratio first appeared in the literature in [15]. It is calculated in the same way as the equivalence ratio based on intermediates and products in the previous section, but CO$_2$ and H$_2$O are entirely omitted from the summation of atoms. Consequently, it can be used as a measure of the reactivity of the mixture, since it is only based on species that have not been fully oxidized. The oxygen equivalence ratio will only be zero if/when the complete conversion to CO$_2$ and H$_2$O has taken place.

THE INFLUENCE OF EGR

In order to avoid increasing the equivalence ratio due to the presence of C and H atoms originating from EGR, a special procedure was implemented which omits the CO$_2$ and H$_2$O in the EGR composition from the summation of atoms in the $\phi$ calculation. However, in the summation of O atoms in the denominator of the $\phi$ formula, no attempt was made to distinguish between oxygen originating from the fresh air and oxygen from lean EGR products.

GENERAL T- $\phi$ MAP ANALYSIS

The temperature and pressure were held constant in each calculation point of the map. The same temperature before and after combustion was superimposed, so the conditions are non-isochoric and non-adiabatic. Therefore, in some regions of the map, the actual T-$\phi$ combination will never be obtained in practice from combustion with a certain $\phi$. In order to acquire a measure of the temperature that would be obtained in practice after combustion with a certain $\phi$, the adiabatic mixture temperatures at constant pressure were calculated independently using the EQUIL code of the Chemkin-2 package. Then, the adiabatic T-$\phi$ trajectories were plotted on the maps shown in Figures 3-4, representing the maximum temperature that can be achieved after combustion. The equilibrium calculation starts from a temperature of 900 K, typical for in-cylinder conditions at the SOI for diffusion combustion.

The T-$\phi$ region with the highest combustion efficiency is shown in Figure 3, which presents CO, soot - NO, CO$_2$ and C$_2$H$_2$ species. The region stretches from 1500-2500 K for lean to stochiometric conditions. At temperatures lower than 1500 K at lean conditions there will be smaller amounts of CO$_2$ due to the lower concentrations of important radicals, acting as oxidizers e.g. OH, Figure 4. Thus, there will be a lot of incomplete combustion products, e.g. CO and C$_2$H$_2$, as shown in Figure 3. Those species are not present in large concentrations at temperatures between 1500-2500 in lean to stoichiometric regions, thus one can conclude that this is the most favorable region for complete conversion to products. At high temperatures (>2500 K) CO levels increase again due to dissociation of the complete combustion product CO$_2$. Figure 3 shows that the region of highest combustion efficiency tends to be at higher temperatures for richer mixtures.

The most efficient combustion region is located between the high soot-NO formation regions, since soot is a product of incomplete combustion and product dissociation via important exothermic reactions, e.g. CO + OH = CO$_2$ + H contributes to the high NO concentration at high temperatures. The OH released can then form NO in the Zeldovich reaction: N + OH = NO + H, as illustrated in Figure 4.
Figure 3. CO, Soot – NO, CO\textsubscript{2} and C\textsubscript{2}H\textsubscript{2} mole fractions showing the T-\(\phi\) region with the highest combustion efficiency, at 50 bar after 1 ms.

Figure 4 shows that the T-\(\phi\) region with the highest NO concentrations coincides with the region of the highest OH concentrations, illustrating the “soot – NO dilemma”, i.e. in the region with high NO concentrations a lot of OH will be available to oxidize the soot previously formed in locally rich regions. However, outside this high temperature region, NO will not be formed but soot may be, and only small amounts of OH radicals will be available to oxidize it later in the cycle.

Figure 4. The T-\(\phi\) regions with the highest NO and OH concentrations coincide. OH radicals are needed for the oxidation of soot previously formed in locally rich regions.

**3D CFD FREE PISTON ENGINE SIMULATIONS**

The 3D CFD simulations were carried out for a Free Piston Engine, FPE, which is characterized by rapid turning at TDC, mainly in the expansion stroke. A FPE has no crank mechanism, and the piston motion is controlled by Newton’s second law, providing the possibility to vary the compression ratio without any hardware modifications. Nevertheless, most conclusions about the combustion process that will be drawn here are also valid for crankshaft driven engines.

In order to meet stringent emissions legislation, the FPE is designed to run in the HCCI mode, i.e. the piston bowl is of a flat design (see Figures 7-8). However, since HCCI combustion is not easy to control, diffusion combustion is planned to be utilized during the first stage of engine testing.

**FREE PISTON VS. CRANKSHAFT-DRIVEN MOTION**

Figure 5 compares the piston motion of the FPE to a corresponding crankshaft-driven engine. The most pronounced difference is that for the FPE the piston is closer to TDC during the whole compression stroke. Then, just after TDC the expansion is very rapid. The maximum free piston speed is lower than for a conventional engine with the same speed and stroke, but the peak value is reached more quickly.

Figure 5. Predicted free piston position and velocity as compared to a corresponding crank-shaft driven engine at 31.96 Hz/1918 rpm.

**DETERMINATION OF THE FREE PISTON MOTION**

In order to simulate the FPE the CFD code was modified by replacing the conventional crank shaft controlled piston motion by a piston motion profile calculated using a MATLAB/SIMULINK model. This model employs Newton’s second law, accounting for the forces acting on the piston/translator, i.e. friction forces, electrical forces, and in-cylinder gas forces. The onset of combustion is modeled with an ignition delay integral and the heat release by Wiebe functions. Those simplified models used in the dynamic modeling have been tuned iteratively with the help of heat release curves from CFD modelling (the DOS model). Figure 6 shows the Wiebe function used to simulate diffusion combustion, together with the heat release predictions from the CFD modeling. A detailed description of the MATLAB/SIMULINK model can be found in [16].
ENGINE CHARACTERISTICS AND COMPUTATIONAL GRID

Although the FPE does not employ a crank mechanism, virtual CAD notation will be used to indicate timings hereafter, since it is widely used. However, the quoted CADs are merely time equivalents calculated as $\text{CAD} = \text{time} \times \text{frequency} \times 360$. The main engine characteristics and operating point are listed in Table 2. Table 3 presents some of the computational models parameters.

<table>
<thead>
<tr>
<th>Table 2. Main engine characteristics and operating point</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore [cm]</td>
</tr>
<tr>
<td>Number of exhaust valves</td>
</tr>
<tr>
<td>Number of inlet ports</td>
</tr>
<tr>
<td>Swirl angle [deg]</td>
</tr>
<tr>
<td>Number of injector orifices</td>
</tr>
<tr>
<td>Nozzle hole diameter [mm]</td>
</tr>
<tr>
<td>Injected fuel mass/stroke [mg]</td>
</tr>
<tr>
<td>Intake boost pressure [bar]</td>
</tr>
<tr>
<td>Compression ratio</td>
</tr>
<tr>
<td>Stroke [cm]</td>
</tr>
<tr>
<td>Engine speed [Hz]</td>
</tr>
<tr>
<td>Spray umbrella angle [degree]</td>
</tr>
<tr>
<td>Injection duration [CAD]</td>
</tr>
<tr>
<td>Power [kW]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3. Parameters of the computational models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Grid Cells in the 72 degree sector grid</td>
</tr>
<tr>
<td>50 radial</td>
</tr>
<tr>
<td>32 azimuthal</td>
</tr>
<tr>
<td>75 vertical</td>
</tr>
<tr>
<td>K-H Breakup Constant ($B_1$ before wall impingement)</td>
</tr>
<tr>
<td>K-H Breakup Constant ($B_1$ after wall impingement)</td>
</tr>
<tr>
<td>R-T Breakup Constant ($C_3$)</td>
</tr>
<tr>
<td>Breakup Length Constant ($C$, distant)</td>
</tr>
<tr>
<td>Initial Sauter Mean Radius</td>
</tr>
<tr>
<td>Initial Sauter Mean Radius Distribution</td>
</tr>
<tr>
<td>Wall/Head/Piston temperature [deg. C]</td>
</tr>
<tr>
<td>Number of Injected Parcels</td>
</tr>
<tr>
<td>Spray Cone Angle [degree]</td>
</tr>
</tbody>
</table>

A 72-degree sector polar mesh (Figure 7) was used since it offers good resolution of the spray. The initial swirl ratio was taken from a full 360 degree mesh simulation, including inlet ports and exhaust valves (see Figure 8).
RESULTS - VARYING THE SPRAY UMBRELLA ANGLE, CONSTANTS OF THE BREAK-UP MODEL, INITIAL SMR AND DROPLET SIZE DISTRIBUTION

Two spray umbrella angles; 140 deg. and 153 deg. were examined. The results in terms of emissions towards the end of the cycle (105 CAD ATDC), combustion efficiency and pressure-volume work for the simulated duration (-105 CAD to 105 CAD ATDC) are summarized in Table 4 and Table 5 for constants $B_1$ in the K-H break-up model of 10 and 40, respectively. Table 4 shows that the wider spray angle is required to get high combustion efficiency, avoiding severe spray piston interaction (see Figure 9, showing liquid tracers and gas $\phi$). When introducing EGR (case 3) the accompanied delay causes incomplete combustion. Case 4 is not using an initial droplet size distribution. However, the effect on combustion characteristics and average droplet size is minor, see Table 4 (compare case 4 and 2) and Figure 10, respectively.

Table 4. Results for SOI at 10 CAD BTDC, $B_1=10$

<table>
<thead>
<tr>
<th>Case #</th>
<th>Spray Angle</th>
<th>Soot [ppm]</th>
<th>NO [ppm]</th>
<th>CO [ppm]</th>
<th>Comb $\eta$ [%]</th>
<th>P-V work [J]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\alpha=140$ deg.</td>
<td>0.2</td>
<td>17</td>
<td>1100</td>
<td>62</td>
<td>205</td>
</tr>
<tr>
<td>2</td>
<td>$\alpha=153$ deg.</td>
<td>0.07</td>
<td>39</td>
<td>600</td>
<td>99.4</td>
<td>333</td>
</tr>
<tr>
<td>3</td>
<td>$\alpha=153$ deg. + 40% EGR</td>
<td>0.2</td>
<td>5</td>
<td>2010</td>
<td>90</td>
<td>287</td>
</tr>
<tr>
<td>4</td>
<td>$\alpha=153$ deg. + CONST. DROP SIZE</td>
<td>0.08</td>
<td>38</td>
<td>590</td>
<td>99.7</td>
<td>333</td>
</tr>
</tbody>
</table>

Table 5. Results for SOI at 10 CAD BTDC, $B_1=40$

<table>
<thead>
<tr>
<th>Case #</th>
<th>Spray Angle</th>
<th>Soot [ppm]</th>
<th>NO [ppm]</th>
<th>CO [ppm]</th>
<th>Comb $\eta$ [%]</th>
<th>P-V work [J]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>$\alpha=153$ deg.</td>
<td>0.15</td>
<td>24</td>
<td>1040</td>
<td>89</td>
<td>292</td>
</tr>
</tbody>
</table>

Figure 11 shows the parcels together with the oxygen and product $\phi$ of the gas phase for case 2. The oxygen $\phi$ is illustrative of the regions of incomplete combustion; first in regions in the core of the fuel vapor, and at 5 CAD ATDC near the piston. The high swirl transports the combustion region outside the cutplane at TDC. Two separate simulations were carried out for an identical case, illustrating the stochastic behavior of the spray, i.e. the position and size of the spray parcels of Figure 11 differ for the same CAD of the identical simulations. Naturally, this will cause other slight changes, e.g. the combustion efficiency differs by 0.17 %. The random number generator which is used to generate the probability of the collisions as well as the initial droplet size is responsible. Also in experiments there is always some cycle-to-cycle variation in the jet penetration and symmetry [17].

The impact when the constant $B_1$ in the K-H model was changed from 10 to 40 is profound as shown in Table 5 (compare case 5 and 2). Figure 9 shows poor evaporation, i.e. very low product $\phi$ of the gas for $B_1=40$, illustrating the importance of K-H instabilities downstream in the spray. Another parameter that greatly affects the spray penetration is the Sauter Mean Radius, SMR, of the droplets exiting the nozzle (see Figure 12).

Figure 9. Spray parcels (circles) and product $\phi$ distribution at 5 CAD BTDC for different spray angles, EGR and K-H model constants ($B_1$)

Figure 10. Average Sauter Mean Radius vs. CAD when using an initial droplet size distribution vs. constant size for the same input SMR

Figure 11. Spray parcels and oxygen/product $\phi$ distribution at different CAD for case 2
Figure 12. Spray parcels and product equivalence ratio distribution at 5 CAD BTDC for different initial Sauter Mean Radii ($B_1=10$, $B_2=140$, $\alpha=140$) mass in T-\(\phi\) regions plotted on soot – NO maps

Figure 13 shows soot-NO maps combined with in-cylinder T-\(\phi\) regions (circles), illustrating the effect of EGR (bottom row, case 3) vs. EGR free (top row, case 2) mixtures. All other parameters such as SOI etc. were identical. As expected, when including EGR the combustion is delayed in the cycle and the peak temperatures reduce.

It should be noted that the smaller species mole fractions when including EGR in the maps are affected by mixture dilution and does not necessarily mean that e.g. less soot is formed if the T-\(\phi\) are identical.

CONCLUSIONS

THE APPLICABILITY OF T-\(\phi\) MAPS TO THE COMBUSTION PROCESS IN REAL ENGINES

The map approach is a useful tool for visualizing and establishing links between in-cylinder T-\(\phi\) conditions and emission levels. The maps were made relevant to engines by changing the pressure in a certain number of time intervals. Nevertheless, the combustion process in the map is still quite different from that in a real engine. In an engine, the local equivalence ratio and temperature changes with time, and the mass migrates between T- \(\phi\) regions. In the map, each PSR point is kept at constant T- \(\phi\) conditions throughout their time courses. For example the regions where NO was formed do not cool down as the do in the expansion stroke of an engine. This means that for example NO conversion into...
NO₂ by reaction 9 in Table 1, which is promoted by low temperatures (negative \( E_a \)), relevant to the expansion stroke (especially for HCCI combustion) cannot be captured using the map approach, as illustrated in Figures 14-15. Figure 14 shows that in the maps NO₂ is only formed in high temperature regions where NO was once formed (above 2100 K), whereas in the (HCCI) engine simulation of Figure 15, NO₂ formation begins at ~40 CAD ATDC (Figure 15a) and continues to increase from then, although the maximum temperature is only 1700 K, dropping to 1200 K (Figure 15b).

To conclude, total NO\(_x\) emissions can be predicted from map analysis, but the distribution among the NO\(_x\) species is changed (Figure 15a) and cannot be predicted. For soot and CO, which are formed and then oxidized in different T-\( \phi \) regions, analysis based on the map is less straightforward. Therefore, the maps cannot be used as absolute values for predicting emission levels in engine simulations. Since the maps should be used only as conceptual tools, we believe that transient maps, despite being more accurate than static maps, are not precise tools.

HCCI VS. DIFFUSION COMBUSTION IN T-\( \phi \) MAPS

Figure 16 clearly shows that HCCI combustion is characterized by lower temperatures and equivalence ratios than diffusion combustion. Hence, soot formation is virtually non-existent and NO formation only occurs fairly far into the “peninsula” at high temperatures. The peak CO levels, which occur around TDC, are much higher for diffusion combustion due to the presence of more mixture in rich regions. HCCI combustion shows a cluster of points at low T-\( \phi \), a region where CO concentrations are high. Hence the main CO formation regions are quite different. Nevertheless, the engine-out emissions of CO are generally lower for diffusion combustion, since there is more scope for oxidation due to the higher levels of OH (Figure 5) and O radicals formed at high temperatures.

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