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A Study on the Emissions of Alternative Aviation Fuels

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ABSTRACT

Currently, the aviation sector is seeking for alternatives to kerosene from crude oil, as part of the efforts combating climate change by reducing greenhouse gas (GHG) emissions, in particular carbon dioxide (CO_2), and ensuring security of supply at affordable prices. Several synthetic jet fuels have been developed including sustainable bio-kerosene, a low-carbon fuel. Over the last years, the technical feasibility as well as the compatibility of alternative jet fuels with today's planes has been proven However, when burning a jet fuel, the exhaust gases are a mixture of many species, going beyond CO_2 and water (H_2O) emissions, with nitrogen oxides (NOx), carbon monoxide (CO), unburned hydrocarbons (UHC) including aromatic species and further precursors of particles and soot among them. These emissions have an impact on the local air quality as well as on the climate (particles, soot, contrails). Therefore, a detailed knowledge and understanding of the emission patterns when burning synthetic aviation fuels is inevitable. In the present paper, these issues are addressed by studying numerically the combustion of four synthetic jet fuels (Fischer-Tropsch fuels). For reference, two types of crude-oil based kerosenes (Jet A-1 and Jet A) are considered, too. Plug flow calculations were performed by using a detailed chemical-kinetic model validated previously. The composition of the multi-component jet fuels were imaged by using the surrogate approach. Calculations were done for relevant temperatures, pressures, residence times, and fuel equivalence ratios φ. Results are discussed for NOx, CO as well as for benzene and acetylene as major soot precursors. According to the predictions, the NOx and CO emissions are within about ± 10% for all fuels considered, within the parameter range studied: $T = 1800$ K, $T = 2200$ K; $0.25 \leq \varphi \leq 1.8$; $p = 40$ bar; $t = 3$ ms. The aromatics free GtL (Gas to Liquid) fuel displayed higher NOx values compared to Jet A-1/A. In addition, synthetic fuels show slightly lower (better) CO emission data than Jet A-1/A. The antagonist role of CO and NO_x is apparent. Major differences were predicted for benzene emissions, depending strongly on the aromatics content in the specific fuel, with lower levels predicted for the synthetic aviation fuels. Acetylene levels show a similar, but less pronounced, effect.

Keywords: kerosene, alternative aviation fuels, emissions, NOx, soot, CO, CO_2, benzene, reaction mechanism

INTRODUCTION

It is expected that demands of energy will increase worldwide, while fossil resources are decreasing at the same time. To address this challenge, many efforts are assigned to increase efficiencies of existing combustion concepts. Furthermore, the use of alternative and renewable energy resources is attracting much interest, also to counteract climate change attributed to the burning of fossil fuels, *e.g.* to limit the global temperature increase to less than 2°C [1]. Efforts are undertaken aiming to meet the energy demands in the field of energy [2-9], road transportation [10-12], and aviation [13-16]. As a consequence, concerning the aviation sector, ACARE (Advisory Council for Aeronautical Research in Europe) has announced its goal of reducing CO_2 emissions by 50% in 2020 and by 75% by 2050 relative to year-2000 aircraft [17]. The 'Flightpath 2050' initiative of the European Commission [18] aims at a 90% reduction in NOx emissions, besides others.

For these reasons, meanwhile, a wide range of fuel candidates and fuel blends is discussed, also considering different feedstock and processes [19-20]. Five types of synthetic kerosenes are certified and approved: (i) CtL (coal); (ii) FT-SPK (Fischer-Tropsch, synthetic paraffinic kerosene) *e.g.* GtL (natural gas) or BtL (biomass); (iii) HEFA (hydro processed esters and fatty acids); (iv) SIP (synthesized iso-paraffins), *i.e.* farnesane; and (v) AtJ, alcohol-to-jet.

Today, the technical feasibility of synthetic jet fuels is proven [13-16, 19-28]. Due to the certification, synthetic jet fuels are assumed to perform appropriate with respect to the combustion in the aero engine and to the whole fueling system including material (sealing) and thermo stability aspects of the fuel itself. However, as emissions depend on the type of aero engine, emission tests are not part of the approval protocol.

The combustion of any fuel and its emissions are directly linked to its specific composition, besides the combustion determining parameters, such as temperature, pressure, and equivalence ratio. On one hand, any alternative aviation fuel is composed of hydrocarbons, and thus, similar to Jet A-1/A. On the other hand, the amount of hydrocarbons of a certain kind as well as the chemical family and the H/C ratio might differ considerably [19-21]. Hence, the emission characteristics might also differ when burning these fuels in a jet turbine.

In this context, synthetic aviation fuels available are offering an emission pattern with a reduced detrimental factor on the environment because they contain no fuel-bound nitrogen and almost no sulfur or aromatics. The last affects the emission behavior leading to a considerably reduced number of particulates; *i.e,* having a better performance with respect to the local air quality when compared to crude-oil kerosene [19].

In the last years, several experimental studies were done focusing on the emissions of combustors and turbine engines operated with alternative jet fuels. For an overview of major relevant studies, see [28-29] and references therein. The emissions measured include gaseous emissions, mostly CO, CO_2, NO_X, UHC, and particle emissions, in mass, number, and size, besides sulfur containing species, aromatics, and aldehydes. Studies on emission pattern in exhaust plumes are limited. The fuels may be studied both neat and in blends with petroleum-derived fuels, as a response to the approval protocol.

These investigations have shown differences in the emission pattern of alternative aviation fuels compared to the one of Jet A-1/A. It was also pointed out that a clear trend in a specific emission, *e.g.* NOx [27] is not straightforward due to the existing interactions between physical and chemical properties when burning the liquid fuel mixture in a highly turbulent system, depending on thrust, too.

In the present study, the emission pattern of four synthetic jet fuels (Fischer-Tropsch fuels) is investigated numerically by exploiting a detailed chemical-kinetic reaction mechanism. The goal is, thus, to get more insight into trends and potential differences in the emission pattern when burning different synthetic fuels. The reaction model was shown previously to describe correctly combustion relevant properties, in particular laminar flame speed, ignition delay time, and product species, for several synthetic aviation fuels [13-16], for a wide range of operating parameters.

For this purpose, plug flow calculations were performed for relevant temperatures, pressures, residence times, and fuel equivalence ratios φ. The composition of the multi-component jet fuels were addressed by following the surrogate approach [16, 19]. For reference, two types of crude-oil based kerosenes (Jet A-1 and Jet A) were considered also. Results are presented for emissions of NOx, CO, benzene and acetylene, as major soot precursors. The predicted trends are discussed with respect to global trends and differences in the combustion behavior of a specific fuel. In addition, an overview is given on CO and NOx measurements reported in literature. Thus, this work might contribute to help fostering the transition from crude-oil based jet fuels to synthetic jet fuels having a less harmful impact on the environment.

EMISSIONS

Aviation fuels may contain numerous hydrocarbon molecules, their oxidation leading to the release of several pollutants. The emissions spectrum is dependent on the interactions between physical and chemical processes, and turbulence when burning the vaporized fuel in a gas turbine [20]. Physical properties (*e.g.* surface tension and viscosity) affect fuel's placement, in particular atomization and evaporation; chemical properties (*e.g.* molecule family) affect fuel's combustion, in particular type and amount of exhaust gases (emissions), laminar flame speed (stability), and ignition delay time (safety) [20]. These properties are dominated by the specific fuel's composition and the operational parameters: temperature, fuel equivalence ratio, pressure, and reaction time. In addition, the emissions are dependent on the different flight operations (power settings), shown schematically in Fig. 1. Emissions at power settings most known are those from LTO-cycle (landing–takeoff, ICAO) measurements [30].

The present work is focusing on the following pollutants: CO, NOx, and unburned hydrocarbons (UHC) addressing acetylene and benzene considered as the major precursors of particles and soot [31-37]. Soot is formed when the fuel is burned under excess of fuel (fuel rich, $\varphi > 1$); NOx species are produced when the fuel is burned under excess of air ($\varphi < 1$). Note that the main exhaust gases products - CO_2 and water (H_2O) - are not considered in the study as well as sulphur containing species (SO_2) which are not present in synthetic aviation jet fuels.

Emission Index Calculation

In order to provide a better comparability of the emissions for different power settings and fuel mass flows, the emission species mass flow is normalized by the fuel mass flow. This is called the emission index, whose unit is given as g/kg_{fuel}.

For experimental studies and flight measurements, the emission index of nitrogen oxides (NOx) is calculated from the emission index of carbon dioxide (CO_2), which is straightforward to determine from the carbon content of the used fuel [39]. Equation 1 provides an example of an emission index (EI) calculation from measurement results [39-40].

$$\mathrm{EI}_n = \frac{\mathrm{E}_n}{\mathrm{E}_{\mathrm{CO_2}}} * \frac{\mathrm{M}_n}{\mathrm{M}_{\mathrm{CO_2}}} * \mathrm{EI}_{\mathrm{CO_2}} \qquad \text{Eq. (1)}$$

Often, the pure emission index is additionally referenced on the International Civil Aviation Organization (ICAO) thrust levels. In order to limit emissions of NOx, CO, and hydrocarbons, ICAO publishes boundary values in Annex 16 Volume II [30]. The limits imposed are dependent on the maximum rated thrust of the engine at sea level static conditions without water injection, the engine age, and the engine pressure ratio [30].

The emission indices given in the present study were calculated to allow a comparison with measurement results provided by literature. Thus, they are not intended to represent a specific engine. The simulation results allow a direct reference of the calculated emission mass in grams on the used fuel mass. However, a difference to measured values is to be expected because the simulation does not consider fuel viscosity, spray behavior as well as burner geometry or staged combustion. Additionally, measurements are mostly taken at the exit plane of the engine or in the developing exhaust plume, not directly behind the burner [39, 41-43].

APPROACH – SELECTED ALERNATIVE FUELS, SURROGATES, AND SIMULATION CONDITIONS

Within this study, a variety of six fuels, by exploiting the surrogate approach, were considered. The detailed compositions of the surrogates used are presented in Table 1.

Two of the utilized surrogates were developed in order to model crude-oil based kerosene: One surrogate represents Jet A-1 [44], the other Jet A [21]. Two different surrogates are used to account for the composition variations of crude-oil based kerosene depending on source, production process, and standard [22-23]. Additionally, the comparison aims at minimizing the deviations between surrogate and real fuel behavior caused by modeling.

Furthermore, four alternative fuel models were used in the calculations. These surrogates model a CtL (Fully synthetic Jet Fuel by Sasol) [24], two different GtLs (Syntroleum S-8, Royal Dutch Shell GtL) [24-25], and a mixture of Royal Dutch Shell GtL and naphthenic cut [25], a product of coal liquefaction. The GtL+naphthenic cut (GtL+n-c) surrogate models a 50% mixture by volume. These mixtures may be used to operate aircraft without the need of blending with crude oil kerosene to adjust density and aromatics content to the required amounts [25]. The selected CtL serves as a synthetic reference fuel with defined origin and composition. The Shell GtL surrogate was chosen as a representative of the Fischer-Tropsch based fuels. The Syntroleum S-8 surrogate was used to contrast the Shell GtL surrogate with a two components surrogate. Additionally, S-8 is a synthetic kerosene often analyzed; its composition is considered similar to HEFA (hydrotreated esters and fatty acids) based synfuels. Therefore, the possibility to model both fuel types with the same surrogate has been pointed out by Naik *et al*. [26].

MODELING AND SIMULATION

For the simulation of the combustion of the six fuels, the software Chemical Workbench, version 4.1, developed by Kintech Lab Ltd. was used [45]. As a model reactor, the calorimetric bomb reactor (CBR) was combined with an equivalence ratio mixer module, to adjust the desired equivalence ratios. The CBR module [45] uses the assumptions of isobaric and isothermal conditions. Therefore, pressure and temperature are set to predetermined values. In order to maintain constant temperature and pressure at different equivalence ratios, the heat flux from or to the reactor is assumed, the energy equation is not considered by the program [45]. The CBR calculates homogeneous distributions of the reactants and thus a perfect mixture. Product production rate is limited by reaction rate, not by mixing or flow processes.

Within the current study, calculations were done for temperatures of 1800 K and 2200 K at p = 40 bar; the reaction time was set to 3 milliseconds. These values were chosen in order to approximate conditions typical to jet engine combustors [38, 46-47]. Fuel equivalence ratios were varied between 0.25 and 1.8, in order to depict different thrust levels and flame zones. A mixture of 79 mol% nitrogen and 21 mol% oxygen was used to represent dry air.

The reaction model used is composed of two parts: (i) the hydrocarbons reaction mechanism validated and used in the Alfa-Bird study [13-16, 24]; and (ii) a nitrogen reaction part taken from the public-domain mechanism, GRI, version 3.0 [48]. The hydrocarbons reaction mechanism consists of 6346 reactions comprising 1437 species, the nitrogen sub model adds 108 reactions and 17 nitrogen containing species. Note that calculations with a nitrogen sub model considering thermal NO production only gives considerably lower NOx values than the ones achieved with the full nitrogen sub model, even at high temperatures (2200 K) [49].

In the present work, the focus is on the trend of predicted emissions, within the combustion of several synthetic kerosenes, not on absolute concentration numbers. In general, it is assumed that the performance of a chosen reaction model will not lead to erroneous conclusions, when studying the combustion of similar fuels under the same conditions. In addition, similar, the uncertainty ranges of a model will not differ [50-51].

RESULTS AND DISCUSSION

By applying the detailed reaction scheme described earlier, the combustion behavior of the fuels is studied as a function of temperature and equivalence ratios, at a constant pressure (40 bar) and up to 3 milliseconds. Calculated emissions profiles of the four alternative fuels and the two kerosenes (Jet A-1/A) are presented as a function of time: CO (Fig. 2), NOx (Fig. 4), benzene (Fig. 6), and acetylene (Fig. 7). In addition, emission indices of CO (Fig. 3) and NOx (Fig. 5) are given, for a discussion with measurements (Tables 3-4).

In summary, no differences in CO emissions exceeding 10% at relevant time scales between the six fuels were predicted. For NOx emissions, the overall difference between all fuels investigated was about ± 10%, similar to CO emissions. However, major differences are predicted concerning benzene emissions, a major precursor of soot particles, with the levels strongly dependent on aromatics content in the fuel considered, and with additional difference resulting from the kind of aromatic compounds.

Adiabatic flame temperature

Concentrations of emissions may be strongly dependent on specific combustion parameters, *e.g.* temperature, pressure, and residence time. For example, concerning NOx emissions, the dominant NOx formation pathway is thermal-NOx, also referred to Zeldovich NOx, according to:

$O+N_2 \rightleftharpoons NO+N$,

$N+O_2 \rightleftharpoons NO+O$,

$N+OH \rightleftharpoons NO+H$.

Due to the high activation energy reflecting the strong triple bond within the nitrogen molecule, the thermal NOx pathway starts to open at high temperatures, $T > 1800$ K, and becomes dominant at even higher temperatures. Hence, concentrations of NOx emissions follow the adiabatic flame temperature of a specific fuel-air mixture.

For these reasons, adiabatic flame temperatures are calculated for all fuels considered, for synthetic jet fuels and for kerosene from crude-oil (Jet A-1 and Jet A). Calculations are conducted at five different equivalence ratios ranging from fuel lean (φ = 0.25) to fuel–rich (φ = 2.0). All fuels show very similar combustion temperatures (Table 2a). Consequently, similar NOx values are expected; however, care must be taken in interpreting measured values due to the interaction between physical and chemical properties of the liquid fuels [27-29].

It is difficult to connect a specific φ value to a specific power state of a jet engine. Therefore, Table 2b provides a list of possible equivalence ratios leading to those adiabatic flame temperatures used for the calculations in this study (T = 1800 K and 2200 K, respectively). Thus, the results provided later on, in terms of emission indices, can be applied much easier for LTO cycles due to the wide range of equivalence ratios considered; especially Take-off (100% thrust) and Climb (85% thrust) [30] provide conditions similar to the ones considered in the present study, with high burner temperatures.

CO Emissions

CO emission calculations by using the detailed reaction scheme are conducted for the six fuels considered. All calculations are performed at relevant temperatures ($T = 1800$ K and $T = 2200$ K) at high pressures $p = 40$ bar, and residence times up to 3 milliseconds. Equivalence ratios are ranging between $\varphi = 0.25$ and $\varphi = 2.0$.

Results are given in Figs. 2 and 3. The color code applied to the designation of the fuels is as follows: Jet A-1 (black), Jet A (red), CtL (green), GtL+n-c (light blue), GtL (dark blue), and S-8 (orange). The fuel equivalence ratio φ is depicted by the kind of symbols used. Note that for monotonous graphs, the axes are cut in order to show areas of higher dynamics in greater detail.

As a result, no differences larger 10% at relevant time scales between the fuels were calculated. Both GtL-fuels showed lower emission values than Jet A-1/A. Apparently, this finding correlates with the low aromatics content as well as the high content of *n*- and *iso*-paraffines. CtL and GtL+n-c, with cyclic or aromatic components, are closer to Jet A-1/A.

<u>CO emissions calculated at *T* = 1800 K</u>

CO emissions calculated at $T = 1800$ K and for lean equivalence ratios ($0.25 \leq \varphi < 1.0$) are predicted to peak very early followed by a strong decrease at longer reaction times (Fig. 2a). Under these conditions, the fuels can be separated into two groups: (i) GtL and S-8 displaying lower emissions; and (ii) CtL and GtL+n-c, the remaining two alternative aviation fuels, as well as Jet A-1 and Jet A. The maximum calculated peak values of about 83,000 ppm are caused by Jet A-1, followed by Jet A. The lowest CO emissions are predicted for lower φ values. With decreasing φ values, the differences (absolute and relative) between the fuels are reduced. For $t = 0.003$ s, CO emissions are below 100 ppm for all fuels, at fuel-lean and stoichiometric mixtures.

For fuel rich conditions ($\varphi > 1.0$) and T =1800 K, the predicted CO emissions of all fuels rise with reaction time (Fig. 2b). The predicted maximum difference between the highest and the lowest CO emissions is between 5,000 and 7,000 ppm. This corresponds to a difference of about 5% referring to the maximum value of the family of curves at t = 0.003 s for φ = 1.8 and 7% for φ = 1.4, respectively. The Jet A emission curves are calculated as the highest for all fuel rich equivalence ratios; at φ = 1.4 and φ = 1.6, the lowest emissions are calculated for GtL+n-c. For higher φ values (φ = 1.8, open triangle), CO emissions of GtL and S-8 curves are approaching those of GtL+n-c.

CO emissions calculated at *T* = 2200 K

At T = 2200 K, emission values are much higher, for lean and fuel rich mixtures (Fig. 2c-d). While the highest peak values under fuel lean conditions are predicted for Jet A-1, Jet A-1 shows the lowest emissions for times $t \geq$ 20 µs. However, for stoichiometric mixtures (Fig. 2c, open triangles), Jet A-1 emissions are lower than the ones of Jet A, but higher than the corresponding synthetic jet fuels emissions. The emission curves of the alternative fuels are close. At φ = 1, GtL and S-8 emissions are predicted to be the lowest, while both GtLs approach Jet A for lower equivalence ratios. GtL+n-c shows similar behavior compared to pure GtL and S-8; CtL is closer to Jet A-1.

For fuel-rich mixtures, the emissions predicted increase over time, as well as for T =1800 K. For φ = 1.6 and φ = 1.8, the CO emissions of Jet A and CtL differ by less than 1% within the first 100 µs; then, Jet A emissions increase much more than the CtL ones approaching the values calculated for Jet A-1. For φ = 1.4, emissions of Jet A and of GtL+n-c cut are close to each other, with lower levels compared to CtL, before reaching amounts similar to the ones of Jet A-1. Syntroleum S-8, GtL, and GtL+n-c (sorted by rising emission values) exhibit the lowest calculated emissions, with about 5% difference at the end of the simulation time.

CO emissions - Comparison with measured values

Due to the difficulty of connecting an equivalence ratio to an ICAO power setting (see above), CO emissions indices are depicted in Fig. 3 for equivalence ratios ranging from φ = 0.3 to φ = 1.8. With respect to the high values at fuel rich conditions, note that an oxidation of CO to CO_2 possible after the burner exit plane was not considered.

The emission indices calculated for fuel lean conditions reach values similar to values provided from measurements (Table 4). The compositions of the fuels CtL (Fully Synthetic Jet Fuel - FSJF) and FT-SPK+50% n-c served as basis for the surrogate models of the fuels CtL and GtL+n-c used in the present study. They show similar emission levels compared to the simulated ones. Note that the temperature provided in the table is the burner inlet temperature used in the experiment [27]. The actual combustion temperature is higher and similar to the temperatures used here for simulation. The simulated emission values of CtL are higher than the values for GtL+n-c while the provided measurements indicate the opposite. This may result from different spray behaviors attributed to the fuels not considered in the simulation [27-29].

Nitrogen Oxide Emissions

NOx emissions of the six fuels were calculated for the same parameter range as for CO emissions; results are given in Figs. 4 and 5. The same color code was applied to label the fuels. All simulations were done for a reaction time of 3 ms. However, the diagrams provided display results for times up to 0.5 ms and 1.0 ms, respectively, accounting for the continuous time dependent behavior of NOx emissions of all fuels. Thus, differences in the fuels emission profiles are easier to follow.

NOx emissions calculated at $T = 1800$ K

Overall, low NOx emissions are calculated: with values around 6 ppm at stoichiometric equivalence ratios, and even lower values at lower fuel equivalence ratios. The predicted maximum deviation between all fuels studied is about 0.5 ppm corresponding to 8%.

For fuel lean conditions ($0.25 \leq \varphi < 1.0$), higher emissions are predicted with higher equivalence ratios, with a reduction in increase with rising equivalence ratios (Fig. 4a). At the lowest equivalence ratio considered ($\varphi = 0.25$), the calculated NOx emissions of Jet A-1/A are the highest, followed by the ones of CtL and Gtl+n-c It is interesting to note that, with rising equivalence ratios (for $\varphi < 1.0$), NOx emissions of Jet A increase less than those of the other fuels; hence, for $\varphi = 0.6$ and $\varphi = 0.8$, Jet A produces the lowest NOx emissions. On the other hand, NOx emissions simulated of GtL and S-8 show a higher increase with rising equivalence ratios. Therefore, at $\varphi = 1.0$, GtL and S-8 clearly exhibit the highest NOx emissions, whereas the lowest NOx emissions are predicted for CtL and GtL+n-c.

With fuel equivalence ratios increased further ($\varphi > 1.0$), lower NOx emissions are predicted (Fig. 4b). For fuel rich mixtures ($\varphi = 1.8$), calculated NOx emissions are below 0.25 ppm at $t = 3$ ms. In addition, the GtL+n-c and CtL fuels produce the highest NOx amounts calculated. Decreasing differences between the fuels are predicted for higher equivalence ratios. This behavior cannot be caused by decreasing adiabatic flame temperatures since the reactor model is isotherm with a predefined constant reaction temperature (set to 1800 K or 2200 K). Instead, the effect is caused by specific combustion properties of the fuels investigated.

Therefore, a reaction path analysis of the reaction mechanism used was conducted for fuel lean ($\varphi = 0.5$), stoichiometric, and fuel rich ($\varphi = 1.6$) mixtures at 1800 K. The results reveal the domination of the prompt NO production path [49]. The production path significances of NO are found to be almost identical for all conditions predicting only minor differences in the order of 5% or below. Predicted nitrogen oxide consumption differed even less with a maximum deviation of 2.9%. Furthermore, the relative importance of the NO production paths changed only marginally between the fuels studied, Jet A-1, GtL, and CtL [49].

NOx emissions calculated at $T = 2200$ K

For higher temperature and lean conditions, NOx emissions increase with decreasing φ values up to $t = 0.05$ ms (Fig. 4c). Then, the higher slopes of the emission curves for low equivalence ratios result in higher NOx emissions at $t = 1.0$ ms albeit the higher equivalence ratios initially show higher emission values. Jet A-1 emissions are the lowest for all fuel lean equivalence ratios. Jet A emissions are calculated as highest for $\varphi = 0.25$ but increase less than GtL, S-8 and GtL+n-c with rising equivalence ratios. The biggest deviation between all fuels is predicted with about 25 ppm for $\varphi = 1.0$.

Stoichiometric conditions show the biggest difference from lowest emission curve to highest emission curve, with about 10%. For fuel rich conditions (Fig. 4d), the emission levels simulated decrease with increasing equivalence ratios, as already seen for calculations at $T = 1800$ K. Here, GtL and Jet A show almost identical simulation results whereas Jet A-1 produces the lowest emissions, as already seen for fuel lean conditions. The emission values of CtL are calculated as the second lowest. The highest emissions are predicted for S-8. The initial differences between the different fuels decrease over time under fuel rich conditions.

NOx is produced by more than 60% via the thermal-NOx pathway as calculations with a nitrogen sub model considering thermal nitrogen oxide production only reveal [49].

NOx emissions - Comparison with measured values

The relation of the emission values at high equivalence ratios to the fuel flow leads to further reduced emission indices compared to fuel lean conditions (Fig. 5). The calculated emission indices for T = 1800 K are all below the provided literature values (Table 4). Only for T = 2200 K and for equivalence ratios below φ = 1.1, the values are in the same order of magnitude. Especially for high equivalence ratios, the calculated values are too low. This finding might result from the high *iso*-octane contents in the fuels leading to elevated CH_i-levels with increased reburning and reduced free oxygen concentrations. On top of that, turbulence and the resulting zones of higher combustion temperature are not considered in the homogeneous reactor model used in the study. Further discrepancies might be caused by influences due to the burner geometry and imperfect fuel atomization, causing areas of high temperature in real combustion systems.

Calculations conducted at p = 1 bar for varying fuel lean equivalence ratios at T = 1800 K predict higher emission amounts (six to twelve times higher depending on equivalence ratio, compared to calculations conducted at 40 bar) [49]. Resulting emission indices are of the same order of magnitude as results from Bhagwan et *al.* [27]; see Table 4. The relative difference between the surrogates remains below 10 %, similar to the trends at high pressure.

Emissions of soot particles

Radiation by soot particles is the major mechanism how heat is transferred to the combustor walls in a gas turbine engine. However, soot particles have an impact on the local air quality and on radiative forcing, due to its effects on contrails properties as well as on cirrus cloud formation [57]. For these reasons, information on the sooting characteristics of synthetic jet fuels relative to Jet A-1/A is highly needed.

Acetylene (C_2H_2) and benzene (C_6H_6) plays an important role in the formation of polyaromatic hydrocarbons (PAH) considered as major building blocks in soot formation [31-37]. Therefore, benzene and C_2H_2 emission profiles serve as an indicator for a fuel's sooting tendency.

Benzene emissions

The simulations depict large differences in the benzene profiles (Fig. 6). Jet A-1 shows the highest peak emission values. Jet A shows the longest lasting emission values, resulting in the highest emissions after the initial peak. Only fuels containing aromatic or cyclic components show emission levels similar to Jet A-1/A. Benzene emissions are greatly reduced over reaction time, for all temperatures and equivalence ratios. Higher equivalence ratios expectedly lead to higher benzene emissions. For low equivalence ratios, the emissions are reduced faster.

At 1800 K, about 10 ppm are left at fuel rich conditions. For the highest equivalence ratio (φ = 1.8) Syntroleum S-8 shows increasing values over time; thus, S-8 still show the lowest calculated emissions. For lean conditions, CtL has the second highest peak values whereas for fuel rich conditions Jet A-1 has the second highest values. Above φ = 1, S-8 emissions are as high as the ones of GtL, being both negligible compared to the emissions calculated for Jet A-1/A and CtL. In the fuel lean regime, the S-8 values are lower. Also, GtL+ n-c is always below Jet A-1/A and CtL. Note that CtL contains cyclic components, but no aromatic species.

For higher temperatures (T = 2200 K) the peak values of Jet A-1 and CtL are increased, with the ones of the other fuels reduced. Jet A-1 and CtL share the same aromatic species, *n*-propylbenzene.

Acetylene emissions

For the lower considered temperature (T = 1800 K), GtL+n-c shows the highest peak values, followed by CtL, Jet A-1, GtL, S-8, and Jet A (Fig. 7a-b). Jet A reaches its peak value last, and its values decrease the slowest. For fuel lean conditions, no significant acetylene amounts are left at t = 3 ms, with the lowest values resulting from the GtL+n-c, also displaying the fastest decrease. This applies to fuel lean and rich conditions.

For fuel rich conditions, the difference between all fuels at t = 3 ms is below 5%. Increased amounts of fuel result in increased Jet A-1 emission levels compared to other fuels. The Jet A emissions reduce slowest, just as seen earlier for benzene. It is noteworthy that Jet A is the only fuel with toluene as aromatic component (Table 1, composition of fuel surrogate).

A temperature increase to $T = 2200$ K results in higher peak values and reduced build up and decomposition times (about 10 times faster). Jet A-1 has the highest peak values followed by CtL, GtL+n-c, Jet A, GtL, and S-8. Again, acetylene decomposition is the slowest for Jet A. For fuel rich conditions, the differences between all fuels at the end of the calculation time are even smaller than 5%.

For both temperatures considered, the conventional fuels (JetA-1/A) show the highest emissions at simulation end. At $T = 1800$ K, GtL and S-8 show about 2-3% higher values than CtL and GtL+n-c, whereas S-8 and GtL display the lowest values for fuel rich conditions ($\varphi \geq 1.4$) at 2200 K.

Discussion of soot precursor emissions

The simulations indicate reduced levels of the soot precursors considered especially for fuels without cyclic or aromatic components. This is in accordance with experimental results [18, 24-25]. The differences calculated between alternative and crude-oil based fuels concerning acetylene are small, while the range of difference in benzene emissions is strongly time dependent. For benzene, a remarkable difference in behavior of both conventional kerosenes (Jet A-1/A) is predicted resulting from the different composition (Table 1). This also applies for acetylene, at least at $T = 1800$ K. For benzene, the differences between Jet A-1/A are bigger for all conditions than between Jet A-1 and CtL. The differences at $T = 2200$ K were predicted to be strongly time dependent. GtL and S-8 are found to be similar in results simulated behavior regarding the considered soot precursors.

SUMMARY AND CONCLUSIONS

The present study was done to get more insight into the emissions when burning synthetic fuels, in sense of qualitative trends and, in particular, into potential differences between them. Two crude-oil based and four synthetic aviation jet fuels were studied numerically by following the surrogate approach and applying a detailed chemical kinetic reaction model validated in previous work. The focus was on the emissions of major pollutants: CO, NOx, benzene, and acetylene (soot particles). The simulations were done at typical parameters, *i.e.* $p = 40$ bar, $T = 1800$ K and $T = 2000$ K, and fuel equivalence ratios φ ranging from 0.25 to 1.8, for reaction times up to 3 milliseconds.

Concerning NOx emissions, no significant differences were found between Jet A-1/A (two conventional fuels), with trends similar and the overall difference between all fuels being predicted to be about 10%. The aromatics free GtL-fuels displayed higher NOx values compared to Jet A-1/A.

Regarding CO emissions, no significant differences of synthetic fuels were predicted, too. A difference of about 10% was calculated with synthetic fuels showing slightly smaller (better) values than the two crude-oil based fuels studied. Simulation results and measured values from different sources indicate the same order of magnitude for fuel equivalence ratios φ slightly below 1.

Benzene emissions were strongly dependent on the fuels aromatics content, with additional differences between different aromatic species. Acetylene showed a less intensive effect but was also dependent on the type of aromatic species contained in the fuel (imaged in surrogate composition).

The antagonist role of CO and NO_x is apparent, with surrogates having higher NO_x values (especially GtL and S-8) showing lower CO emissions and rising CO values under fuel rich conditions, where NO_x emissions decrease.

Regarding all emissions and conditions, both GtL fuels showed similar results. The differences between the two crude-oil based kerosenes (Jet A-1/A) were sometimes predicted to be bigger than the difference to the synthetic fuels. CtL and GtL+n-c were the synthetic fuels closest to Jet A-1/A in terms of simulation behavior. They also are the only surrogates for fuels possibly fit for use according to regulations.

These results are considered to be helpful in guiding the development of synthetic aviation fuels, with respect to emissions. Thus, these findings might foster the transition from crude-oil based jet fuels to synthetic jet fuels having a less harmful impact on the environment.

Nomenclature

p	Pressure
t	Time
T	Temperature
EI	Emission Index
M	Molar mass
E	Emission value in ppm
EGT	Exhaust gas temperature

Greek letters

φ	Fuel equivalence ratio

Subscripts

ad	adiabatic
end	End of simulation
n	Emission species

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Table 1 Composition of fuel surrogates used in p.w.

Fuel Surrogate / mol%	Jet A-1 [44]	Jet A [21]	CtL [24]	GtL [24]	GtL+n-c [24]	S-8 [25]
n-Decane	68.24	42.67	39.5	57.7	24.5	53.1
2,2,4-Trimethyl-pentane	-	33.02	13	33.2	21	46.9
n-Propylcyclohexane	19.34	-	37.3	9.1	54.5	-
n-Propylbenzene	12.42	-	10.2	-	-	-
Toluene	-	24.31	-	-	-	-

Table 2a Fuels studied: Adiabatic flame temperature T_{ad}, K

Equivalence ratio / Fuel	$\varphi = 0.25$	$\varphi = 0.5$	$\varphi = 1.0$	$\varphi = 1.5$	$\varphi = 2.0$
Kerosene from crude oil					
Jet A-1 [44]	1121	1656	2360	2123	1780
Jet A [21]	1121	1657	2360	2124	1781
Alternative jet fuels					
CtL [24]	1120	1654	2357	2117	1773
GtL [24]	1118	1650	2353	2109	1765
GtL+n-c [24]	1118	1651	2354	2111	1766
S-8 [25]	1118	1650	2352	2107	1764

Table 2b Fuels studied: Equivalence ratio φ needed to reach adiabatic flame temperature T_{ad}

T_{ad}/ K / Fuel	1800	2200	1800K	2200
Kerosene from crude oil				
Jet A-1 [44]	0.575	0.82	1.39	1.97
Jet A [21]	0.575	0.82	1.4	1.97
Alternative jet fuels				
CtL [24]	0.58	0.825	1.39	1.96
GtL [24]	0.58	0.83	1.38	1.95
GtL+n-c [24]	0.58	0.83	1.38	1.94
S-8 [25]	0.58	0.83	1.37	1.94

Table 3 Various literature values of measured carbon monoxide (CO) emission levels. The emissions are shown as emission index. The significant discrepancy between different power settings is noteworthy

Fuel	**Emission index in g/kg$_{\text{fuel}}$**	**Environment Conditions**	**Engine**	**Year; Source**
conventional	51.8 ± 4.6	ICAO Idle	CFM56-3	1998; [42]
conventional	24 ± 4.8	ICAO Idle	CFM56-5C2	1998; [42]
conventional	3	Cruise	various, average value	2008; [52]
JP-8	2.3 – 53.7	ICAO Idle to Max	T 700	2009; [53]
JP-8	2.8 – 31.0	ICAO Idle to Max	T 701 C	2009; [53]
JP-8	1.4	laboratory, 827 K, 24 bar	Lean direct injection low emissions concept	2013; [54]
JP-8	0.6	laboratory, 827 K, 10 bar	Lean direct injection low emissions concept	2013; [54]
Jet A-1	0.2 - 16.9	lab., $T = 578$ K, $p = 3$ bar, $\varphi = 0.48$-0.82	PEX experimental combustor	2014; [27]
CtL (FSJF)	< 0.1 - 10	lab., $T = 578$ K, $p = 3$ bar, $\varphi = 0.55$-0.88	PEX experimental combustor	2014; [27]
GtL	0.7	lab., $T = 578$ K, $p = 3$ bar, $\varphi = 0.56$	PEX experimental combustor	2014; [27]
GtL+50%n-c	0.2 - 12	lab., $T = 578$ K, $p = 3$ bar, $\varphi = 0.55$-0.79	PEX experimental combustor	2014; [27]

Table 4 Literature values of measured nitrogen oxide (NOx) emission values. Emission index is given in g/kg$_{\mathrm{fuel}}$

Fuel	**NOx emission index g/kg$_{\mathrm{fuel}}$**	**Environmental Conditions**	**Engine**	**Year; Reference**
conventional	18± 3	altitude 915-9000 m	Fleet average	1987; [56]
conventional	21	altitude 915-9000 m, average thrust 40%	Fleet average	1987; [56]
conventional	15±3	altitude > 9000 m	Fleet average	1987; [56]
conventional	6.4 – 11.7	Cruise, 40-130 s from exhaust	various, maximum and minimum	1993/94; [39]
conventional	10.9 – 16.8	Cruise	various, fleet average	1993/94; [39]
conventional	14.1	Cruise	various, Fleet average	2006; [55]
conventional	14	Cruise	various, average value	2008; [52]
JP-8	4.4	Sea Level Static, EGT 643 K	GTCp 85-98CK	2009; [41]
JP-8	2.0 - 9.9	ICAO idle to max	T 700	2009; [53]
JP-8	2.8 - 15.0	ICAO idle to max	T 701 C	2009; [53]
JP-8	8.0 - 16	laboratory, T = 827 K, p = 24 bar	Lean direct injection low emissions concept	2013; [54]
JP-8	5.0 - 10	laboratory, T = 827 K, p = 10 bar	Lean direct injection low emissions concept	2013; [54]
Jet A-1	1.0 - 8.0	lab., T = 578 K, p = 3 bar, φ = 0.4-0.82	PEX experimental combustor	2014; [27]
CtL	4.3	Sea Level Static, EGT 643 K	GTCp 85-98CK	2009; [42]
GtL	3.5 - 13.7	ICAO idle to Max	T 701 C	2009; [54]
CtL (FSJF)	1.0 - 7.6	lab., T = 578 K, p = 3 bar, φ = 0.5-0.88	PEX experimental combustor	2014; [27]
GtL	1.6 - 4.3	lab., T = 578 K, p = 3 bar, φ =0.56-0.68	PEX experimental combustor	2014; [27]
GtL+50%n-c	0.4 - 7.6	lab., T = 578 K, p = 3 bar, φ =0.44-0.78	PEX experimental combustor	2014; [27]

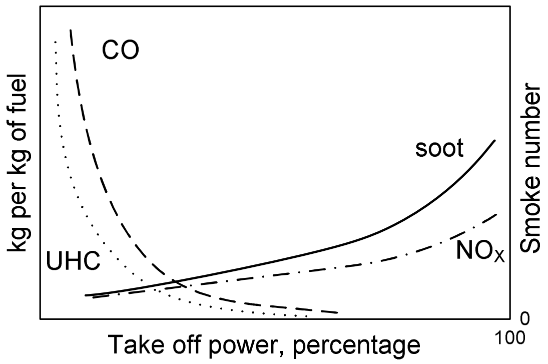
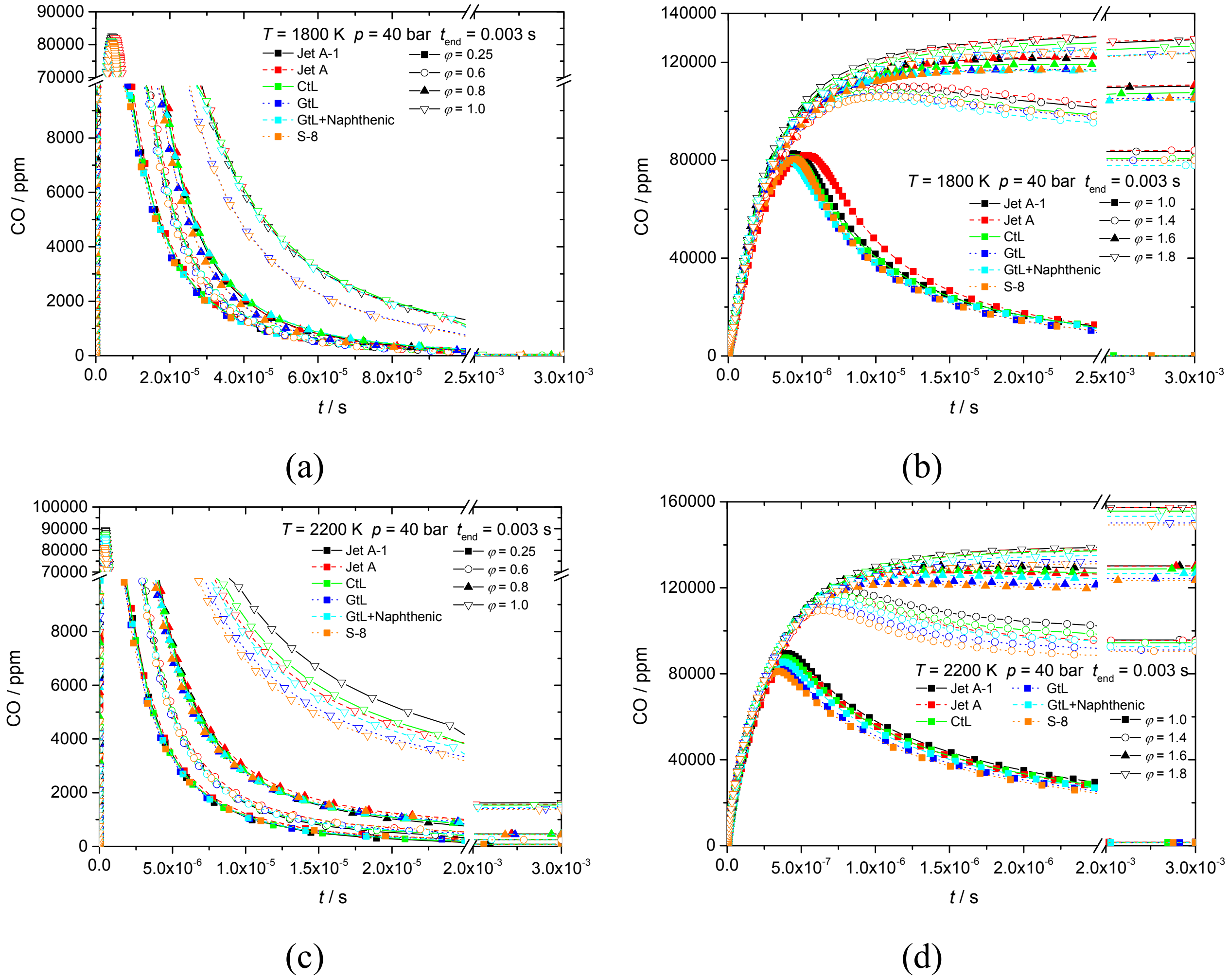


Fig. 1: Emissions characteristics in a gas turbine, principle power dependency [38]



(a)

(b)

(c)

(d)

Fig. 2: CO emissions: Calculated for four alternative aviation fuels as well as for Jet A-1 and Jet A, at $T = 1800$ K and at $T = 2200$ K for $p = 40$ bar. CO emissions calculated for the GtL fuels are the lowest

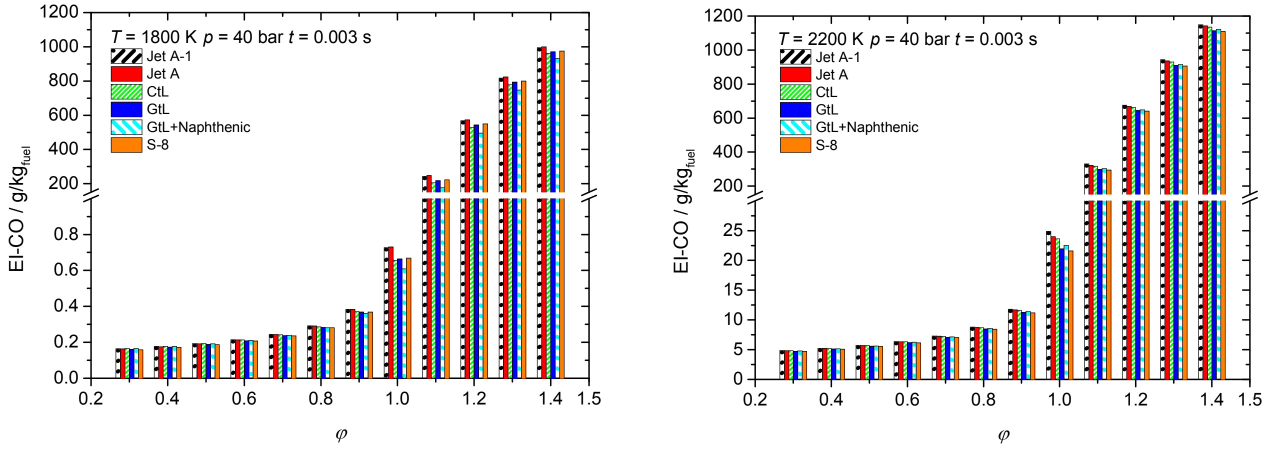


Fig. 3: CO emission indices, as derived from CO emissions calculated of the six fuels. Note the similarity of the emission levels between the six fuels for all conditions considered

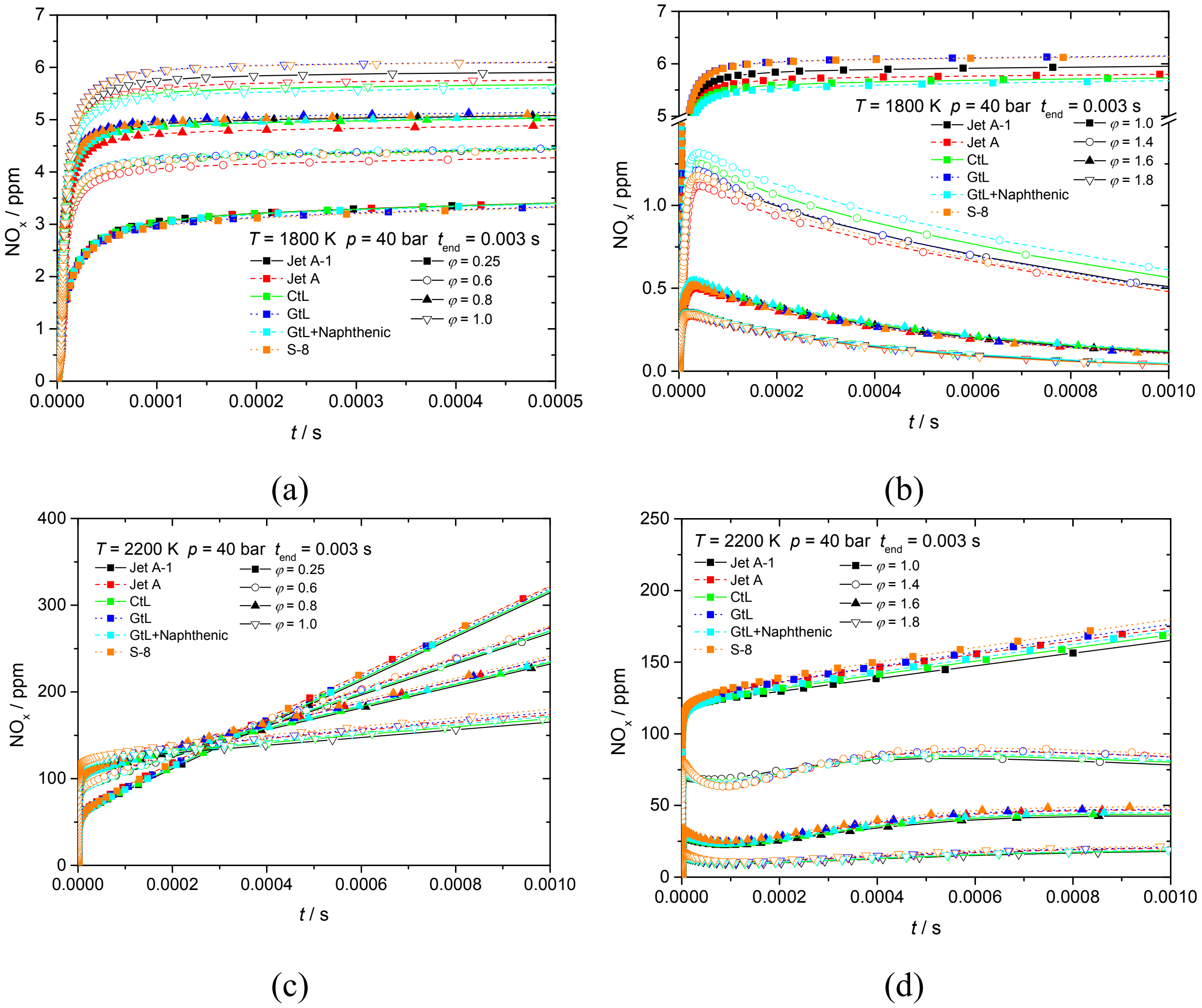


Fig. 4: NOx emissions: Simulated at T = 1800 K and at T = 2200 K. Curves follow the depicted trends monotonically

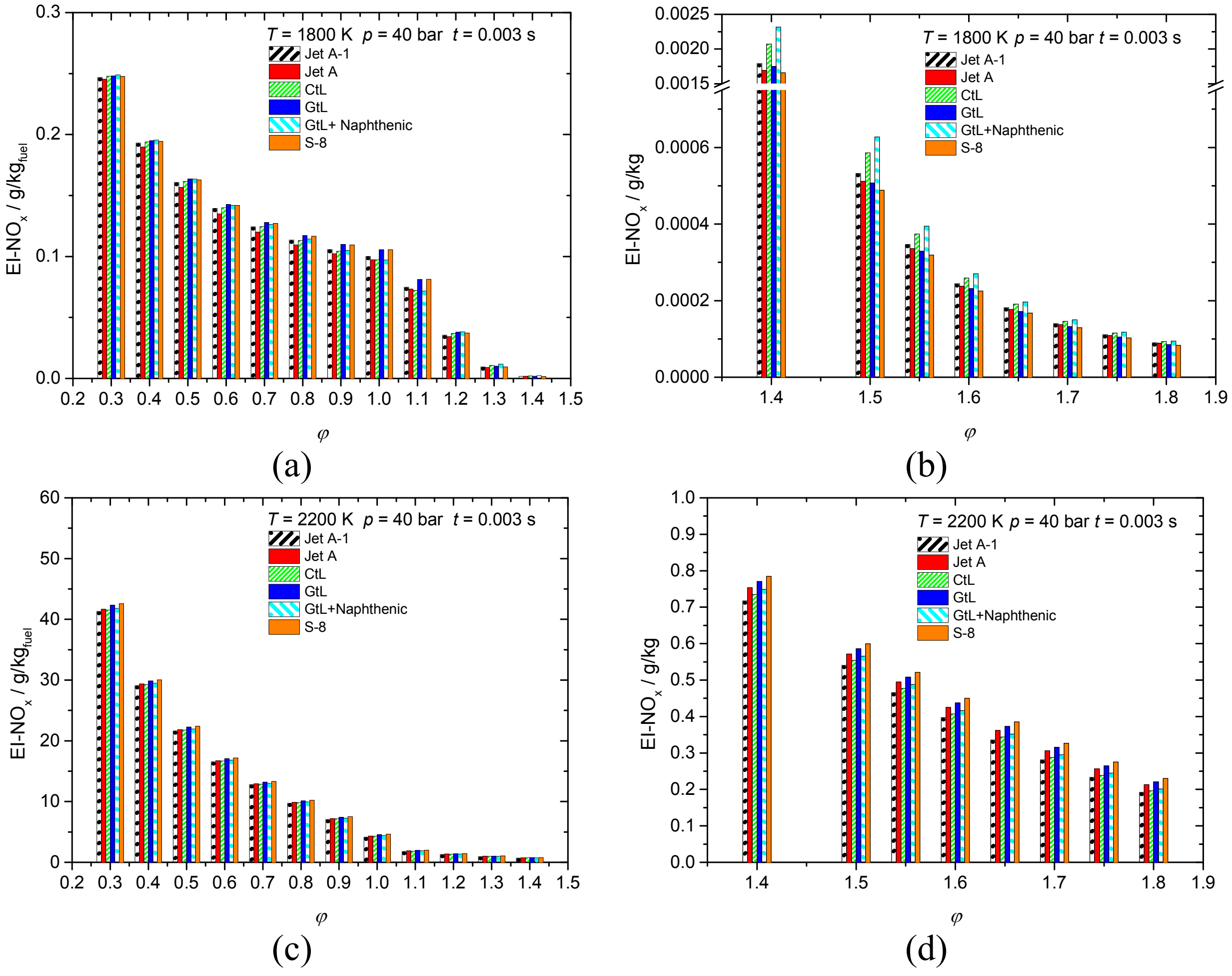
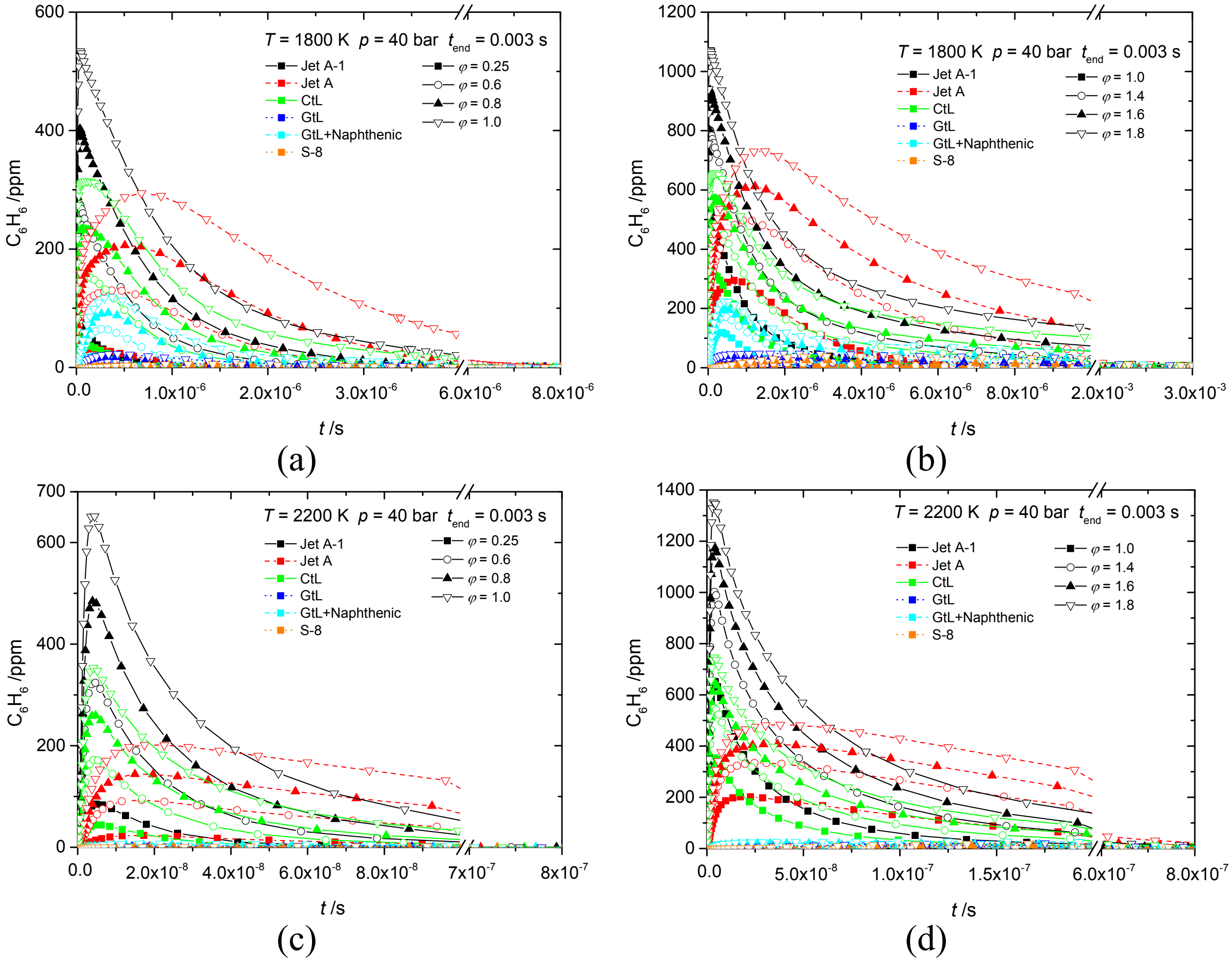


Fig. 5: NOx emission indices as derived from NOx emissions calculated of the six fuels, a: $T = 1800$ K, $0.25 \leq \varphi \leq 1.4$; b: $T = 1800$ K, $1.5 \leq \varphi \leq 1.8$; c: $T = 2200$ K, $0.25 \leq \varphi \leq 1.4$; d: $T = 2200$ K, $1.4 \leq \varphi \leq 1.8$



(a) (b)

(c) (d)

Fig. 6: Benzene emissions simulated at $T = 1800$ K (a-b) and at $T = 2200$ K (c-d). Only minor amounts of benzene remain at $t = 0.003$ s. For the parameter considered, Jet A-1 shows the highest peak emissions, whereas the GtL-fuels show the lowest peak emission values

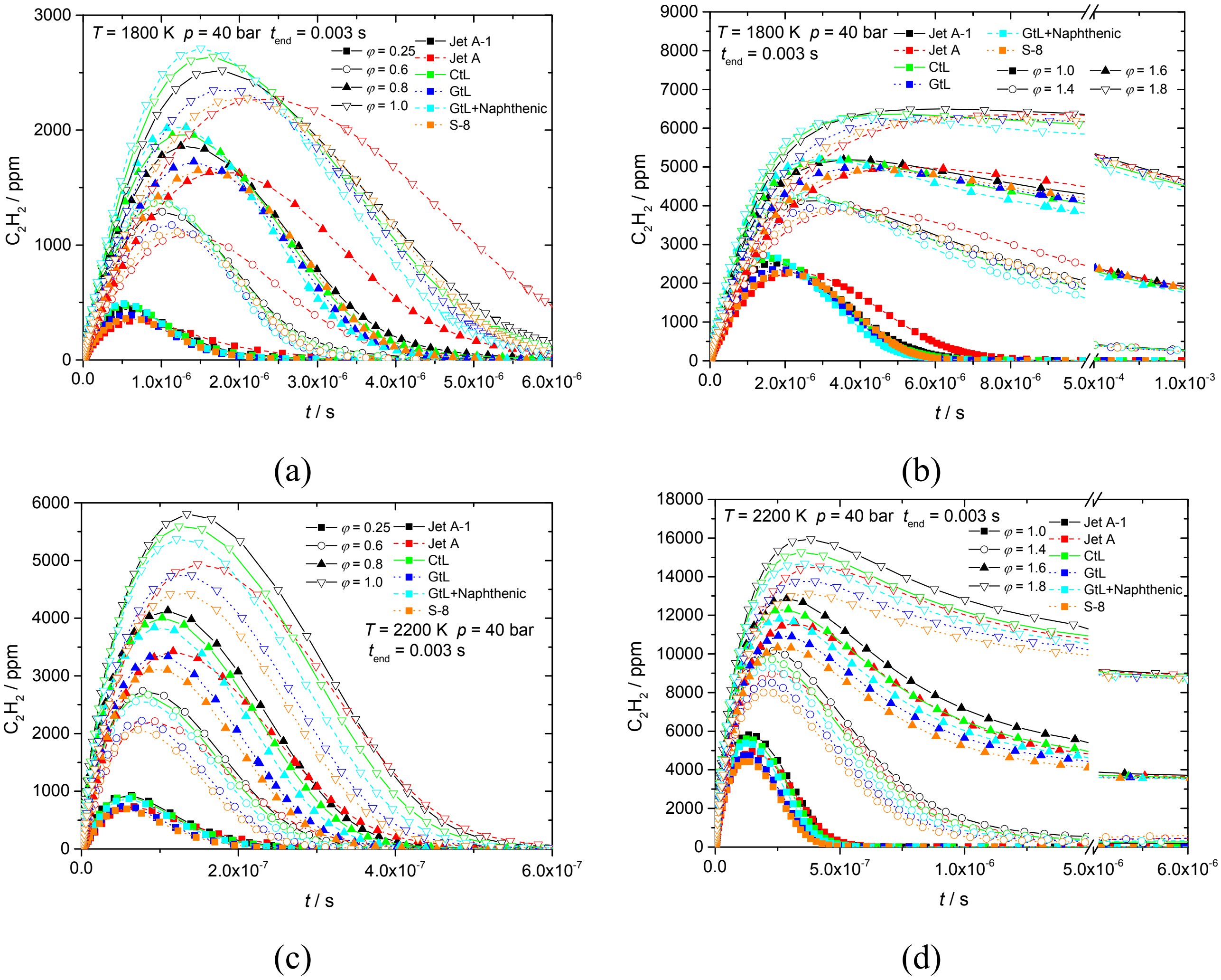


Fig. 7: Acetylene emissions simulated at $T = 1800$ K (a-b) and at $T = 2200$ K (c-d). Only minor amounts of acetylene remain for fuel lean mixtures, with significant acetylene levels for fuel rich mixtures