

HIL COMPATIBLE ENGINE MODELS FOR DUAL FUEL APPLICATIONS

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ABSTRACT

More and more, alternative fuels, fuel mixtures and dual-fuel engines are gaining in importance. This means a huge challenge to thermodynamic modeling of combustion and species transport. The computational performance is reached by an optimized filling and emptying approach applying tailored models for in-cylinder combustion and species transport in the gas path. The impact of the thermodynamic characteristics induced by the different fuels is described by an appropriate set of transport equations in combination with specifically prepared property databases. The accuracy of a lumped fuel approach is compared for a six, three and one species transport. The simulations are performed with a 6 cylinder medium speed engine. The real-time factor of this engine is in the range of 0.2 for all species transport approaches, what enables this method to support HiL based function development and calibration.

INTRODUCTION

Methanol, ethanol and renewable biofuels as well as blends of it are gaining importance as sources of energy. Also attempts to exploit shale gas have been made. The characteristic of shale gas with methane as one of its major components makes it especially attractive for use in internal combustion engines. Because of these trends we are facing an increasing number of dual fuel approaches, especially for stationary, marine, locomotive but also truck applications. There are two basic design concepts for dual fuel engines, following a recent technology review presented by Shah et al. [1]. Both concepts are based on a typical compression ignited direct injection Diesel engine where gas is additionally injected either directly into the Diesel spray in the cylinder at higher pressure or at low pressure into the intake port featuring a premixed homogeneous air gas mixture. Properly designed dual fuel engines can achieve superior full-load fuel efficiency and BMEP than spark ignited engines and can achieve a substantial reduction in NOx and particulate matter emissions compared to compression ignited engines but they need a sophisticated control system. The combustion of dual fuel fired Diesel engines deviates decisively from pure Diesel engines. For port injected gas engines and low ratios of Diesel to gaseous fuel, the pilot injected Diesel does not serve as main energy source but it is supposed to ignite the premixed gas air mixture. Out of this, two different combustion regimes can be identified. First, a Diesel-like combustion takes places influenced by spray penetration, droplet breakup, its evaporation, gas air mixture entrainment and ignition. Here the description of the ignition delay is essential as it deviates in dual fuel

operation due to different gas properties of the gas air mixture (Liu and Karim[2]). The second combustion regime is comparable to the one of spark ignited gasoline or gas engines. The ignition takes place around the Diesel pilot spray cones and a flame front propagates through the combustion chamber. Here, the description of the flame turbulence is important as it is influenced by the Diesel spray inducing additional kinetic energy.

For dual fuel engines with port injection of the gaseous fuel, the concentration of the premixed gas has to be limited to avoid knocking (see Karim and Zhaoda [3]) in the case of high compression ratios of the engine. This leads to even more complex combustion patterns as larger amounts of Diesel fuel are injected over a longer period of time causing a coexistence of inhomogeneous and homogeneous types of combustion. Unlike in port injected dual fuel engines, in dual fuel engines featuring direct injection of both fuels in the vicinity of the TDC, the inhomogeneous type of combustion prevails for both fuels (Shah et al. [1]). However, this type of dual fuel combustion still differs from the pure Diesel-like inhomogeneous combustion due to distinct mixture preparation characteristics and different chemical kinetic mechanisms inherent to dual fuel combustion.

A broad variety of phenomenological combustion model approaches can be found from literature with the attempt to transform the complexity of dual fuel combustion into a simple set of equations, with respect that it is not purely super-imposing existing models for Diesel and premixed gas combustion. The interference of the two combustion regimes leads to either new governing equations or requires at least a thorough re-parameterization of existing approaches.

The increasing requirements on control development and calibration leads to “model based development” as a key strategy in the modern development process (Kordon et al. [4]). It is based on real-time capable, semi-physical engine plant models, drivetrain models run on a virtual test bed equipped with established automation, data management and monitoring tools. Focus on the dual fuel combustion model development presented in this paper was on real-time capability, model accuracy and time for model setup.

In order to efficiently comply with the above requirements an innovative computationally optimized filling and emptying approach presented in Wurzenberger et al. [5] was used as modeling basis.

Further addressed in this paper is the species transport and an appropriate treatment of all mixture properties.

1. MODEL

The generic concept of "storage" and "transfer" elements (Merker and Schwarz [6]) is used for modelling the gas path. These element types are alternatively connected to each other. Typical examples for storage elements are volumes, cylinders, walls, fuel films or rotating shafts and for transfer elements compressor, turbine, intercooler, air cleaner, ports, or restrictions, see Figure 1.

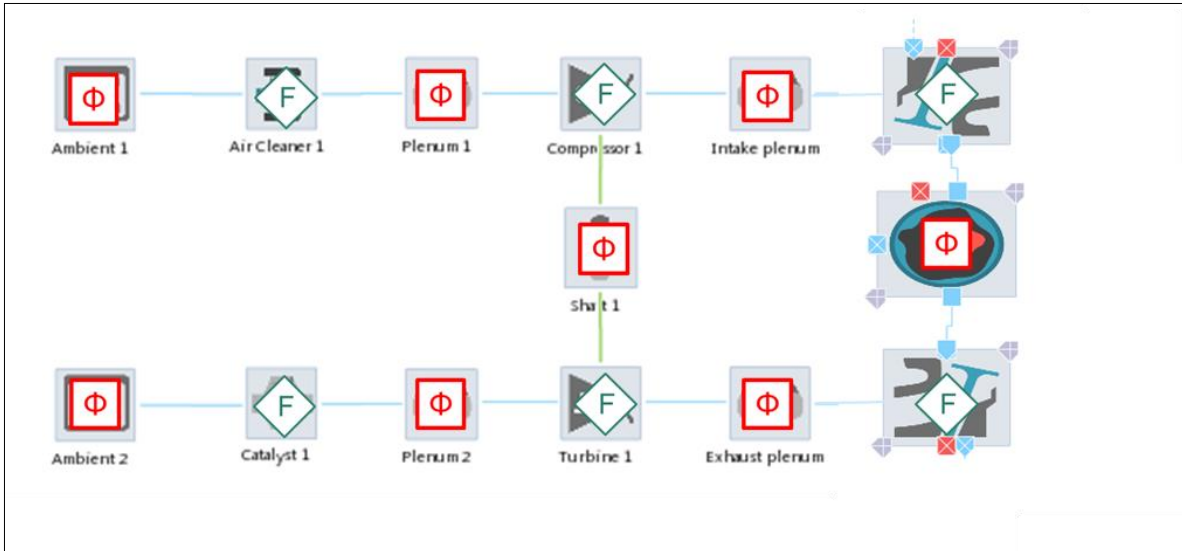


Figure 1: Engine gas path description using storage (Φ) and transfer (F) elements

1.1. Balance Equations

States Φ and their transient variation are represented by the storage components and the fluxes F by the transfer components (Figure 1). The fluxes are evaluated depending on the attached states and feed back into the conservation balances of the storage components. The application of this generic concept to describe an arbitrary gas path network translates to balance equations for mass, enthalpy. The change of mass in a storage component over time is the sum of all incoming fluxes components reduced by the sum of all outgoing fluxes to the upstream side of the attached transfer components. An explicit distinction between downstream and upstream side in transfer components is made in order to take into account sources/sinks within these components. Thus, this approach enables modeling of typical engine components like compressor, turbine, intercooler or injectors in a straight forward manner.

In order to calculate species balance equations tailored for multi fuel applications the species mass fraction vector is compiled according to

$$w = \left[(w_{FB}, w_{CP}, w_{FV})_1, \dots, (w_{FB}, w_{CP}, w_{FV})_L, w_{P,1}, \dots, w_{P,n} \right]^T \quad (1)$$

where L individual fuels are characterized by three mass fractions for fuel burned w_{FB} , combustion products w_{CP} and fuel vapor w_{FV} , respectively. The fraction of fuel burned together with the fraction of combustion products is used to track the information on combustion air fuel ratio. The additional mass fractions $w_{P,n}$ are used to transport any properties (e.g. pollutants) through the gas network in a passive manner without feedback to all thermodynamic evaluations.

Above definition of the species vector allows an arbitrary scaling depth of the species transport. A dual fuel model requires a 6-species (two times three species) transport approach to track the properties of both fuels. The 6-species approach is computationally less demanding than the application of general species transport

methods (see Wanker et al.[7]) including chemical equilibrium calculation during the run-time. One important requirement is real-time capability therefore computational performance is a decisive factor. Because of this it will also be compared with a 3- and 1-species approach. A 3-species transport approach can be applied under the assumption that the influence of varying fuel composition is negligible regarding combustion product and fuel vapor properties. Thus, only a lumped fuel is transported and contributions of different fuels are mapped to the species vector (massfraction burned fuel, combustion products and fuel vapor) of this lumped fuel. A1-species transport approach (transport of fuel burned only) can be applied under the assumption that influences of fuel vapor can be neglected.

The species balance equation is applied in an explicit form for the species mass fraction. This is given by

$$\frac{dw_s}{dt} = \frac{1}{m} \cdot \left[\sum_{i=1}^I \dot{m}_{DS,i} \cdot (w_{DS,i,s} - 1) - \sum_{j=1}^J \dot{m}_{US,j} \cdot (w_s - 1) \right] \quad (2)$$

where w_s represents the mass fraction of species s in the species vector of Eq. (2). The fractions $w_{DS,i,s}$ of species s belongs to the downstream side of the attached transfer component in case the corresponding mass flux is positive. For the case of changed flow directions ($\dot{m}_{DS,i} < 0$) the mass fractions are taken from the considered storage component itself (w_s). The same rule for defining the species fractions is applied for the fluxes going out of the component into the upstream side of the attached transfer components.

1.2. Medium Properties

The enthalpy equation applies several thermodynamic properties that need to represent dual (multi) fuel characteristics. The properties of the gas mixture are evaluated according to

$$x = x_{\text{Air}} \cdot w_{\text{Air}} + \sum_{l=1}^L x_{\text{FV},l} \cdot w_{\text{FV},l} + \sum_{l=1}^L x_{\text{CP},l} \cdot w_{\text{CP},l} \quad (3)$$

$$x = [u, h, R]$$

where the property x (representing mass specific internal u energy, enthalpy h and gas constant R) of the overall fluid mixture is composed out of the properties of air and the mass weighted sums of fuel vapor and combustion products of all involved fuels, respectively. The mass fraction of air (w_{Air}) is evaluated depending on the given mass fraction of fuel vapor and combustion products of all L fuels. This is given by

$$w_{\text{Air}} = 1 - \sum_{l=1}^L w_{\text{FV},l} + \sum_{l=1}^L w_{\text{CB},l} \quad (4)$$

In Eq. (3), the thermodynamic properties of fuel vapor and air are assumed to be solely dependent on temperature. Thus, they are taken from a database following the NASA polynomial format. The fluid properties of combustion products are assumed to depend on temperature, pressure and the excess air ratio from the time when

combustion took place. This excess air ratio λ_{CP} is evaluated out of the balanced conservation variables for combustion products and fuel burned. It is given for the l 'th fuel by

$$\lambda_{CP,l} = \frac{w_{CP,l} - w_{FB,l}}{w_{FB,l} \cdot AF_{stoich,l}} \quad (5)$$

where $AF_{Stoich,l}$ represents the stoichiometric air to fuel ratio of the considered fuel.

The thermodynamic properties of the combustion product associated to a specific fuel are evaluated following an assessment of the corresponding species composition. Here, a thermodynamic equilibrium is assumed at temperatures above 1700K (Heywood [8]) and “frozen” composition at temperatures below. Thus, with a given ratio of C, H, O, N, representing a considered fuel and air mixture and assuming that combustion products consist of twelve relevant species the combustion product equilibrium composition is calculated to populate look-up tables in a temperature range from 200K to 4000K, a pressure range from 1bar to 200bar and an excess air ratio range between 0.3 and 10000.

The present study applies three individual fuel property tables generated for Diesel (represented by $C_{10}H_{17}$) for LPG (65% butane and 35% propane mixture) and methane (CH_4), respectively. The consistency of the multi-fuel relies on the fact that during run-time individual fuel property tables can be blended based on the actual fuel composition. The mixture properties of fuel blends are evaluated by mass weighting of the properties of the individual “pure” fuels. This approach is also applied for blending combustion products although they rely on equilibrium calculations. That this approach features nearly perfect coincidence with the general species transport was proven in a paper from Kutrašnik T. And Wurzenberger J.C. [13]

The 3-species approach transports only species of one lumped fuel. Furthermore, contributions of different fuels are not constant in different engine components or different strokes of the cylinders and also not in different dual fuel operating modes. Since, these effects cannot be traced by the reduced number of transported species, it is necessary to select in advance an appropriate set of “lumped” single fuel properties. Here, properties of either “pure” fuels or a particular fuel blend can be chosen. In general, the errors are even more significant for the properties of fuel vapor. These inaccuracies apply to the properties of fuel vapor and combustion products. However it is easily possible to adapt the lower heating value, the stoichiometric air fuel ratio and also the heat of evaporation to the actual fuel blending as inflows of both fuels into the cylinder are generally known.

2. RESULTS

The work was performed with the MAN D 0826 LOH 15 turbocharged and intercooled 6 cylinder engine, see Figure 2. The air path topology is assembled out of base library components that are parameterized with geometry data, manufacture data (e.g. compressor and turbine) and with the help of the given ROHR data. The application of the latter turned

out to be especially beneficial since it significantly shortened the entire model parameterization and model tuning process by raising the final model accuracy at the same time.

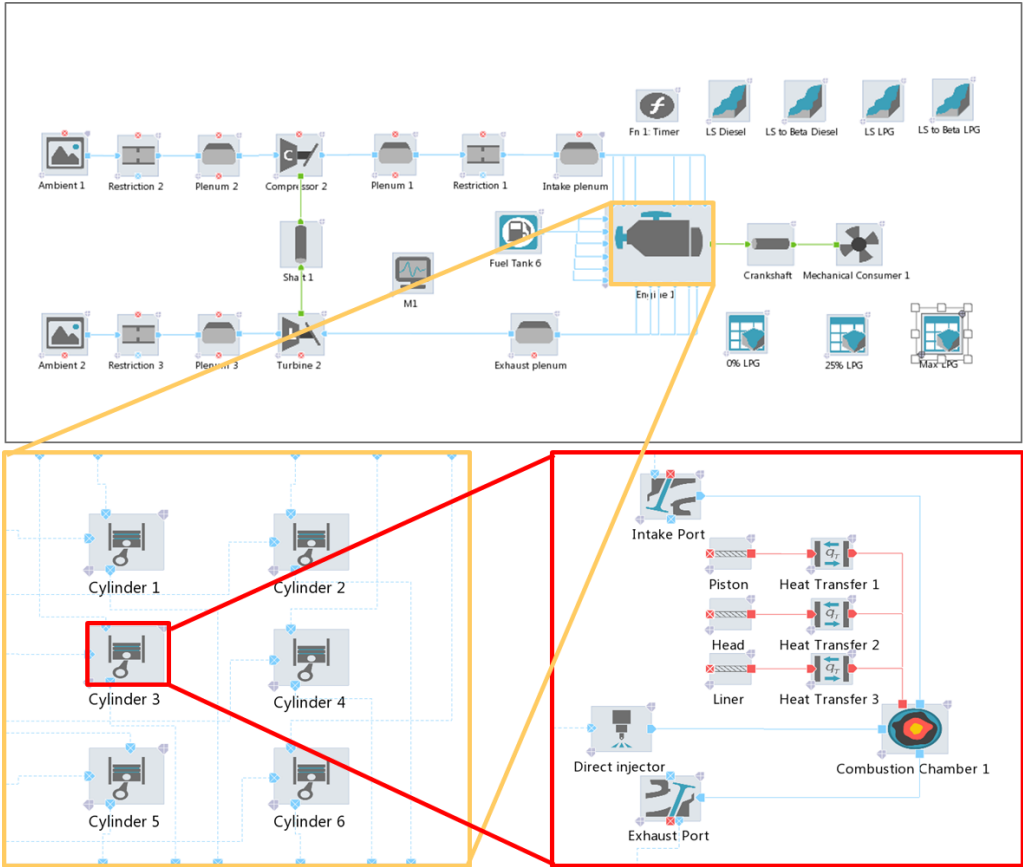


Figure 2: Schematic of the CRUISE M engine model topology split into three different model layers for engine air, path, cylinder bench and individual cylinder

2.1. Model Validation

Figure 3 and Figure 4 compare measured and simulated in-cylinder pressure traces for two different load points (1400rpm, 10bar and 1800rpm, 6bar) and 3 different mixture ratios of LPG and Diesel (0%LPG, 25%LPG and 41%LPG). The deviation of the simulation results from the measured data is negligible. Measured ROHR tables were used for the combustion modelling. It indicates an appropriate description of the entire gas path including the turbocharger, the charge air cooler and of the in-cylinder gas exchange process leading to corrected conditions at intake valve closure. In addition, the application of a 6-species transport model (fuel vapor, combustion products and fuel burned for LPG and Diesel) can be seen as justified.

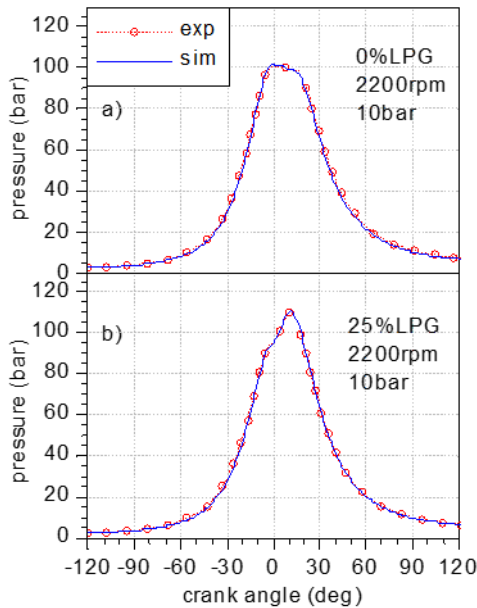


Figure 3: Comparison of measured and simulated pressure traces at 1400rpm and 10bar for 2 different LPG ratios

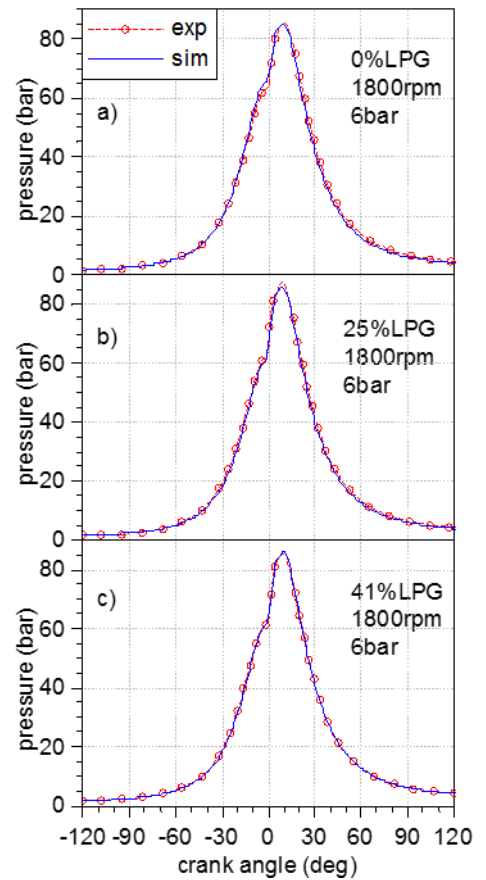


Figure 4: Comparison of measured and simulated pressure traces at 1800rpm and 6bar for 3 different LPG ratios

2.2. Species Transport and Gas Properties

The impact of different models depths for species transport and different approaches for gas properties is elaborated for various operating conditions regarding excess air ratios, compression ratios and gas fuel.

2.2.1. High Excess Air Ratio

Figure 5 shows the impact of different modeling depths for species transport on the predictability of pressure and temperature traces at load point of 2200rpm, 10bar, a LPG fraction of 25% and an excess air ratio of approximately 2.1 (compare Figure 4). Three different species transport models are compared. The detailed 6-species transport model, presented in this study, a standard 3-species transport model and a reduced 1-species transport model. The latter two approaches apply property look-up tables specifically generated for a considered mixture of LPG and Diesel. For all species

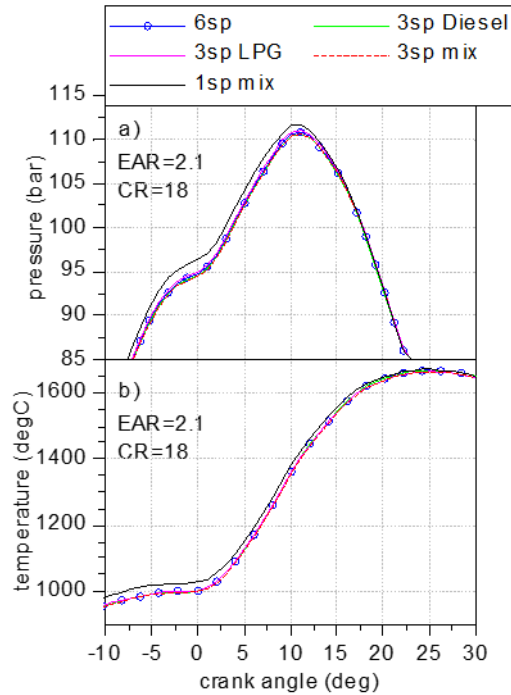


Figure 5: Pressure and temperature traces of LPG Diesel simulated with three different species transport modeling depths at excess air ratio of 2.1 and compression ratio of 18

start of combustion of about 40degC and an over prediction of pressure at start of combustion of about 2bar. The observed deviation in pressure traces of the 1-species approach leads to difference in IMEP in the range of 3%.

The comparison of the 3-species and 6-species approach shows nearly identical results for pressure and temperature traces. It is even more important that the results of the 6-species approach coincide very well with the 3-species results irrespective of the selected gas property database (Figure 5). The results using the fuel mixture specific database (3sp mix) nearly coincide with the results using the properties referring to pure Diesel or LPG. This can be explained mainly by two facts. First, the lower heating value, the stoichiometric air fuel ratio and also the heat of evaporation are adapted to the actual fuel blending based on the inflows of both fuels into the cylinder. Second, the given in-cylinder excess air ratio equals approximately 2.1. At this operating condition the overall fraction of CO₂ and H₂O is small compared to the fractions of N₂, and O₂. Thus, different fuel compositions that are reflected in different CO₂ to H₂O ratios do not significantly influence values of the overall gas properties. The comparison in Figure 5 indicates that the 3-species transport approach can be sufficient to model dual fuel engines operated at very lean conditions until the lower heating value, the stoichiometric air fuel ratio and also the heat of evaporation are adapted properly.

transport approaches all model parameters including the explicitly given ROHR's are kept constant. This ensures that differences in the results originate from different species transport and gas property treatments.

It can be observed that the reduced 1-species approach, as it does not consider any transport of fuel vapor, is not capable to catch the simulated pressure and temperature traces of the two other approaches especially during compression and combustion phase.

The simplification to assume compression of pure air with residual combustion product without considering compression of fuel vapor leads to an under prediction of the temperature at

2.2.2. Low Excess Air Ratios

Operating conditions with lower excess air ratios are simulated to ensure a more comprehensive analysis of the influence of different species transport approaches and the influence of different gas property databases. Furthermore, in addition to the Diesel-LPG blend also a Diesel-CH₄ blend is investigated. This is motivated by two facts. First, it is expected that the availability of CH₄ as fuel will increase as described in the introduction. Second, the differences in fuel vapor and combustion product properties between CH₄ and Diesel are more significant than between LPG and Diesel.

Analyses are performed for two excess air ratios of approximately 1.45 and 1.25. The latter value typically corresponds to the lower end of the excess air ratio characteristic applied in modern engines featuring inhomogeneous combustion. The investigation is made for an engine speed of 2200rpm. This is motivated by the fact that at this engine speed the turbocharger characteristics allow sufficiently high boost

pressures to reach IMEP values of approximately 23 and 30bar for the excess air ratios of 1.45 and 1.25, respectively. These operating conditions are investigated because they also correspond to modern high performance engines and because elevated temperatures and pressures additionally emphasize differences in gas properties. The share of LPG is increased to mass fractions of 61% and 71% for the excess air ratios of 1.45 and 1.25, respectively. For the analyses with CH₄ the amount of total energy added by the gaseous fuel and the cyclic fuel delivery of Diesel is retained leading to CH₄ mass fractions of 59% and 69% for the excess air ratios of 1.45 and 1.25, respectively. Due to relatively high concentrations of gaseous fuel in the homogeneous air gas mixture and due to the relatively high compression ratio of 18, auto-ignition will take place before the injection of Diesel (see Karim and Zhaoda [3], Zhang et al. [9]). Therefore more realistic conditions of the same engine with a reduced compression ratio of 14 are analyzed in addition

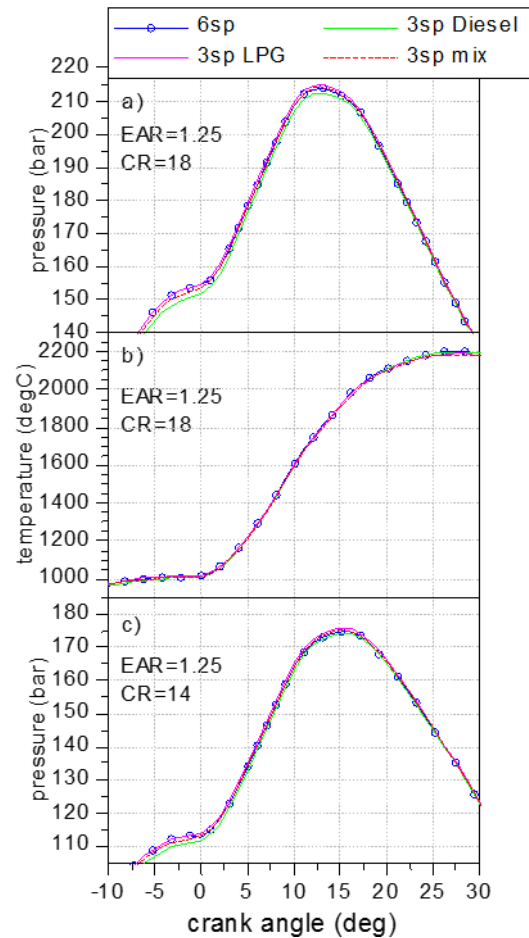


Figure 6: : Pressure and temperature traces of LPG Diesel simulated with three different species transport modeling depths at excess air ratio of 1.25 and compression ratios of 18 and 14

to these operating conditions—motivated by the numerical exploration of species transport and gas property phenomena.

Figure 6 shows results for a blend of 71% LPG and 29% Diesel at 2200rpm at an excess air ratio of 1.25 and at two compression ratios of 18 and 14. Figure 6a reveals that - at an angle of -3deg BTDC - pressure traces of the 6-species model coincide nearly perfectly with the results of the 3-species model using the LPG property database. The 3-species model using a fuel mixture specific property database and the 3-species model using the Diesel property database under-predict the pressure for 1.4bar and 3.1bar, respectively. This is related to the fact that in the compression stroke only LPG is compressed and thus the use of the LPG property database leads to more accurate results. The same trend can be observed for the temperature at the end of compression (Figure 6b). The observed trends change during combustion as increasing fractions of burned Diesel influence the composition of combustion products. Here, the results of the 3-species model using the fuel specific property database are closest to the reference results of the 6-species model, whereas the 3-species model using properties based on pure Diesel and pure LPG under-predicts and over-predicts the peak firing pressure in the range of 1.4bar, respectively. However, as the conditions at -3deg BTDC were not identical for the 6-species model and the 3-species model using the fuel specific property database, good agreement of the peak firing pressures cannot be considered as the proof of consistency of these two results. This is also revealed in the trend of the peak firing temperature. The 3-species model using pure Diesel based properties under-predicts the temperature by 4degC, the 3-species model using pure LPG or fuel mixture based properties under-predicts the reference temperature by 12degC and 14degC, respectively.

The same pressure trace characteristics as exposed for a compression ratio of 18 is also valid for a compression ratio of 14 (Figure 6c). Here, smaller deviations can be observed. Thus, there is very good agreement between peak firing pressures predicted by the 6-species model and the 3-species model using a fuel specific property database. The 3-species model using Diesel based or LPG based properties under-predict and over-predict the peak firing pressure by 0.7bar and 1bar respectively. Although differences in the results for both compression ratios are not negligible, it can be concluded that they are relatively small.

2.2.3. *Computational Speed of the Models*

The computational performance of the models is assessed on a single core of a standard office PC with 2.4GHz. When applying an integration increment of 1deg in the cylinder and a time step of 1ms in the gas path a real-time factors of the 6 species, 3 species and 1 species model equal to 0.22, 0.182 and 0.157 respectively for the analyzed engine speed of 2200rpm. These real time factors are sufficient - ensure ample margins towards real-time violations - to execute the model for example on an ETAS HiL system as presented by Hoepfner et al.[10] who applied the same tool to support HiL based control function development for a large engine.

CONCLUSION (Should begin 3 lines below the text)

Out of the performed simulations the following conclusions can be drawn:

- All species transport modeling depths—from the detailed 6-species to the lumped 3-species and also 1-species approaches—are real-time capable.
- In comparison to the given experimental data the 6-species approach shows very good agreement proving that the model accurately captures the compression and combustion characteristics of dual fuel engines operated at various speeds, loads and gas to Diesel mixing ratios.
- The 3-species approach can be seen as a promising simplification to the 6-species approach especially at higher excess air ratios. The prerequisite for its application is a thorough preparation of appropriate mixture properties database.
- The 1-species approach is recommended only for very crude analysis simulations since it shows significant deviations to the 3-species and 6-species approaches.
- The numerically efficient 6-species approach is also ready to support more complex combustion models. Surrogate ignition delay models derived from detailed auto-ignition chemistry simulations (see Walther et al. [11]) fit perfectly to further refine the explicit rate formulas. Here, the real-time capability of the simulation framework used in this work is also demonstrated (see Pötsch [12]) for the more complex mixture controlled combustion models.

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DEFINITIONS/ABBREVIATIONS

Acronyms

0D/3D	Zero/Three Dimensional
BMEP	Brake Mean Effective Pressure
BTDC	Before Top Dead Center
CFD	Computational Fluid Dynamics
CNG	Compressed Natural Gas
CRA	Crank Angle
ECU	Engine Control Unit
HiL	Hardware in the loop
IMEP	Indicated Mean Effective Pressure
LPG	Liquid Petroleum Gas
sp	Species

Latin

Letters

AF	Air to fuel ratio (kg/kg)
B	Help variable in energy balance (K.kg/J)
cp	Mass specific heat capacity (J/(kg.K))
CR	Compression ratio (-)
EAR	Excess air ratio (-)
F	Flux vector (various)
h	Mass specific enthalpy of overall gas mixture (J/(kg.K))
\dot{H}	Enthalpy flux (W)
IMEP	Indicated mean effective pressure (Pa)
K	Help variable in energy balance (1/kg)
m	Mass (kg)
\dot{m}	Mass flux (kg/s)
p	Pressure (Pa)
R	Mass specific gas constant of overall gas mixture (J/(kg.K))
ROHR	Rate of heat release (J/deg)
t	Time (s)

T	Temperature (K)
u	Mass specific internal energy of overall gas mixture (J/kg)
V	Volume (m ³)
w	Species mass fraction vector (kg/kg)
x	Arbitrary fluid mixture property (various)

Greek Letters

λ	Excess air ratio (-)
ϕ	State vector (various)

Indices

Air	Air
CP	Combustion products
DS	Downstream
FB	Fuel burned
FV	Fuel vapor
i	Index of attached downstream fluxes
I	Total number of attached downstream fluxes
j	Index of attached upstream fluxes
J	Total number of attached upstream fluxes
l	Index of fuel
L	Total number of fuels
n	Total number of passive species
P	Passive
s	Species index
S	Total number of species
$stoich$	Stoichiometric
US	Upstream