

Dual Fuel Engine Simulation - A Thermodynamic Consistent HiL Compatible Model

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ABSTRACT

This work presents a real-time capable simulation model for dual fuel operated engines. The computational performance is reached by an optimized filling and emptying modeling approach applying tailored models for in-cylinder combustion and species transport in the gas path. The highly complex phenomena taking place during Diesel and gasoline type combustion are covered by explicit approaches supported by testbed data. 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. A thermodynamic highly accurate 6-species approach is presented. Additionally, a 3-species and a 1-species transport approach relying on the assumption of a lumped fuel are investigated regarding accuracy and computational performance. The comparison of measured and simulated pressure and temperature traces shows very good agreement. The real-time factor of a 6 cylinder medium speed engine is in the range of 0.2 for all species transport approaches, enabling the support of HiL based function development and calibration.

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INTRODUCTION

Many attempts to exploit shale gas have been made during the last years as it is a promising alternative source of energy to conventional crude oil. The characteristic of shale gas with methane as one of its major components makes it especially attractive for use in internal combustion engines. Apart from the application of spark ignited gas engines also dual fuel operated engines are a promising approach. Here, stationary, marine, locomotive but also truck applications are becoming more and more interesting.

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. The latter concept can also be understood as retrofit approach where besides adaptations in the inlet channel the design of the main combustion chamber remains unchanged. Weaver and Turner [2] discuss comprehensively the advantages and challenges of retrofitted dual fuel Diesel engines compared to purely spark ignited or compression ignited engines. They conclude that 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 NO_x and particulate matter emissions compared to compression ignited engines. Nevertheless, they also state that "performance and emissions in dual fuel engines vary depending on the operating conditions and the sophistication of the 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 place 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 [3]). 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 [4]) 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.

Simulation models dealing with the specifics of dual fuel combustion have been developed for many years. The most complex descriptions comprise 3D CFD models (see Sing et al. [5], Wang et al. [6]) where the physical depth also requires enormous computational efforts. A significantly simplifying step is the application of 0D phenomenological approaches. Here, a comprehensive approach has been recently presented by Walther et al. [7]. The authors split the combustion into two phases. It starts with a model for Diesel pilot injection followed by a model for flame propagation. The pilot injection model applies a package description (see Stiesch and Merker [8]) where the entrainment of the gas air mixture is motivated by the momentum balance of the spray. Droplet evaporation is modeled using semi-empirical approaches. The changed thermal properties due to the existence of an air methane/biogas mixture are considered in the ignition delay model. It is elaborated by solving chemical kinetics for 29 species and 52 reactions and further transferring its results into an Arrhenius type ignition formula. The flame propagation from the Diesel spray cones (3 and 6 hole nozzles) considers a detailed geometry description of the front surface changing from individual cones into a merged semi-sphere while combustion is progressing. A similarly complex model is presented by Liu and Karim [9] who apply a five zone model together with detailed reaction chemistry for 32 species in 138 elementary reactions. The combustion of the Diesel pilot is described by two superimposed Wiebe-functions where the second one also comprises the combustion of the gas air mixture in the burned zone. A similar multi-zone approach is chosen by Lata and Mistra [10] who also describe combustion by a double-Wiebe function but use an empirical formula for ignition delay instead. A two-zone model is published by Hountalas and Papagiannakis [11, 12]. The authors apply an adopted jet penetration model of Hiroyasu (see Heywood [13]) and an empirical formula for ignition delay. Diesel combustion modeled by two consecutive rate steps (Whitehouse-Way [14]) and gaseous fuel combustion is described by an Arrhenius type equation. This approach also considering the amount of fuel to air at a given combustion excess air ratio. The combustion product composition is estimated by a chemical equilibrium calculation of eleven species. The formation of nitric oxides is based on extended Zeldovich mechanisms and soot is predicted assuming a formation and oxidation reaction rate. Karim and Zhaoda [4] apply a single zone model incorporating

a detailed set of 32 reactions for methane combustion that is not only applied during high pressure but also during the compression phase of the gas air mixture. Rai et al. [15] present a cylinder description based on surrogate models. There, adaptive neuro fuzzy interference systems are trained on 75 measured operating points to predict performance and emissions as a function of load, ignition angle and fraction of gaseous fuel in the overall fuel mixture.

The literature overview reveals a broad variety of phenomenological models. This is surely motivated by the attempt to transform the complexity of dual fuel combustion into a comparably simple set of equations. Here it needs to be kept in mind that plausible approaches do not simply end up in 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. Thus, a common characteristic of all published phenomenological combustion models is a non-negligible effort of parameterization based on experimental high pressure indicating data.

In order to deal with the increasing requirements on control development and calibration, "model based development" is a key strategy in the modern development process (Kordon et al. [16]). 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.

The dual fuel engine model presented in this work is developed specifically to support model based development. Thus, besides real-time capability, the model accuracy and time for model setup are essential features. In order to efficiently comply with the above requirements an innovative computationally optimized filling and emptying approach presented in Wurzenberger et al. [17] was used as modeling basis. The paper at hand presents two additional contributions. First, a HiL capable physically based engine modeling framework for simulating dual fuel operation is presented. Second, a systematic analysis is performed regarding the applicability of species transport and gas property approaches in the light of computational speed and accuracy of the results.

In order to shorten the parameterization effort and to increase also model accuracy the present study combines physical and semi-empirical models of key phenomena with an empirical and explicitly given description of the rate of combustion. The explicitly given description of the rate of heat release allows applying a single zone combustion model whereas the used modeling framework also allows using two-zone models. This approach is especially favorable for the target of supporting model based calibration, where engine prototypes and experimental data are already available and real-time capability is a must. The latter requirement is explicitly addressed in the current study by applying a minimum number of species transport equations and an appropriate treatment of all mixture

properties. In addition, the explicitly given combustion rates are also very favorable for the present analyses on different species transport and gas property treatments.

MODEL

The engine gas path model is based on the generic concept of “storage” and “transfer” components (see Merker and Schwarz [18]). As shown in Figure 1, these two types of components are connected to each other in any alternating manner. With this, network topologies can be assembled for arbitrary engine gas path configurations. Typical examples for storage components are volumes, cylinders, walls, fuel films or rotating shafts. Typical examples for transfer components are compressor, turbine, intercooler, air cleaner, ports, or restrictions.

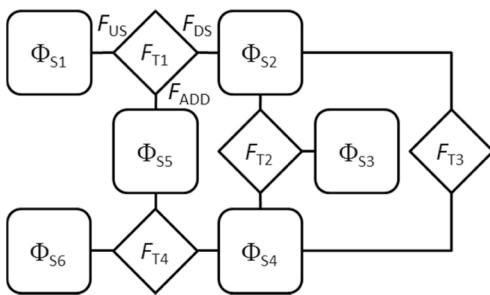


Figure 1. Engine gas path description using storage (.) and transfer (<=>) components (Figure taken from Wurzenberger et al.[19])

Balance Equations

The storage components (see Figure 1) represent states ϕ and their transient variation whereas transfer components represent fluxes F . 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 mass balance is given by

$$\frac{dm}{dt} = \sum_{i=1}^I \dot{m}_{DS,i} - \sum_{j=1}^J \dot{m}_{US,j} \quad (1)$$

where the change of mass m in a storage component over time t is the sum of all incoming fluxes $\dot{m}_{DS,i}$ from the downstream side of the attached transfer components reduced by the sum of all outgoing fluxes $\dot{m}_{US,i}$ to the upstream side of the attached transfer components (the nomenclature of up- and downstream relates to the transfer component). I and J represent the number of fluxes associated to the downstream and upstream side of the attached transfer components, respectively. This 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 dual (multi) fuel applications the species mass fraction vector is compiled according to

$$w = \left[(w_{FB}, w_{CP}, w_{FV})_1, \dots, (w_{FB}, w_{CP}, w_{FV})_L, w_{P,1}, \dots, w_{P,n} \right]^T \quad (2)$$

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.

The applied definition of the species vector allows arbitrary scaling depending on the species transport modeling depth. A dual fuel model requires a 6-species (two times three species) transport approach to track the properties of both fuels. This is significantly less than 29 or 32 species (see Walther et al. [7], Liu and Karim [9]) reported for detailed reaction chemistry analysis. The 6-species approach is also assessed to be computationally less demanding than the application of general species transport methods (see Wanker et al.[20]) including chemical equilibrium calculation during the run-time.

The emphasis on the number of species equations is important as it directly influences the overall computational performance and at the end is also the decisive factor for real-time capability. Therefore, results of the 6-species transport model featuring a high level of fidelity will be compared with results calculated from a 3-species and a 1-species approach. The 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 (w_{FB}, w_{CP}, w_{FV}) of this lumped fuel. Furthermore, the 1-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

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

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.

The enthalpy balance is given in an explicit form for the time derivative of temperature. Additionally, all property derivatives with respect to the state variables are extended to handle a multi-fuel system. This leads to

$$\frac{dT}{dt} = \frac{B}{m} \cdot \left[\begin{aligned} &+ \dot{H} + (K \cdot m - 1) \cdot p \cdot \frac{dV}{dt} \\ &- \left(u + K \cdot T \cdot m \cdot \frac{dm}{dt} \right) \\ &- m \cdot \left[\left(K \cdot m \cdot T \cdot \sum_{s=1}^S \frac{dR}{dw_s} + \sum_{s=1}^S \frac{du}{dw_s} \right) \cdot \frac{dw_s}{dt} \right] \end{aligned} \right], \quad (4)$$

where T is the temperature, p is the pressure and V represents the current volume. The internal energy of the entire gas mixture is given by u and R is its mass specific gas constant.

The help variables K and B are evaluated for the entire gas representing all fuels. They are given by

$$K = \frac{\partial u}{\partial p} \cdot \frac{1}{V \cdot \left(1 - \frac{p}{R} \cdot \frac{\partial R}{\partial p} \right)}, \quad B = \frac{1}{K \cdot m \cdot R \cdot \left(1 + \frac{T}{R} \cdot \frac{\partial R}{\partial T} \right) + \frac{\partial u}{\partial T}} \quad (5)$$

where additional dependencies of the mass specific gas constants and the internal energy on changes in the state variables are taken into account.

The variable $\dot{H}$ represents generic enthalpy fluxes over the boundaries of the considered balance volume. It is given by

$$\dot{H} = \sum_{i=1}^I \dot{m}_{DS,i} \cdot h_{DS,i} - \sum_j \dot{m}_{US,j} \cdot h, \quad (6)$$

where the enthalpy fluxes are evaluated with the given mass fluxes and the mass specific mixture enthalpies of the fluid. In analogy to the species conservation equation, the mass

specific enthalpy is chosen depending on the flow direction. It is taken either from the upstream transfer component (if $\dot{m} > 0$) or from the storage component itself (if $\dot{m} < 0$).

Fluid 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

$$x = x_{\text{Air}} \cdot w_{\text{Air}} + \sum_{l=1}^L x_{\text{FV},l} \cdot w_{\text{FV},l} + \sum_{l=1}^L x_{\text{CP},l} \cdot w_{\text{CP},l}, \quad x = [u, h, R] \quad (7)$$

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

$$w_{\text{Air}} = 1 - \sum_{l=1}^L w_{\text{FV},l} + \sum_{l=1}^L w_{\text{CB},l} \quad (8)$$

In Eq. (7), 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

$$\lambda_{\text{CP},l} = \frac{w_{\text{CP},l} - w_{\text{FB},l}}{w_{\text{FB},l} \cdot AF_{\text{stoich},l}}, \quad (9)$$

where $AF_{\text{Stoich},l}$ 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 [13]) 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 (i.e. H, O, N, H₂, OH, CO, NO, O₂, H₂O, CO₂, N₂, Ar) the combustion product equilibrium composition is calculated to