

Evaporation and Cold Start Behavior of Bio-Fuels in Non-Automotive Applications

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ABSTRACT

Worldwide increasing energy consumption, decreasing energy resources and continuous restriction of emission legislation cause a rethinking in the development of internal combustion engines and fuels. Alternative renewable fuels, so called bio-fuels, have the potential to contribute to environmentally friendly propulsion systems. This study concentrates on the usage of alcohol fuels like ethanol, methanol and butanol in non-automotive high power engines, handheld power tools and garden equipment with the focus on mixture formation and cold start capability. Although bio-fuels have been investigated intensely for the use in automotive applications yet, the different propulsion systems and operation scenarios of nonautomotive applications raise the need for specific research. A zero dimensional vaporization model has been set up to calculate the connections between physical properties and mixture formation. This model is able to calculate the vaporization behavior of different mixtures based on the chemical composition and the single component properties of fuels. Calculation cases for different applications and boundary conditions have been taken into account to evaluate the influence of fuel properties on the vaporization potential. In order to validate the results of the calculations, experimental investigations of the vaporization behavior have been performed. These investigations were made by using a cold start procedure on different four stroke engines. The results of the simulation give information about the cold start behavior of different fuels and are necessary to understand the mechanisms of vaporization during the cold start process.

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INTRODUCTION

A characteristic property of non-automotive high power engines, handheld power tools, and garden equipment is a high power to weight ratio whereby the high energy density of conventional fuel has major influence. The restriction of emission legislation, the decreasing energy resources and the dependency on mineral oil also pose problems which affect engines used in these applications. The narrow boundary conditions for the usage of power units in these specific applications are responsible for the fact that internal combustion engines can hardly be replaced by alternative power units. The technical standard of state of the art internal combustion engines is on a high level, which implies that further direct improvements concerning efficiency, emissions and environmental compatibility cause a very high technical and financial effort. An indirect way to achieve improvements on these topics is to change the

fuel type. Alternative renewable fuels, so called bio-fuels, have, in dependency on their production process and raw material, a better well-to-wheel-CO₂-emission-balance than conventional ones. Especially alcohol fuels and the influence of different alcohol-gasoline blends on the whole combustion system have been investigated intensely for the use in automotive applications. Nevertheless, different fuel-mixture-generation systems, lower electronic control possibilities and different operation scenarios of non-automotive engines raise the need for specific research.

The used reference fuel is a specific gasoline with very low oxygen content, good oxidation resistance and very tight specifications concerning density, distillation range and vapor pressure. The usage of such a fuel is necessary to avoid cross influences depending on basic fuel transformations during the research period.

Table 1. Properties of reference fuel and alcohol fuels

	units	reference fuel (E0)	methanol	ethanol	2-butanol
RON	[-]	100	109	108.6	105
MON	[-]	87.6	90	89.7	90.9
ρ at 293.15 Kelvin	[kg/m ³]	754.5	791	785.2	806
carbon content	[w%]	87.03	37.5	52.14	64.82
hydrogen content	[w%]	12.97	12.6	13.13	13.6
oxygen content	[w%]	<0.1	49.9	34.73	21.58
boiling temperature	[°C]	35-191	64.7	78	99
stoichiometric air requirement	[-]	14.46	6.5	9	11.16
lower heating value	[MJ/kg]	42.67	19.86	26.85	33
mixed heat value at $\lambda=1$ (293.15Kelvin, 1013mbar)	[MJ/m ³]	3,27	3,14	3,18	3,21
related enthalpy of vaporization at $\lambda=1$	[kJ/kg _{air}]	20-30	179.6	102	60
vapor pressure at 310.95 Kelvin	[kPa]	58.6	32	16	5.3

Based on the comparison of physical and chemical properties of the reference fuel and alcohol fuels (shown in Table 1), the influence on the engine behavior and the problematic aspects of alcohol fuels are elaborated. The engine specific properties, like research octane number and motor octane number of alcohol fuels are higher than the octane numbers of the reference fuel. This implies that alcohols are able to tolerate higher compression ratios due to higher knock resistance of these fuels. A result of high compression ratios is an increasing efficiency of the engine which has already been verified in other studies [1], [2] and [3]. Additionally, alcohol admixtures have an influence on engine out emissions. Because of higher cooling effects, due to higher vaporization enthalpies, a differing mixture formation and a lower carbon to hydrogen ratio of alcohol fuels, engine out emissions are changing. With reference to [4], [5] and [6] a methanol, ethanol and 2-butanol addition helps to lower CO and CO₂ emissions. This phenomenon is caused by the lower carbon to hydrogen ratio of ethanol, methanol and 2-butanol. In contrast to the lower CO and CO₂ emissions, HC emissions tend to increase with the use of bio-fuels. The responsible reasons are the worse evaporation properties of alcohol fuels. This causes a worse mixture formation. Additionally, the lower exhaust gas temperature of bio-fuels limits the HC post oxidation. Due to the high oxygen content of alcohols, the stoichiometric air requirement is also lower. On this account, more fuel mass is necessary to achieve a stoichiometric air fuel ratio. In combination with the vaporization enthalpy a related enthalpy of vaporization at $\lambda=1$ was introduced. This value describes the energy, which must be provided by air to evaporate the whole fuel mass. As shown in Table 1, the related enthalpy of vaporization at $\lambda=1$ is much higher for alcohol fuels than for the reference fuel. The vapor pressure of methanol, ethanol and 2-butanol is significantly lower

than the vapor pressure of the reference fuel. This value has a great influence on the mixture formation and vaporization behavior and confirms the fact that alcohol fuels have a worse cold start capability than gasoline.

Motivation

The combination of lower vapor pressures and higher related evaporation enthalpies of alcohols raise the need for further investigations of the evaporation behavior of alcohol-gasoline blends. The mixture formation and evaporation behavior have a direct influence on the cold start capability, the combustion process, and the raw emissions and are thus central issues for the whole engine process. To assess the evaporation behavior of alcohol-gasoline blends, the correlation between dominant physical properties and evaporation behavior has to be investigated. An experimental investigation of the mixture formation process of different fuels is shown in [7]. This study concentrates on the measurement of the air fuel ratio at the spark plug. The effort to assess the influence of different fuels and engine strategies on the mixture formation and cold start capability is high. To elaborate the influence of single fuel components on the mixture formation the experimental method is not suitable.

Based on the idea to characterize the influence of bio-fuels according to their properties, a zero dimensional vaporization model has been set up. In dependency on the cold start procedure the simulation model helps to interpret the influences of different fuel properties and components on the vaporization behavior and cold start capability of an engine.

Outline

To give an overview of the essential tasks of this research, Figure 1 illustrates the relations between simulation, necessary input data, and the experimental verification of the simulation results.

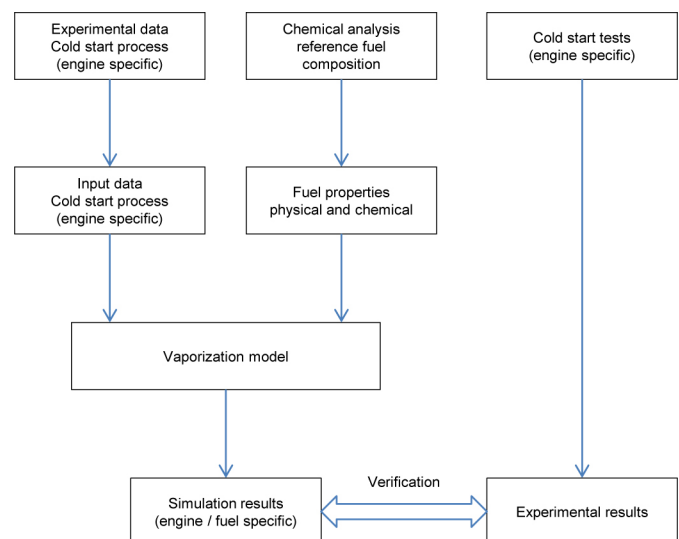


Figure 1. Overview of the relevant tasks of the research

The physical and chemical properties, like vapor pressure and stoichiometric air fuel requirement, have to be calculated according to the composition of the requested fuel. A chemical analysis is

commissioned for determining the liquid fuel composition. Furthermore, engine specific input data is required for the calculation of the vaporization behavior. These input data are boundary conditions, relevant for cold start processes. They are pressure and temperature courses which are derived from the experimentally investigated cold start process of two different engines. Additionally, the provided liquid fuel flow has been recorded. Due to different fuel mixture-generation systems, varying starting applications and differing throttle valve positions, the boundary conditions have to be adapted engine specifically. Based on current fuel properties, it is possible to calculate the maximum possible gaseous mass of each fuel component which evaporates under the give boundary conditions. This value is interpreted as the vaporization potential of each fuel component. Additionally, cold start tests of the test engines will be conducted. The comparison of the simulation results with the experimental results provides information about the accuracy and prediction cabability of the vaporization model.

PROBLEM DEFINITION

As mentioned above and with reference to the fuel properties shown in Table 1, the cold start capability of bio-fuels is worse than gasoline. The condition to ignite an air fuel mixture is the upper and lower explosive limit of a fuel. The lower explosive limit (LEL) defines volume fraction of the gaseous fuel which is necessary to ignite the mixture. It is also possible to express this value as an air-fuel equivalence ratio. Therefore, the stoichiometric air fuel requirement and the molar mass of the fuel are required. The black line in Figure 2 shows the approximated LEL of different gasoline ethanol blends in terms of lambda.

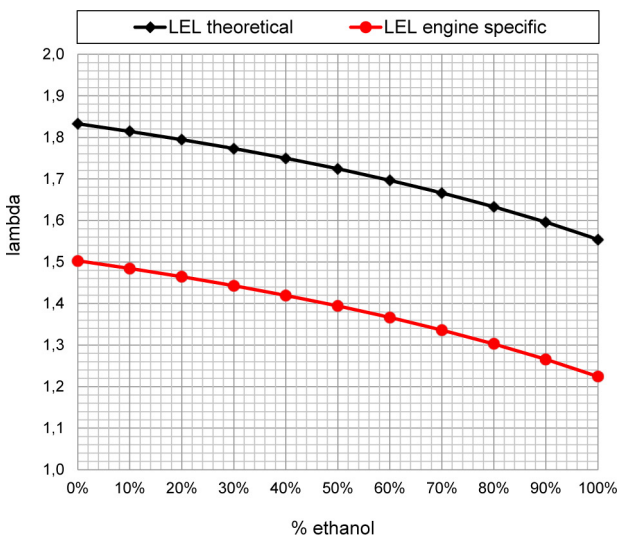


Figure 2. LEL at ideal conditions (black line), and engine specific LEL (red line; test engine 1) in dependency of the ethanol content

The explosive limit of an air fuel mixture in a combustion engine (red line) is lower than the theoretical LEL and varies from engine to engine. This is caused by different ignition energies, turbulences, velocities at the spark plug and the pressure and temperature course history, which has been applied on the air fuel mixture. The air and gaseous fuel equivalence ratio of the cylinder is subjected to local variations. A usage of a cylinder averaged air and gaseous fuel

equivalence ratio leads to additional variations of this value. The current gaseous fuel mass at the ignition point is a function of the applied pressure and temperature course of the process. To reach an ignitable air fuel mixture, the current air and gaseous fuel equivalence ratio must be richer than the required air fuel equivalence ratio of the explosive limit of the real engine. This fact raises the need to determine the engine specific explosive limit experimentally. The reachable evaporated fuel is engine specific and depends on pressure and temperature course, mixture formation process and vaporization behavior of the fuel. Based on the assumption, that the droplet heat flow, the droplet size and the local fuel distribution of different fuels are similar, the gaseous fuel mass is a function of the vaporization behavior.

To evaluate the cold start capability of different fuels, a consideration of the vaporization behavior of different fuels during the cold start process is conducted. Therefore, a comparable value has to be defined. On the basis of the boundary conditions of the cold start process, the maximum possible fuel mass which can evaporate (vaporization potential) at each crank angle step can be calculated.

Maximum means the mass which is able to evaporate at equilibrium conditions and infinite time. To create a basis of comparison between calculated evaporation behavior and the theoretical and engine specific explosive limits, the equivalence ratio of air to gaseous fuel (λ_{gaseous}) is chosen.

The research of [8] concentrates on the engine temperature variation due to different fuels. Therefore, in-cylinder crank angle based temperature measurements were applied to evaluate the influence of different fuels. In this study, the cycle averaged temperature has the significance to describe the connection between fuel vaporization properties, like vapor pressure and vaporization enthalpy, and cooling effects.

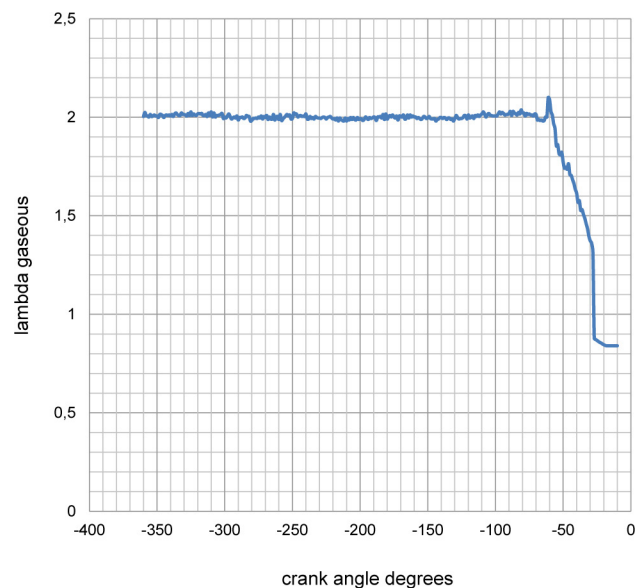


Figure 3. λ_{gaseous} course over the cold start process of test engine 1

The conditions at the time of ignition are not sufficient for the calculation of λ_{gaseous} at time of ignition and, therefore, cold start capability. This would only be true if equilibrium state can be

reached due to a long time for evaporation at these conditions. Therefore, the trace of the conditions over the whole process, from injection to ignition, has to be taken into account.

Figure 3 shows the calculated crank angle based vaporization potential over the cold start process at a defined ambient air temperature.

To express the vaporization potential of the whole cold start process, the process averaged calculated vaporization potential ($\lambda_{\text{gaseous,ave}}$) is one relevant value for the comparison. This value can be calculated in dependency of different ambient air temperatures. Figure 4 shows the theoretical and engine specific ignition limit for the reference fuel E0. Additionally, the calculated $\lambda_{\text{gaseous,ave}}$ course of E0 is illustrated. The intersection between this course and the engine specific upper explosive limit defines the real cold start limit of the engine. At higher temperatures the engine is able to start. The intersection between the calculated lambda course and the idealized explosive limit defines the theoretical cold start limit at ideal conditions, implying equilibrium conditions.

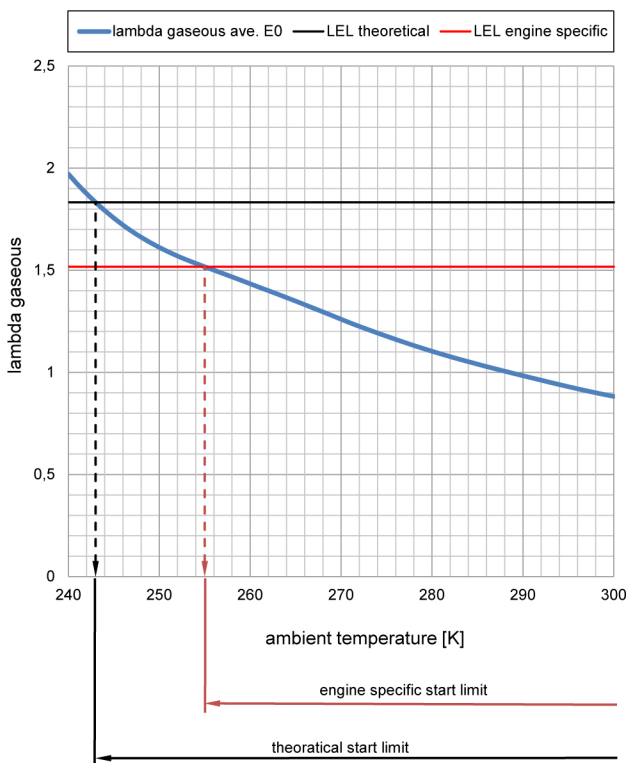


Figure 4. Averaged lambda gaseous versus idealized and engine specific LEL calculated for E0 (test engine 1)

VAPORIZATION MODEL

The global calculation workflow of the simulation model is shown in Figure 5. The fuel databases supply information about the properties of alcohol fuels and the reference fuel. To offer the possibility to elaborate the influences of different fuel components on the vaporization behavior, it is essential to treat the reference fuel as a mixture of different hydrocarbons. In this case, the physical and chemical properties of the reference fuel have to be calculated from the properties of the different fuel components. Therefore, a chemical analysis, which gives information about the chemical composition of

the reference fuel, is launched. With reference to [9], the components with a weight proportion higher than 0.5% have to be taken into account to represent the properties of gasoline. For the further calculations, relevant fuel components and their properties are shown in Appendix Table 1. The liquid fuel and air temperature represent the current temperature of the application. The engine specific boundary conditions describe the cold start process of the requested engine.

The first calculation steps concentrate on the adaption of the boundary conditions on the current air temperature and on the calculation of the general fuel properties. Therefore, the current liquid fuel and air temperature are required. Based on the engine specific boundary conditions, which are experimentally investigated at different temperatures, and the current air temperature, the pressure and temperature conditions of the cold start process have to be re-calculated for each crank angle step. Therefore, a thermodynamical analysis of the starting process is taken into account.

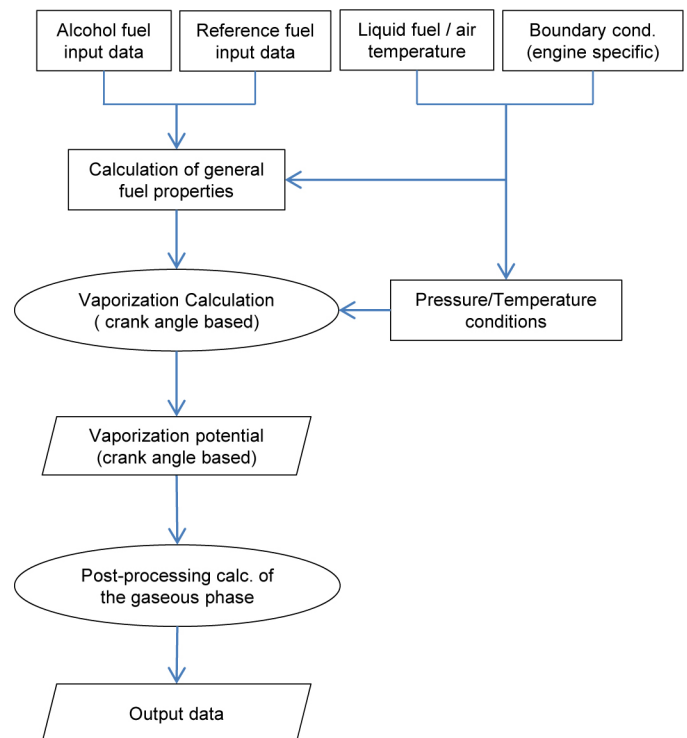


Figure 5. Global calculation workflow of the simulation model

To calculate the general fuel properties, the given alcohol gasoline ratio, the liquid fuel temperature and the engine specific injected liquid fuel mass are required. Based on the dependence of air density on temperature and pressure and due to the varying densities of different fuels, the provided air and liquid fuel equivalence ratio will be re-calculated according to the current liquid fuel and air temperatures. At this point, the pressure and temperature conditions, the liquid fuel composition, the fuel properties like stoichiometric air fuel requirement, mass fraction and molar fraction of each component and the provided air fuel ratio at the mixture generation system are defined. This information is transferred to the crank angle based vaporization calculation. The definition "crank angle based" means that the vaporization calculation will be conducted for each degree crank angle with consideration of the relevant boundary conditions.

For the detailed explanation of this step, the calculation methodology is shown in Figure 7. The output data of the vaporization calculation is the vaporization potential, which is described by the crank angle based gaseous mass of each fuel component.

To derive the crank angle dependent equivalence ratio of air to gaseous fuel (λ_{gaseous}) and to determine $\lambda_{\text{gaseous,ave}}$, additional calculations of the gaseous phase are required. The post-processing calculation of the gaseous phase is therefore implemented. A description of this calculation step is shown in Figure 8. The final output data are the $\lambda_{\text{gaseous,ave}}$, the stoichiometric air requirement of the gaseous phase, the chemical composition of the gaseous phase and a mass balance of the liquid and fuel phase.

Vaporization Calculation (Crank Angle Based)

The calculation of the vapor pressure of different fuels is a central point. A differentiation of the calculation of the vapor pressure according to the fuel has to be considered. Therefore, the procedures for the calculation of the vapor pressure of the reference fuel and gasoline ethanol blends are described.

Vapor Pressure Approximation of Reference Fuel

[9] and [10] show that it is possible to calculate the vapor pressure of gasoline based on the liquid composition of the fuel by using Raoult's law (1).

$$p_{\text{vap,fuel}} = \sum_i x_i * p_{\text{vap},i} \quad (1)$$

Raoult's law takes into account the vapor pressure of each component according to his liquid molar fraction, which is defined in (2).

$$x_i = \frac{n_i}{\sum_i n_i} \quad (2)$$

For this calculation, the vapor pressure profile over the temperature of each component is required. It is possible to use correlations like the Antoine equation to approximate the vapor pressure profile. The coefficients for the correlations were collected for all 28 components of the reference fuel and for methanol, ethanol and 2-butanol. The sources for this data are [11], [12] and [13].

Vapor Pressure Approximation of Gasoline Ethanol Blends

Alcohols like methanol, ethanol and 2-butanol have a different behavior than the other hydrocarbons which occur in the reference fuel. For the calculation of the vapor pressure profile, activity coefficients are necessary to represent the secondary effects between alcohols and gasoline hydrocarbons. With reference to [14], the extended Raoult's law (3) is suitable for solving this task.

$$p_{\text{vap,fuel}} = \gamma_{\text{gasoline}} * x_{\text{gasoline}} * p_{\text{vap,gasoline}} + \gamma_{\text{alcohol}} * x_{\text{alcohol}} * p_{\text{vap,alcohol}} \quad (3)$$

[14] also shows that the activity coefficients do not have a strong dependency on the chemical gasoline composition. So it is possible to take over the elaborated activity coefficient for gasoline ethanol blends from this publication. The coefficients for methanol and 2-butanol blended fuels were determined from experimental data of [15].

The results of the calculated vapor pressures with consideration of the extended Raoult's law are shown in Figure 6. Especially the pressure curves of ethanol and methanol blended fuels show a positive deviation. That means that low additions of methanol and ethanol higher the vapor pressure of the mixture. The pressure curve of 2-butanol blended fuels shows a very low deviation. At this point, it can be assumed that 2-butanol blends have the worst vaporization potential of the investigated alcohol fuels.

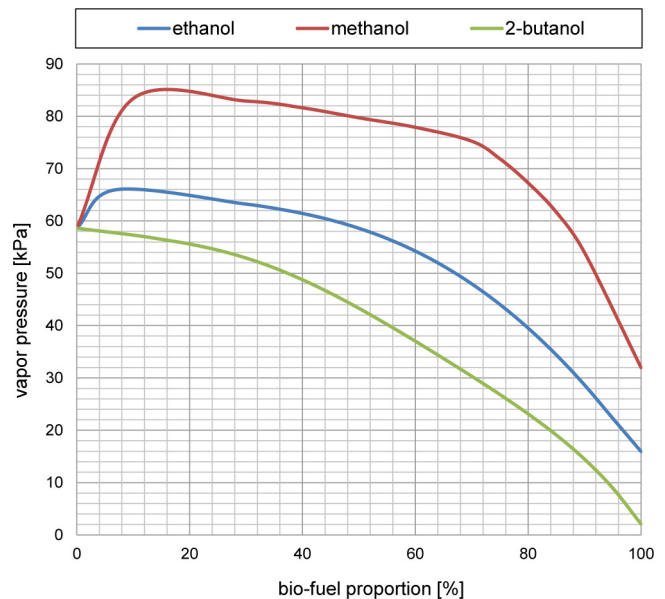


Figure 6. Vapor pressure of alcohol/gasoline blends at 310.95 Kelvin

Vaporization Calculation Workflow

In Figure 7, the calculation flow of the vaporization calculation step is shown. To calculate the vaporization potential, the starting crank angle step and the calculation duration have to be defined. Based on the calculated liquid fuel composition and the boundary conditions it is possible to define the vaporization properties of different hydrocarbons. The temperature condition is decisive for calculating the vapor pressure of each component. The pressure condition is needed to define the partial pressure of each component. The calculation of the vapor pressure of the components is split up into several steps. First, the vapor pressure of the components of the reference fuel must be calculated according to Raoult's law. This results in the vapor pressure of the reference fuel part. This vapor pressure is necessary for the calculations of the extended Raoult's law. The vapor pressure of the reference fuel part and the alcohol part is changing. This is caused by the inclusion of the activity coefficients in the extended Raoult's law. The recalculated vapor pressure of the reference fuel part will be split up into the individual hydrocarbons of the reference fuel. The evaluated vapor pressure of the alcohol fuel can be directly taken into account.