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加速碳中和的能源载体和动力总成技术

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摘要：由于"巴黎协定"和中国碳中和的气候保护目标及对能源独立的追求，需要加速对节能减排和二氧化碳中和的技术研究与开发。目前，在汽车动力系统的节能减排与碳中和方面，主要有3种发展概念：电池驱动；燃料电池驱动；基于二氧化碳中和的内燃机可持续合成燃料驱动。根据能源使用的生命周期，将效率因素简化归纳为决策因素，在时间上无法反映出减少二氧化碳排放及减少化石能源的需求。与必要的能源供应相比，可再生能源的区域可用性有限，因此须以成本效益优势的方式来解决化石能源大规模替代的技术与基础建设问题。除了直接使用可再生电力外，绿色氢气和衍生的合成燃料可以大大加快化石能源的替代。短期内，合成燃料可以实施到全球的现有车辆上（约12亿辆），并持续增加混合汽油、柴油或天然气的混合比例，直到化石能源完全被绿色的氢气、合成燃料或电力所取代。介绍了氢气动力系统（H_2内燃机和燃料电池动力系统）与合成燃料相关的技术解决方案。

关键词：内燃机；合成燃料；甲醇；氢气动力系统
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Accelerated Transition to CO_2 Neutrality —Energy Carriers and Powertrain Technologies

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Abstract: Due to the ambitious climate protection targets of the 'Paris Agreement' (2050) and China (2060) and the pursuit of energy independency, an increased technology-independent research and development of energy efficient and CO_2 neutralization methods is needed[1-2]. Basically, there are three main powertrain concepts for vehicles available: battery electric drive, fuel cell powered electrical drive, and CO_2 neutral sustainable synthetic fuel powered combustion engines. A simplified subsumption of efficiency factors along the process chain from cradle to grave as decision factor does not reflect the most efficient reduction of CO_2 emissions and reduction of fossil energy demand over the timeline. Due to regional limited availability of renewable energy compared to necessary energy supply, a lot of technical and infrastructural problems must be solved in a cost-efficient way in order to enable this large-scale substitution of fossil energy. In addition to the direct use of renewable electricity, green hydrogen and derived synthetic fuels are unique enablers to accelerate the substitution of fossil energy significantly. Synthetic fuels can be implemented short-term and worldwide for the whole existing vehicle fleet (approx. 1, 2 billion vehicles) by utilization of the installed energy logistics. The "drop-in" rate can be successively increased (blending of gasoline, diesel, or natural gas) until complete substitution by green hydrogen, synthetic fuels, or direct use of electricity. This paper is presenting both hydrogen powertrains (H_2 combustion engine and fuel cell powertrain) and synthetic fuels, and technical solutions therefor.

Key words: internal-combustion engine; synthetic fuels; methanol; hydrogen power system

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Considering the global targets for limiting environmental impacts in the transportation sector, there are three possible paths for powertrain developments, which, within those three synthetic fuels in particular permit a rapid reduction in greenhouse gas emissions with an "overnight effect". The infrastructure and logistics are in place, as they are the same that function for fossil fuels. The adaptation of the existing internal combustion engine (ICE) technology is not necessary since most vehicles are capable of using synthetic fuels. At the same time, besides passenger cars, synthetic fuels and hydrogen offer a great potential for all parts of the transportation sector and beyond such as aviation, marine, and agriculture.

While the share of battery electric vehicles will increase in the future, it will take time for a significant replacement of the vehicle fleet and accordingly the environmental benefits of these vehicles to arrive. But on a global scale, synthetic fuels offer an environmental optimization of approximately 1.2 billion vehicles[3]. Considering the further increase of global CO_2 emissions as shown in Fig. 1, it is important to use all possible solutions that can mean a fast and strong decrease in the future, to give other technologies like electromobility more time to build up and establish themselves.

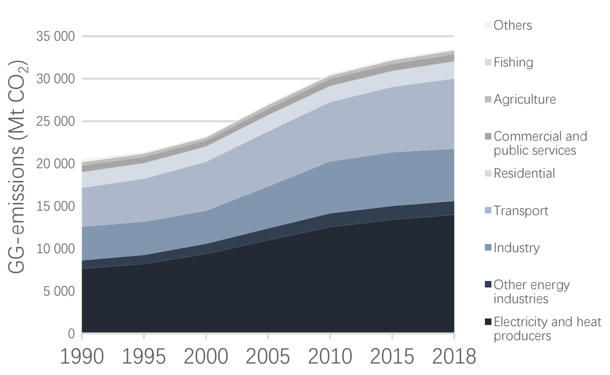


Fig.1　Worldwide CO_2 emissions sorted by sector[4]

Besides the important drop-in property of synthetic fuels, a certain share is possible via blending with other fuels – within the applicable fuel regulations. Which in turn increases the potential for mitigating the environmental impact of the global vehicle fleet. This development is beneficial for a co-evolution of powertrain and fuel technologies with the goal of creating a dedicated synthetic fuel engine, with a higher efficiency and a low-level emission behavior.

This paper is intended to provide a rough overview of the properties, potentials, and technologies for synthetic fuels. Thus, basic production paths are presented and synergies to other sectors is mentioned, which show a similar dependence on fuels. After describing some important properties of synthetic fuels and the applications of drop-in capable and non-drop-in capable synthetic fuels, different potentials and technologies are discussed. On the one hand, the state of research and the expected development of dedicated hydrogen and methanol ICE are explained. On the other hand, the preceding development of fuel cells and biogas ICEs are also discussed. Finally, special synthetic fuels are briefly addressed.

1　Energy carriers of the future

A brief and small introduction to synthetic fuels is provided. In addition to the basic production methods, a few important properties and their potential for the existing fleet are also discussed.

1.1　Production pathways

The basis for synthetic fuels is hydrogen. Green production via solar and wind power enables three further conversion technologies: power-to-gas, power-to-chem and power-to-liquid (see in Fig. 2).

Two main pathways are viable for these conversion technologies. While the ammonia pathway makes easy transport and reconversion of hydrogen possible, the methanol pathway covers more of the conversion technologies, which in turn satisfies the needs of multiple industries and sectors. For drop-in capable synthetic fuels, the Fischer-Tropsch process is essential, as it allows the production of fuels such as gasoline, diesel, and kerosene without a relevant difference from their fossil counterparts. In the long term, dedicated synthetic fuel engines will allow this process to be skipped by using methanol and hydrogen directly. Given this perspective, the methanol pathway is important for the transportation sector in both the short and long term, not only because it saturates the need for drop-in capable and other synthetic fuels, but also because it makes synergies with other industries possible by overlapping power-to-chem and power-to-liquid technologies. For other sectors, such as the chemical industry, an increase in the share of synthetic fuels is as important as that for the transport sector. Methanol, ammonia, and hydrogen in particular are essential base chemicals for a huge number of products. These three chemicals are currently equally dependent on fossil fuels. This co-dependency results in long-lasting cross-sector synergies. Dedicated synthetic fuel engines can maximize these synergies. As an example, methanol can be used as a base chemical and as a fuel for ICE, which in turn reduces the number of conversions for drop-in capable fuels and increases overall efficiency, and furthermore, decreases overall costs. This can further simplify the portfolio of synthetic fuels and increase the capability for mass production.

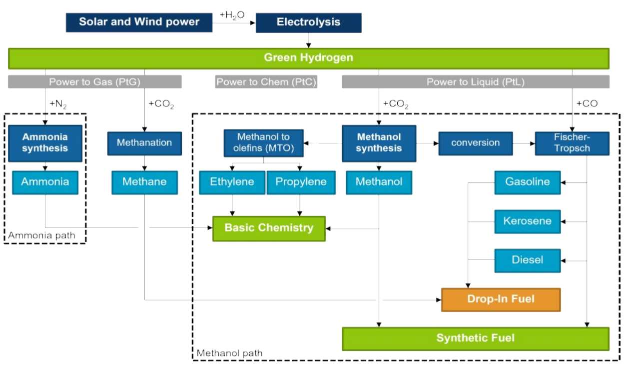


Fig.2 Production Pathways of synthetic fuels[5]

1.2 Relevant properties for internal combustion engines

Like fossil fuels, synthetic fuels also have a variety of properties. Herein, only a few important ones are briefly addressed. For instance, the energy density always plays an important role in the context of the ICEs.

In terms of weight, this is particularly high for hydrogen, while in terms of volume, diesel, gasoline and, following closely behind, methanol, dimethyl ether (DME), and ammonia have a major advantage as shown in Fig. 3. However as seen in Fig. 4, an important point is also the ignition readiness, where ammonia requires a higher energy input of more than 10 times.

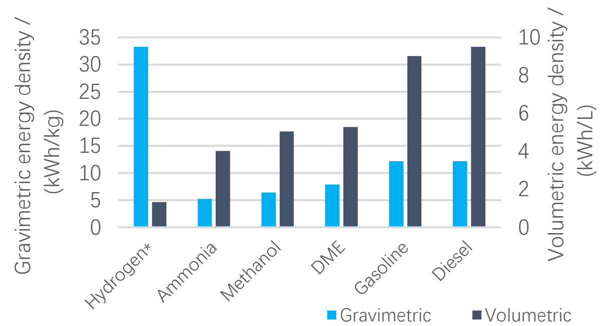


Fig.3 Energy density for chosen synthetic fuels[6]

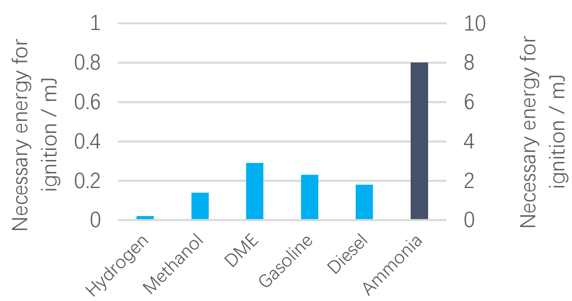


Fig.4 Ignition energy for synthetic fuels[7]

The following Tab. 1 shows other relevant properties. As local zero-emission becomes more of a priority, this issue can be addressed with hydrogen and ammonia in addition to electric mobility, as these fuels have no carbon atoms.

1.3 Fields of application

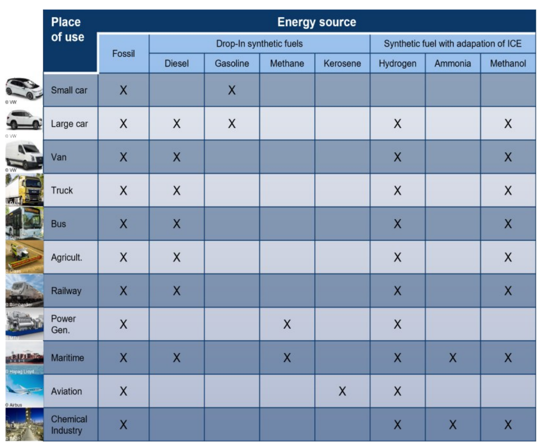
Fossil fuels are used in all areas of the transportation sector. The task of synthetic fuels and hydrogen is to cover all these applications both in the short and long term. For this, synthetic gasoline, diesel, and kerosene are indispensable, at least in the short term. In the future, the application fields could only be supported by methanol and hydrogen. With one exception for small vehicles, this application is perfectly tailored to battery electric vehicles by satisfying most, if not all, user needs.

At the same time, it must be noted that certain applications in the future can only be met by synthetic

Tab.1　Properties of different synthetic fuels

Property	Hydrogen (H_2)	Ammonia (NH_3)	Methanol (CH_3OH)	DME (C_2H_6O)	Gasoline (C_7H_{15})	Diesel ($C_{12}H_{23}$)
n_H/n_C	zero Carbon	zero Carbon	4.00/1.00	3.00/1.00	2.12/1.00	1.90/1.00
Boiling point/°C	−253	−33	65	−24	70–215	170–360
Density (liquid)/(kg/m^3)	71 (@ −253°C)	682 (@ −33°C)	792	740 (@ 24°C)	730–780	820–860
Density/(kg/m^3)	0.08	0.77	—	2.11	—	—
Ignition point/°C	585	630	460	240	220–450	230
Ignition limits in air/(Vol%; 1)	4.0–76.0; 0.4–7.3	15.4–33.6; 0.6–1.4	6.7–36.0; 0.3–1.8	2.8–24.4; 0.3–2.3	1.0–7.6; 0.3–1.9	0.6–5.5; 0.2–1.9
Stoichio-metric air requirement/(kg/kg; kg/MJ)	34.3; 0.286	6.1; 0.324	6.5; 0.326	9.1; 0.330	14.7; 0.359	14.5; 0.339
Mixture heat value (PFI)/(MJ·m^{-3})	3.19	3.11	3.95	3.68	3.66	3.83
Mixture heat value (DI)/(MJ·m^{-3})	4.54	3.96	3.95	3.93	3.66	3.83
RON	130	130	106–119	—	87–102	—
CN	—	—	—	>55	—	48–54

fuels, especially with regard to heavy loads, long ranges and generally high energy needs, such as shipping, aviation and agriculture. A general overview of applications is seen in Fig. 5.



Place of use	Energy source: Fossil	Drop-In synthetic fuels: Diesel	Gasoline	Methane	Kerosene	Synthetic fuel with adapation of ICE: Hydrogen	Ammonia	Methanol
Small car	X		X					
Large car	X	X	X			X		X
Van	X	X				X		X
Truck	X	X				X		X
Bus	X	X				X		X
Agricult.	X	X				X		X
Railway	X	X				X		X
Power Gen.	X			X		X		
Maritime	X	X		X		X	X	X
Aviation	X				X	X		
Chemical Industry	X					X	X	X

Fig.5　Fields of application for different synthetic fuels

1.4　CO_2 impact by accelerated and increased synthetic fuel ratio (EU)

The European passenger car fleet development will serve as an example. Various OEM data were used as a basis for this scenario. Looking at the CO_2 emissions of the entire fleet, even with a larger share of electric vehicles, an increase in greenhouse gas emissions can be expected by 2035. This is also based on the fact that liquid fuel vehicles will still account for the largest share of vehicles in 2035 and that electricity production in Europe will not yet be based solely on renewable energies. At the same time, it is important to mention that tank-to-wheel (TtW) CO_2 emissions will decrease by about 10% in 2035 compared to 2020, due to the increase in the share of electric vehicles.

The right-hand side of Fig. 6 shows the impact of synthetic fuels for the same car population ramp-up. An increase in synthetic fuels of up to 30% by 2025 and up to 50% by 2030 was assumed. While this change has no impact on the production of the vehicle, fuels or electricity, there is a significant elimination of CO_2 emissions in the operation of the vehicles. In order to meet global and local climate targets, synthetic fuels will be able to make a major contribution. Further information on this scenario can be obtained from reference [9] and [10].

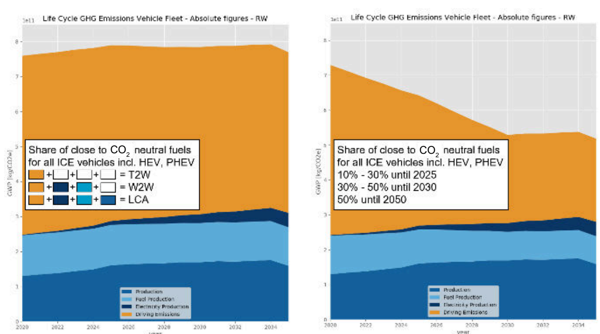


Fig.6　Development of European greenhouse gas emissions of the existing passenger car fleet under different ramp-up scenarios of synthetic fuels[9]

2 Innovation of powertrain technology

For the existing fleet, drop-in capable fuels are essential, as almost no effort is required to be able to use them in existing vehicles. In the long term, taking into account the possible use of synergy effects between different sectors, dedicated synthetic fuel engines will be needed. Herein, some of the technologies that are already available and the research that is taking place within IAV and TU Berlin are addressed.

2.1 Hydrogen internal combustion engines

Since hydrogen serves as the basis for almost all synthetic fuels, it only makes sense to start by looking at technologies that work with hydrogen. Similar to gasoline engines, the hydrogen combustion engine works either via port fuel injection or via direct injection. The same advantages that direct injection brings to the gasoline engine also apply to hydrogen. Here, efficiencies of over 40% have been achieved on current test engines, which is also due to the possibility of very lean operation. However, by eliminating the C atoms in the fuel, CO_2-free operation is also possible with hydrogen in the TtW logic. In the future, further potential can be exploited, and efficiency further increased by changing other parameters, such as increasing the compression ratio. Efficiencies over 50% are expected, as shown in Fig. 7.

A remaining task is to solve NO_x emissions during transient operation, which is also a result of a lean combustion air ratio. Solutions here would be the intelligent integration of hybridization, phlegmatization or electrification of the air path. In addition to soot, however, NO_x emissions are not as relevant as with a diesel engine since basic conditions - such as the necessary temperature - for the generation of both emissions can be completely avoided and emissions can be reduced to a minimum (see Fig. 8). Accordingly, any exhaust aftertreatment systems simplify to fewer components. At the same time, emissions are many times smaller within current certification cycles, as seen in Fig. 9.

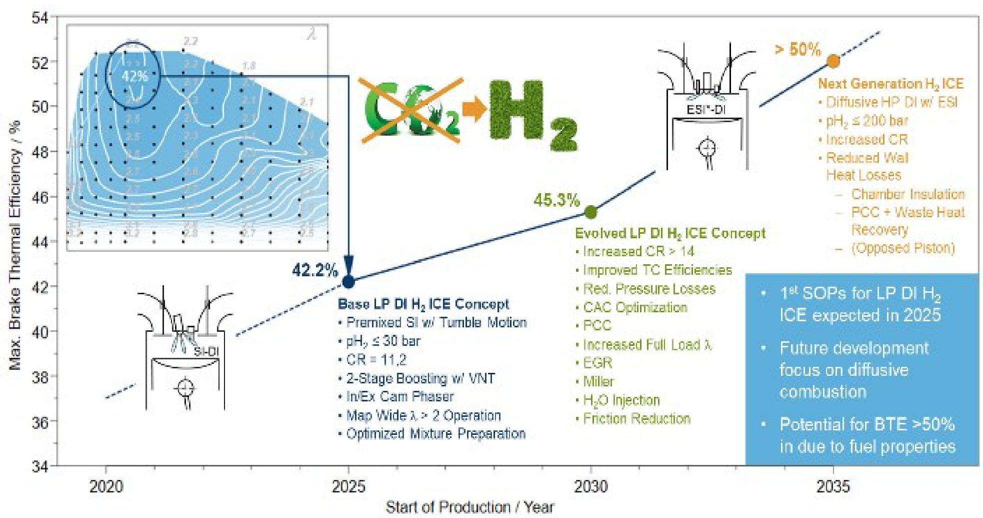


Fig. 7 Potential of hydrogen ICE

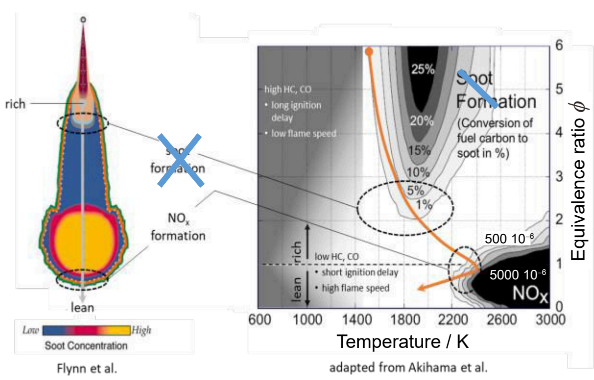


Fig.8 Conditions for generation of soot and NOx[11-12]

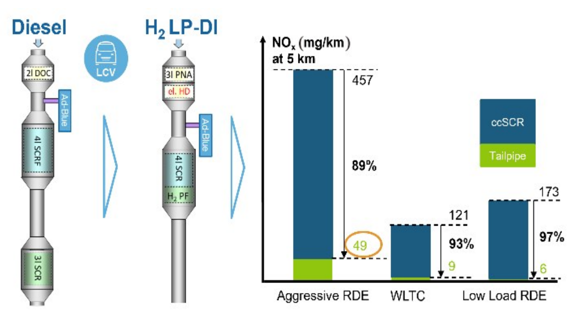


Fig.9 Simplified H2 ICE EAT concept and emission output within certification cycles

Additional research, for example, is the improvement of injectors for operation with hydrogen. As such, in Fig. 10 different profiles are used to adapt the injection depth and distribution to hydrogen combustion. Additional information on these technologies can be obtained from references [8], [9], [13], and [14].

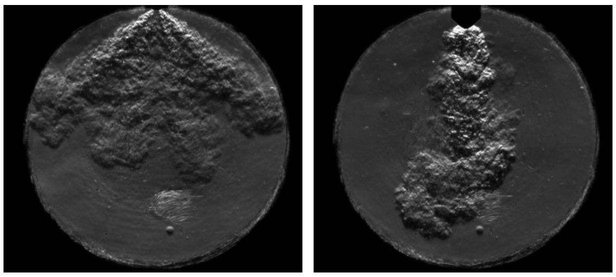


Fig.10　Injection profiles for different injectors and hydrogen in nitrogen[13]

2.2　Hydrogen PEM fuel cell

The second way to use hydrogen in vehicles is to implement a fuel cell. Although there are only a few units of this technology, various vehicles are available on the market. An important advantage over the internal combustion engine is the slightly higher efficiency and the complete absence of emissions. Tasks such as exhaust gas aftertreatment are completely eliminated. Among the challenges are improving the durability and reducing the cost of the system. However, the latter will be further reduced in the future with an increase in production capacities. With the expansion of the hydrogen infrastructure, the usability of both the fuel cell vehicle and the hydrogen combustion engine will also increase.

Ongoing research is improving stack design (such as the membrane-electrode-assembly (MEA)), as well as developing intelligent operating strategies. The development of the efficiency is expected to be well over 55% in the future (see Fig. 11). More information on these topics can be found on references [18] and [19].

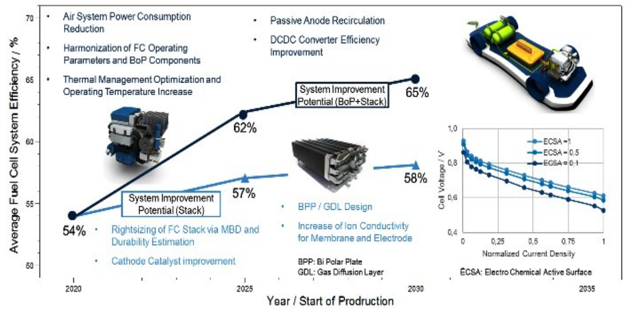


Fig.11　Development of fuel cell system efficiency

2.3　Methanol internal combustion engine

A basic element of several industries and sectors is methanol. The use of methanol in combustion engines has already been successfully demonstrated in several vehicles and prototypes. A green production of hydrogen as a base allows also with this fuel a balance towards zero emissions in the well-to-wheel (WtW) logic.

Excellent properties for combustion, such as very high knock resistance, makes it possible for the combustion engine to operate very efficiently even without complex technologies, which in turn can lead to a possible simplification of the overall system and, accordingly, to cost savings. At the same time, as can be seen in Tab. 2, CO_2 emissions per gFuel are a factor greater than two lower than diesel or gasoline. However, the smaller volumetric and gravimetric energy density in relation to diesel and gasoline leads to the need for a larger tank in order to be able to maintain identical ranges and, accordingly, also to a significantly higher mass flow.

Tab.2　Properties of methanol compared to other fuels

Property	Diesel ($C_{12}H_{23}$)	Gasoline (C_7H_{15})	Methane (CH_4)	Methanol (CH_3OH)
gCO_2/gFuel	3,175	3,043	2,75	1,375
gCO_2/MJ	75,601	73,039	55	69,095
gH_2O/gFuel	1,206	1,206	2,25	1,125
gH_2O/MJ	28,718	28,960	45	56,532
MHV/(MJ/kg)	2,689	2,769	2,733	2,659
RON	30	91…102	130	109…115
Evap. Enth./(kJ/kg)	Ca. 350	Ca. 350	—	1110
Flame speed/(m/s)	0,5	0,3	0,4	0,5
Ad. Flame temp./°C	2650	2300	2250	2200

Other challenges are corrosion and the high evaporation enthalpy. A blending rate of methanol with other fuels is possible in principle but must be matched to the materials used in the injection system. Modern materials can counteract this completely. The high evaporation enthalpy, in turn, leads to difficulties, especially in cold starts. However, technologies such as prechamber ignition can also solve these problems. The implementation of such technologies in the future can result in significant efficiency gains. As such methanol is a great fuel for ICE's, it will make a peak efficiency of up to approximately 50% possible in brake thermal efficiency (BTE) in the future, as seen in Fig. 12.

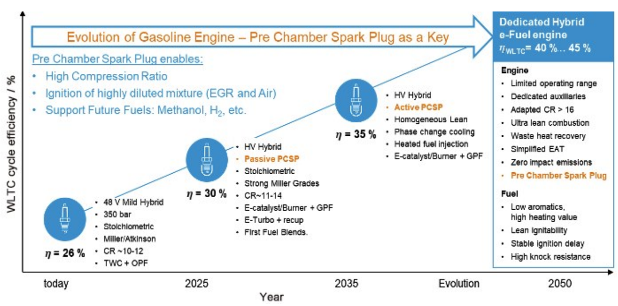


Fig.12 Development of methanol ICE efficiency

2.4 Dedicated (Bio−) methane internal combustion engine

Methane is a common fuel in the field of internal combustion engines. Named manufacturers have many vehicle variants in their portfolio. The advantages are also present in current vehicles, as current models are considered to be very fuel-efficient. With biomethane, it is also possible to design this technology with low CO_2 emissions. The fundamental advantage is the independence from renewable energies and accordingly the further exploitation of other methods to reduce global CO_2 emissions.

With today's methods, dedicated biomethane vehicles are among the more efficient methods of mobility, as seen in Fig. 13. As such, biomethane is a very suitable fuel for long-distance applications due to both its high efficiency and low emissions.

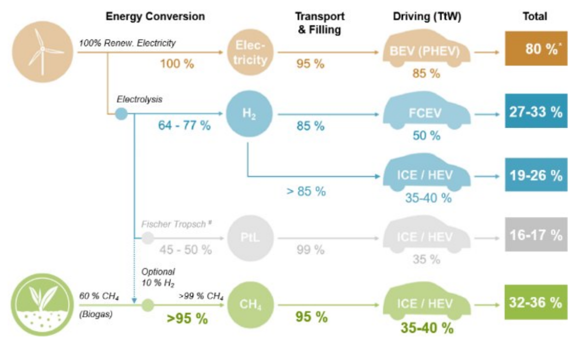


Fig.13 System efficiency of dedicated biomethane vehicle compared to other technologies

Challenges here, however, are the use of additional resources to produce the fuel, as well as the issue of land use. However, with new methods for production (e. g., catalytic hydrothermal gasification), advanced biofuels can be produced even now by using e. g. waste as a source.

The technological level of the engines is currently already at a very high level. Topics such as cold start and further efficiency improvements through engine design measures are being investigated. Here, too, prechamber ignition is a solution for the former. Other solutions include the implementation of an electric turbocharger, as well as a better heat management. Further information on these topics can be found from reference [15].

2.5 DME internal combustion engine

As a fuel that can be produced in the methanol route, DME can replace many applications that are currently diesel-based. The high oxygen content and other combustion characteristics allow furthermore virtually soot-free operation.

Compared to diesel, the energy density of DME is lower, but still within an acceptable range. The cetane number is nearly equivalent, as seen in Tab. 3.

Tab.3 Properties of DME compared to diesel

Property	Boiling point/°C	Cetane number	Density(15°C)/(kg/m³)	Oxygen content/(% m/m)	Lower heating value/(MJ/kg)
EN590 Diesel	180–350	51–54	830	<1	−43.0
DME	−25	55–60	670	35	28.4

Since it is a green production, DME can achieve a CO2 reduction of up to 95% compared to current diesel fuel (see Fig. 14). Current challenges in this drive concept are played by the injection system, since higher mass flows are needed and the lubricity of the DME is very small. However, the injection system can be adapted to address these issues. Other solutions in this system reflect the simplified exhaust gas aftertreatment. In addition to being soot-free, NOx emissions are also significantly minimized. Additional information on these technologies can be obtained from references [20] and [21].

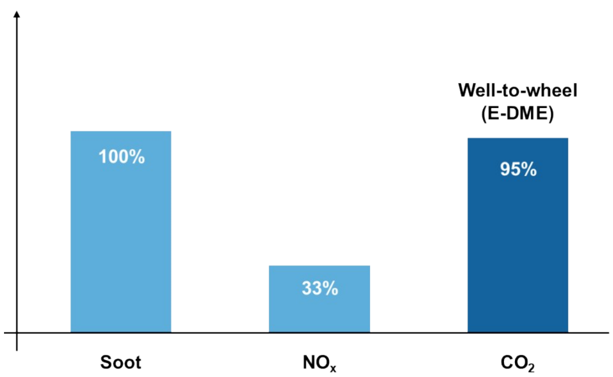


Fig. 14　Emission reduction of DME in comparison with diesel fuel in %

2.6　GANE fuel

GANE fuel is a patented mixture of DME, methanol, water, and other additives. With this fuel, it is possible to combine the advantages mentioned in previous sections. An outstanding characteristic is the very low emission of soot and NO_x, as seen in Fig. 15. The same challenges that pose to methanol and DME also pose here. In order to be able to use the GANE fuel optimally, the fuel system must be adapted accordingly. Further information on the fuel can be found in reference [22].

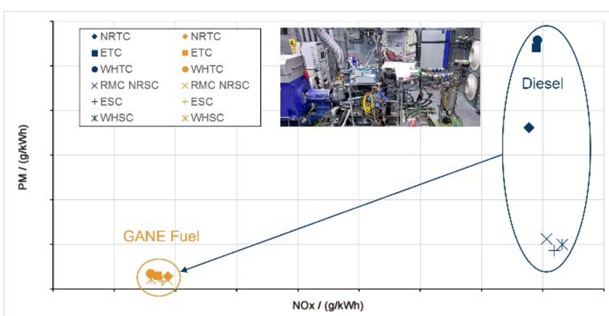


Fig.15　Potential of GANE fuel compared to diesel

3　Summary and outlook

Battery electric vehicles are an important tool to reduce TtW CO_2 emissions within the mobility sector. However, without the required share of locally available renewable energy, there is a risk of missing the CO_2 targets. Simultaneously, there will still be high investments to ensure the infrastructure as well as the distribution of electricity.

An easier way will be to convert the produced electricity on site to liquid or gaseous fuels, as it is the case e. g., in the pilot projects Liquid Sunshine [16] and Haru Oni [17]. The existing worldwide infrastructure and logistics are already in place for this and can be used in their entirety without any adjustments. In this paper, different topics on synthetic fuels were highlighted:

(1) Different production methods exist and differ fundamentally under the ammonia and methanol pathways. The advantage of the methanol pathway is the large coverage of many conversion technologies and the resulting synergy between the transport and other sectors.

(2) Different synthetic fuels are required for different applications, depending on their suitable properties. Some areas of application in the future will only be completely CO_2-emission-free with synthetic fuels, such as aviation.

(3) The introduction of synthetic fuels can bring about a significant reduction in CO_2 emissions with an overnight effect.

(4) A wide variety of technologies and fuels, from blending, drop-in capable fuels, dedicated synthetic fuel ICEs, and fuel cells are already under research and will make it possible for a further significant leap in efficiency of ICEs with values around 50%.

Different scenarios for the introduction and use of synthetic fuels are possible as an admixture to fossil fuels or even as an independent substitute. The integration of CO_2-neutral fuels into the market can support faster compliance with CO_2 targets in the long term and generate a further time buffer for the ramp-up of battery-electric vehicles. Of the 1.2 billion vehicles worldwide, the majority are capable of running on drop-in capable synthetic fuels without adaptation.

However, technology openness, i. e., the simultaneous development of battery-electric vehicles and the ramp-up of CO_2-free fuels, is an essential part of meeting the global targets by 2045, 2050, or 2060.

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