

Feasibility Study of a Fossile Fueled Zero Emission Vehicle

Sebastian Stenger
Energy Technology

Steffi Köhler, Anna-Theresia Nasch, Reinhard Leithner, Stephan Scholl, Ulrike Krewer and
Peter Eilts
Technische Universität Braunschweig

ABSTRACT

This study investigates the technical feasibility of onboard carbon capture in vehicles. In fact there are two different main concepts of hybrid electric vehicles with batteries and range extenders proposed. The first concept uses an Internal Combustion Engine as range extender. Carbon dioxide is separated from the flue gas of this Internal Combustion Engine by chemical or physical absorption. In the second concept a solid oxide fuel cell (SOFC) is used as a range extender. The CO remaining in the anode exhaust gas is not combusted as usual by mixing anode and cathode exhaust gases but shifted with water vapor, sufficient available in the anode exhaust gas flow, to H₂ and CO₂. The H₂ is separated by a membrane permeable only for H₂ and recycled by the methane flow to the SOFC stack. Carbon dioxide can then be separated by simply condensing the water vapor of the anode exhaust gas of the SOFC.

Carbon dioxide can either remain onboard chemically bonded e.g. as carbonate with the absorption media or stored in a pressure vessel after desorption or condensation of the water vapor. As one mole methane produces one mole CO₂, the CO₂ can be stored in one chamber of a double chamber tank. The tank is e.g. divided into two chambers with variable volume by a non-permeable but flexible membrane; on the other side of this membrane methane is stored. At the gasoline station the empty methane chamber is filled with new methane and the CO₂ is discharged simultaneously providing also simple fueling and CO₂ removal methods. Carbonate can also be disposed at the gasoline station and calcinated in centralized plants, i.e. CO₂ can be separated and CaO reused.

Furthermore all concepts are compared in fuel efficiency and general feasibility. The SOFC concept seems to be the most attractive one, because it shows the highest efficiency, uses the simplest CO₂ capture concept and releases the captured CO₂ in gaseous state, providing the simplest CO₂ discharging method.

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INTRODUCTION

In Germany 17 % of the CO₂ released to the atmosphere is emitted by cars [1]. Electric cars powered by batteries or hydrogen consuming fuel cells like PEM-FC can avoid these distributed CO₂-emissions, but are restricted in operating range and/or need a new infrastructure. To avoid these disadvantages electric cars should be provided with range extenders using fuels like diesel or methane, i.e. hybrid cars with CO₂-separation should be used. Hybrid concepts without CO₂-separation are already well established, e.g. Toyota Prius or Opel Ampera. The common hybrid vehicles are using conventional diesel- or gasoline engines with an

additional electric generator and engine and a battery for energy storage.

1.1. Hybrid Vehicle Concepts

Boretti [2] has compared fuel economy and exhaust gas emissions of a full (Toyota Prius) and mild hybrid (Honda Civic) to standard Internal Combustion Engine (ICE) driven vehicles. It was revealed that especially for low driving speeds a significant fuel saving can be achieved for hybrid vehicles. The reasons are:

- Nearly constant efficiency of electric motor over whole speed range
- Storing and Recuperation of braking energy

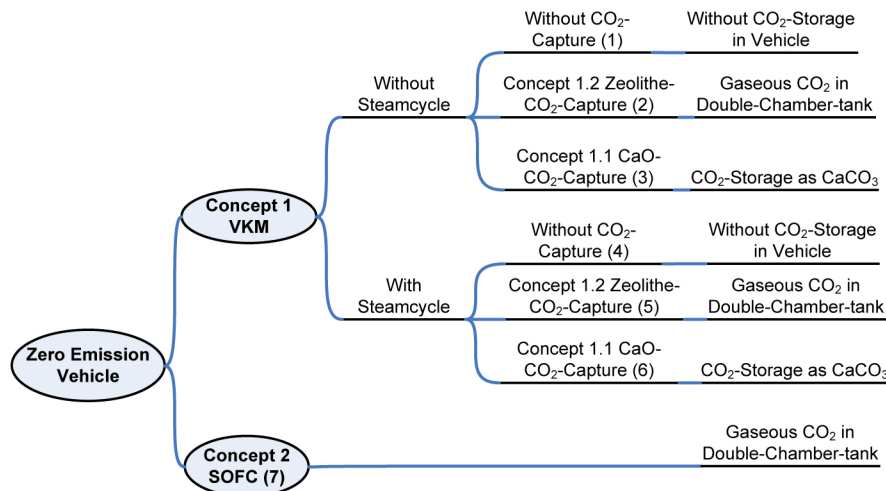


Figure 1. Overview of examined cases

- ICE always running at best point (highest efficiency)
- Acceleration energy provided by battery

In this paper studies on two different concepts for range extenders will be presented:

- Internal Combustion Engine (ICE) as range extender using methane as fuel
- Solid Oxide Fuel Cell (SOFC) using also methane as fuel [3]

1.2. CO₂ - Separation Concepts

In general three CO₂-separation concepts are well known [4]:

a. Post-Combustion Carbon Capture (PCCC)

CO₂ is separated out of the flue gas of hydrocarbons burnt with air consisting mainly of N₂, CO₂ and water vapor.

b. Pre-Combustion Carbon Capture (PRCCC)

CO₂ is separated after gasification and shifting hydrocarbons resulting in a gas mainly consisting of CO₂, H₂, N₂ and water vapor when air was used for gasification or consisting of CO₂, H₂ and water vapor when oxygen was used for gasification. When air was used for gasification CO₂ will be separated by similar methods used for PCCC. When oxygen was used for gasification also these methods can be used but preferably the water vapor will be condensed and H₂ separated by a membrane. The advantages of PRCCC are the lower volume flows and hydrogen as resulting fuel.

c. Oxyfuel Combustion

Oxyfuel combustion means combustion with pure oxygen. The flue gas of hydrocarbons combusted with pure oxygen consists of CO₂ and water vapor. The water vapor can be condensed and nearly pure CO₂ is left.

For standard ICE only PCCC is applicable, but there are many different methods ([5], [6]). Basically there are two

possibilities: First regeneration of the absorbent material onboard leading to a complex desorption process onboard but easy storage and delivery of CO₂ at the gasoline station. Second centralized desorption process avoiding the complex desorption process onboard but leading to a complex change of absorbent material at the gasoline station. As representative methods the following two were selected for the study:

- PCCC using Zeolite and CO₂-storage on board (ZCSOB) in a double chamber methane-CO₂ tank and
- PCCC using CaO, storing CO₂ as CaCO₃ on board and central CO₂ desorption by CaCO₃ calcination (CaOCD)

In the studies also the possibility of improving the efficiency of the ICE by a “bottoming cycle” was included. Further the adsorption heat will only be used in a steam cycle when the ICE waste heat is also used in a bottoming steam cycle and the absorption heat of the carbonization has to be used anyway. Therefore in principle 6 combinations using an ICE with CO₂ separation are possible

- Standard ICE and ICE with bottoming steam cycle (2 option types)
- With 2 different PCCC methods and without CO₂-Capture (in total 3 option types)

The SOFC for a range extender as 7th possibility is only applicable as hybrid, because during the time the SOFC is started (between 10 and 30 min) the vehicle should be running only by battery. All options are summarized in [figure 1](#). The numbers in parentheses are assigned studied cases. [Figure 2](#) comprises the configuration of all cycles examined in one scheme, except the SOFC concept (see [figure 5](#)).

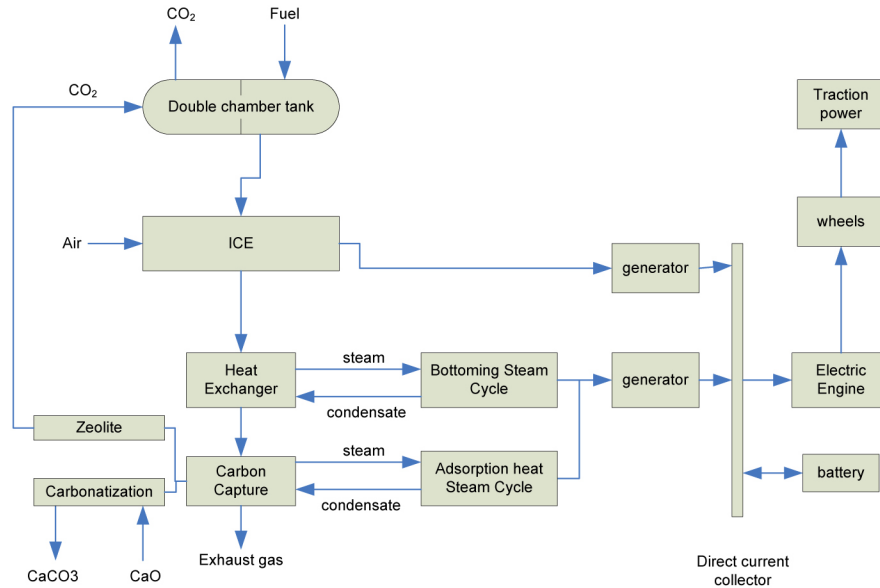
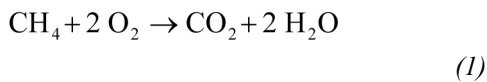


Figure 2. ICE with optional ICE waste heat and adsorption heat recovery by a water steam cycle and carbon dioxide separation by Zeolite or CaO carbonization respectively

1.3. Common Conditions

To establish comparability the following conditions are common for all cases discussed. The power used for driving (at the wheels) shall be 20 kW.

Pure methane is set as the kind of fuel for the ICE and the SOFC as well for all calculations in this study. Specific carbon dioxide emissions of methane can be simply calculated by the equation for the combustion reaction (equation 1):



Mass specific carbon dioxide emissions of pure methane can be obtained by weighting the equation with the molar weights of the involved species.

$$w_{\text{CO}_2} = \frac{M_{\text{CO}_2}}{M_{\text{CH}_4}} = \frac{44}{16} = 2.75 \frac{\text{kg CO}_2}{\text{kg CH}_4}$$

Summarizing these considerations, the following common conditions for the calculation of fuel consumption are given in table 1:

Table 1. Common conditions

	Description	Value
P	Power for driving	20 kW
v_m	Average speed	100 km/h
H_u	Lower heating value of methane	50010 kJ/kg
w_{CO_2}	Specific CO ₂ release of methane	2.75 kg CO ₂ /kg

2. STANDARD ICE AND ICE WITH BOTTOMING CYCLE

The efficiency of a natural gas motor of the envisioned power is assumed to be $\eta_{\text{ICE},BP} = 35\%$ at best point [7].

2.1. Ice without Steam Cycle and Carbon Capture Devices (Case 1)

The conventional ICE as the direct power source of the car without heat recovery and carbon dioxide separation is the state of the art today. Fuel consumption for this standard ICE case can be simply calculated by equation 2:

$$\dot{m}_{F,SICE} = \frac{P}{H_u \cdot \eta_{\text{ICE},BP}} \quad (2)$$

Therefore at the best point in non hybrid mode (using $\eta_{\text{ICE},BP} = 0.35$) a fuel mass flow of 4.11 kg/h methane is required. This fuel consumption and its CO₂-emission are set as a reference value for the calculation of fuel savings for the examined mobility concepts. The corresponding release of carbon dioxide can be simply calculated by equation 3:

$$\dot{m}_{\text{CO}_2,SICE} = \dot{m}_{F,SICE} \cdot w_{\text{CO}_2} \quad (3)$$

In fact the release of carbon dioxide of this ICE at best point conditions is 11.31 kg/h.

2.2. Ice with Bottoming Steam Cycle (Case 4)

The exhaust gas temperature of gas engines is in the range of 490 °C to 545 °C (depending on operating conditions) [7].

which indicates a high potential for heat recovery. The exhaust gas heat can be used for a downstream steam or so called “bottoming cycle” to reduce fuel consumption by improving efficiency. Held [8] observed a fuel saving of 11.5 % and Ambros [9] predicted a fuel consume reduction of 5-8 % by use of this technique. In ([10], [11], [12], [13]) similar efficiency gains were found to be reasonable. The heat of the ICEs water cooling can also be used for the steam cycle but is devaluated because of its low temperature of about 100 °C. According to several studies the efficiency of the water-steam cycle is set to $\eta_{SC} = 6\%$ ([14], [15]). The fuel consumption for an ICE with bottoming cycle can therefore be calculated with equation 4:

$$\dot{m}_{F,ICEWBSC} = \frac{P}{H_u \cdot [\eta_{ICE,BP} + \eta_{SC} \cdot (1 - \eta_{ICE,BP})]} \quad (4)$$

The fuel and CO₂ savings can be calculated by equation 5:

$$S_{ICEWBSC} = 1 - \frac{\dot{m}_{F,ICEWBSC}}{\dot{m}_{F,SICE}} = 1 - \frac{\eta_{ICE,BP}}{\eta_{ICE,BP} + (1 - \eta_{ICE,BP}) \cdot \eta_{SC}} \quad (5)$$

In this Case 3.7 kg/h fuel is consumed which means fuel saving of about 10 % compared to the Case 1 (standard ICE reference case).

3. STORAGE OF METHANE AND CO₂ IN A DOUBLE CHAMBER TANK - EXPANSION OF METHANE AND COMPRESSION OF CO₂

In the ICE cases 2 and 5 using Zeolite adsorption and in the SOFC-concept (case 7) the CO₂ is stored in gaseous state. In both cases expansion of methane and compression of CO₂ are essential.

3.1. Storage of Methane and CO₂ in a Double Chamber Tank

Methane and CO₂ are stored in two chambers of the same tank (pressurized up to approx. 200 bar [16]) divided by a flexible membrane (see fig. 2). During the driving process methane is consumed and CO₂ is stored in the tank. When filling the one chamber with methane at the gasoline station the CO₂ of the other chamber has to be simultaneously discharged to the CO₂-chamber of a similar but bigger tank at the gasoline station. For the feasibility of the concept it is important that the compressed CO₂ has a lower or equal specific volume than the fuel gas. Both gases are at 200 bar in supercritical state. At conditions of 20 °C and 200 bar the density of CO₂ is 937 kg/m³ [17] and of natural at about 330 kg/m³ [18]. The required tank volume for CO₂ can be calculated by equation 6:

$$V_{CO_2} = w_{CO_2} \cdot \frac{\rho_{CH_4}}{\rho_{CO_2}} \cdot V_{CH_4} = 0.968 \cdot V_{CH_4} \quad (6)$$

In fact the density of CO₂ is almost three times the density of methane. Nevertheless the required volume at 20 °C and 200 bar is almost equal. The reduced volume of CO₂ will lead to slightly decreased pressure in the tank compared to methane.

3.2. Methane Expansion and CO₂-Compression

In both cases (CO₂-adsorption by Zeolite and SOFC) at least two stages of compression of CO₂ and methane expansion are necessary to allow intermediate heat transfer from compression to expansion and water condensate separation from CO₂ (see fig. 5). In addition compressors and expanders with pressure ratios of 200 (ca. 1 bar inlet pressure) are not available.

In the Zeolite concept CO₂ is leaving the adsorber with a temperature of 200 °C due to the required desorption temperature level. Therefore CO₂ has to be precooled by e. g. methane and in the SOFC concept the anode flue gas consists mainly of CO₂ and water vapor and has to be cooled down to condensate the water vapor e. g. by the air for the SOFC. For the SOFC concept we will show in detail that it is possible to provide the compression power for the CO₂ by the expansion of methane with an adequate heat management.

4. ICE AS RANGE EXTENDER AND PCCC USING ZEOLITE

One analyzed possibility for mobile capture of carbon dioxide is the capture of CO₂ by a Zeolite and storage in fluid form in a double chamber tank as described above. For use in mobile applications the cycling stability of zeolite is an important issue. It should be at least several thousand cycles. Unfortunately the investigated Zeolite material adsorbs not only carbon dioxide, but also water vapor. This requires a regeneration concept with a selective desorption of water and carbon dioxide, which is generally possible due to different desorption temperatures [19].

The potential of carbon dioxide adsorption with zeolites was determined by preliminary tests. For two different materials of Zeoliths 13X from Silica and Zeolum F9 HA1.5 from TOSOH Corporation Japan isotherms at different temperatures were recorded (figure 3-Japanese material only). It is obvious that carbon dioxide absorption works better at low temperatures. The material from Japan showed better results. The required mass of Zeolite should be as low as possible. First experiments with zeolites and pure CO₂ are promising, since the adsorption capacity is more than 20 wt. % for the best zeolite material at 50 °C.

The carbon dioxide adsorption capacity for real exhaust gases will be lower than the measured 20 wt. % because of the following reasons

- The partial pressure of carbon dioxide in flue gases is significantly lower than that one of pure CO₂
- Adsorption of water will probably further decrease the carbon dioxide adsorption capacity

Further experimental studies are necessary to examine the capacity of the material under real flue gas conditions. For preliminary calculations 8 % CO₂ adsorption capacity are assumed.

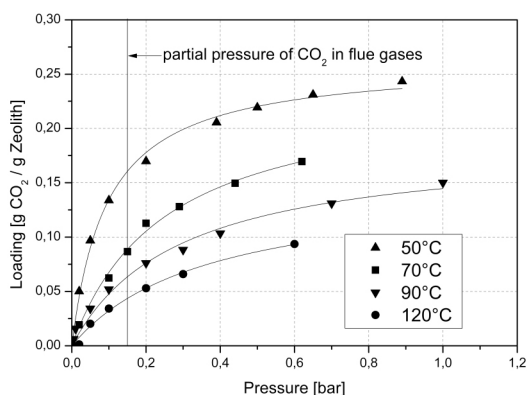


Figure 3. Preliminary CO₂-adsorption isotherms of Zeolum F9 HA1.5 from TOSOH Corporation Japan measured by a magnetic suspension balance (Rubotherm). The isotherms are fitted by the Langmuir equation.

4.1. PCCC using Zeolite without Steam Cycle (Case 2)

The process of PCCC with Zeolites without steam cycle is shown in figure 4. It shows a simplified process flow chart for the required plant layout. Each of the four fixed bed reactors must be able to run in 4 different operation modes and be connected to the adequate gas pipes by appropriate valve positions. The cyclic order of the operation modes is:

- Desorption of Water
- Desorption of Carbon dioxide
- Cooling (active or passive)
- Adsorption of water and carbon dioxide

The operating modes for each reactor at the 4 possible configurations are summarized in table 2.

Table 2. Operations for each fixed bed at any time

	Step 1	Step 2	Step 3	Step 4
Reactor 1	H ₂ O-Des	CO ₂ -Des	Cooling	Adsorption
Reactor 2	CO ₂ -Des	Cooling	Adsorption	H ₂ O-Des
Reactor 3	Adsorption	H ₂ O-Des	CO ₂ -Des	Cooling
Reactor 4	Cooling	Adsorption	H ₂ O-Des	CO ₂ -Des

For better understanding the process flow will be explained following the flue gas flow. The flue gas coming from the combustion consists of N₂, CO₂, H₂O and low contents of the pollutants NO_x, CO and hydrocarbons. If the emission of pollutants exceeds the allowable limits a catalyst has to be arranged before the first reactor. The flue gas coming from the combustion has a temperature of 450 °C (thick line). In step 1 it is directed around the first fixed bed reactor tubes to provide the heat necessary for desorption of water. (The water vapor is discharged from the reactor tubes to the atmosphere-dotted line). After the first reactor the temperature of the flue gas amounts about 315 °C and enters the second reactor (outside the reactor tubes) to provide the heat necessary for the CO₂ desorption. (The CO₂ is discharged from the reactor tubes to the compressor and stored in the double chamber tank-thin line). After the second reactor the flue gas temperature is about 250 °C and has to be cooled down to 50 °C before it enters the fixed bed reactor tubes of the third reactor. In this fixed bed reactor tubes the zeolite adsorbs water vapor and CO₂. (The CO₂-free flue gas can be discharged to the environment together with desorbed water vapor-dotted line). The fourth reactor is cooled down from about 250 °C to 50 °C and will become the next one which adsorbs water vapor and CO₂ (in step 1 reactor 3). In table 2 one can see also the change of operating mode of the other reactors, when step 1 switches to step 2. This switches are initiated automatically after a certain time because the absorbent materials of reactor 3 (step 1) is loaded so much that the CO₂ content in the outlet exceeds a certain limit and desorption of reactor 1 and 2 (step 1) is finished. Of course the reactors have to be designed according to these limits. When switching from step 1 to step 2 reactor 3 changes from adsorption to H₂O desorption operation mode, reactor 2 from CO₂ desorption to cooling operation mode and reactor 1 from H₂O desorption to CO₂ desorption operation mode. The switches from step 2 to step 3 and to step 4 follow the same regularity. After the fourth step the system starts again with step 1.

The whole system must be controlled by a process automatisation unit to keep the parallel operating processes running. It is estimated, that with a proper heat management there is only a negligible efficiency loss due to pressure losses etc. compared to the reference case.

4.2. PCCC using Zeolite with Ice Waste and Adsorption Heat Recovery Steam Cycle (Case 5)

Heat for the CO₂-desorption and a heat recovery steam cycle can be supplied by ICE and CO₂-Adsorption by zeolites. Anyhow it can be expected that the fuel saving potential of this heat recovery concept will be lower because the heat with the highest temperature is needed for desorption