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Critical assessment of power trains with fuel-cell systems and different fuels

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Abstract

Legal regulations (USA, EU) are a major driving force for intensifying technological developments with respect to the global automobile market. In the future, highly efficient vehicles with very low emission levels will include low-temperature fuel-cell systems (PEFC) as units of electric power trains. With alcohols, ether or hydrocarbons used as fuels for these new electric power trains, hydrogen as PEFC fuel has to be produced on board. These concepts including the direct use of methanol in fuel-cell systems, differ considerably in terms of both their development prospects and the results achieved so far. Based on process engineering analyses for net electricity generation in PEFC-powered power trains, as well as on assumptions for electric power trains and vehicle configurations, different fuel-cell performances and fuel processing units for octane, diesel, methanol, ethanol, propane and dimethylether have been evaluated as fuels. The possible benefits and key challenges for different solutions of power trains with fuel-cell systems/on-board hydrogen production and with direct methanol fuel-cell (DMFC) systems have been assessed. Locally, fuel-cell power trains are almost emission-free and, unlike battery-powered vehicles, their range is comparable to conventional vehicles. Therefore, they have application advantages cases of particularly stringent emission standards requiring zero emission. In comparison to internal combustion engines, using fuel-cell power trains can lead to clear reductions in primary energy demand and global, climate-relevant emissions providing the advantage of the efficiency of the hydrogen/air reaction in the fuel cell is not too drastically reduced by additional conversion steps of on-board hydrogen production, or by losses due to fuel supply provision.

Keywords: PEFC power trains; Process simulation

1. Introduction

From today's perspective, the present status of our industrialized world requires new approaches to solve most urgent energy and environmental problems.

A medium- to long-term approach to solving our energy and environmental problems envisages using fuel-cell systems for power generation. This approach is being developed on a worldwide basis for both stationary and mobile applications. It seems to promise sustainable options for the future. The challenges this approach is supposed to meet could dominate energy conversion systems introduced in the energy market for the foreseeable future.

Possible advantages of such a scenario are:

- providing power for both stationary and mobile applications,
- preserving material and energy resources,
- minimizing environmental problems on a local basis (i.e. emissions, summer smog, noise),
- reducing emissions (greenhouse effect) on a global basis, and
- considering new fuel concepts.

On the other hand, the economic and technological challenges include:

- competing with established low-cost technologies showing considerable development promise (efficiency improvement, reduction of pollutant emissions),
- solving specific problems associated with the new technology,
- promoting social acceptance of the new technology, and
- discussing the application prospects of new fuels.

2. Fuel-cell drive systems for road traffic

New drive systems with fuel cells and the energy carriers required could play a major part in improving the

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overall social environment. This is especially the case of improved conventional energy carriers and drive systems should reach to its limit then the new systems proposed offer a new quality of traffic in society. At present, however, only a working hypothesis can be offered towards the discussion of possible advantages of fuel-cell drive systems as compared to conventional combustion engines. The following include perceived benefits:

- high electrical efficiency,
- no (or low) local emissions,
- no mechanical vibration (little acoustic noise),
- low maintenance requirements,
- good driving characteristics,
- effective on-board energy supply,
- high flexibility due to modular design of fuel-cell stacks.

The technical systems under discussion will have to be evaluated on the basis of three reference criteria: performance, life cycle, and cost. The present evaluation is only valid under the condition that there will be sufficient user-friendliness, good driving and environmental behaviour and long-term availability of resources and primary energy carriers. In particular, electrically powered fuel-cell drive systems will have to compete with

- combustion engines (on the basis of clean primary energy carriers),
- hybrid drive systems (with higher drive weight and higher cost), and
- electric drive systems with batteries (with higher cost, shorter range and higher drive weight).

The use of hydrogen as a fuel is expected to have advantages with respect to fuel-cell technology in terms of a sustainable material and energy supply compared to conventional approaches. If hydrogen could be produced on a non-fossil basis, this would offer an option for overcoming the greenhouse effect. Apart from niche market solutions, however, the energy market, in general, will require other energy carriers for the next 20 to 30 years. For example, natural gas as the primary energy carrier for stationary applications, or methanol, or hydrocarbons in the tanks of vehicles for the on-board production of hydrogen to be used in mobile fuel cells.

In the future, highly efficient vehicles, running at very low emission levels will include low-temperature fuel-cell systems as units of electric power trains (Fig. 1). Pressurized or liquefied hydrogen can be used directly as an energy carrier for power trains that offer good performance, including high efficiencies, zero emission and sufficiently dynamic operation. With methanol, ethanol or hydrocarbons used as fuels for these new electric power trains, hydrogen as the PEFC fuel has to be produced on board (with heated steam reformer, HSR, or partial oxidation reformer, POR, as well as catalytic burner and gas cleaning units). Methanol might also be used directly for electricity generation inside the fuel cell. These concepts differ completely in terms of both their development capabilities and the results achieved so far.

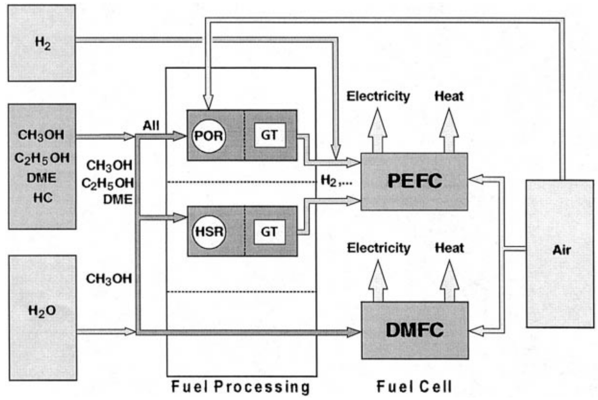

Fig. 1. Possibilities for use different fuels in fuel cells, POR: partial oxidation reformer; HSR: heated steam reformer, GT: gas treatment, PEFC: polymer electrolyte fuel cell, DMFC: direct methanol fuel cell.

Passenger cars with fuel cells could run on various energy carriers such as hydrogen, methanol, gasoline or diesel, although energy carriers such as ethanol, dimethylether or various crude oil fractions may offer feasible solutions also. As compared with conventional cars, fuel-cell cars would be equipped with novel drive units, this is, the fuel-cell unit (PEFC) and, in addition, fuel processing or gas production unit in the case of methanol or hydrocarbons (clean gasoline or clean diesel), when used instead of hydrogen. These new fuel-cell systems for road traffic are confronted with the following key requirements:

- low manufacturing costs (< 70 DM/kW_{el}),
- light and compact construction (< 6 kg/kW_{el}, < 6 l/kW_{el}),
- efficient energy management,
- efficient water management,
- efficient gas processing,
- quick start-up and systems dynamics,
- compliance with environmental standards,
- adequate life cycle (> 10 years),
- mass production,
- driving comfort and
- safety considerations.

The efficiency rates achieved in various units of gas-producing systems, including gas after treatment and fuel-cell systems with net power generation for the electrically powered drive systems, are interrelated process parameters which determine the energy management in the New European Driving Cycle (NEDC) in terms of both the drive system and the overall energy requirements at the (wheel basis).

If fuel-cell systems, that is, PEFC systems that are ready for operation at ambient temperature with optimum operational temperatures between 60 and 80°C, are integrated in electrically powered drive systems, the overall energy management depends on various performance parameters that determine not only the energy and emission balances but also the material balances. Major variable performance parameters showing particular impact on the power yield in the fuel-cell system are:

- temperature,
- pressure in anode and cathode unit,
- excess air in cathode unit,
- fuel–gas processing in anode unit,
- fuel–gas rarefaction or pollution (e.g., CO),
- design of membrane and electrode,
- quality and quantity of electrode catalyst, and
- energy and water management.

All these parameters influence the current/potential characteristics of the cells, thus defining the energy efficiency rate of power generation as a function of the drive load. At the same time, they determine the overall energy management for fuel gas supply, net electricity generation of the fuel-cell system, current transformer and electrically powered drive with electric motor and, if appropriate, transmission mechanism.

3. Process analysis of fuel-cell systems for different fuels

An assessment of the effect of the energy-conversion chain has to cover both the conversion of primary energy into the fuel at the filling station and analyses of

- on-board fuel conversion into hydrogen-rich gas,
- conversion inside the fuel cells (electricity generation) and
- determination of the fuel-cell efficiency during the driving cycle.

For process engineering analysis, the commercial simulation program PRO/II was used; it solves the equations of energy and mass balances. This program is only suitable for stationary conditions. Input data defines the conditions that are required to solve the balances. The program recognizes a number of components, such as heat exchangers, compressors, pumps and chemical reactors. Through a meaningful combination of these components, it is possible to describe a fuel cell or a complete system in terms of process engineering and to balance the process as a function of different defined parameters.

4. Hydrogen production and treatment

The following energy carriers

- methanol
- dimethylether (DME)
- ethanol
- gasoline
- diesel and
- propane

can be utilized for hydrogen production in a reformer with autothermal reforming, that is a partial oxidation reformer (POR,) above a temperature of 550°C. At a sufficiently high air ratio (λ), as well as a sufficiently high temperature of the fuel air/water mixture, it is possible to avoid carbon formation for low amounts of water [1]. At the high temperature used, there is probably methane formation, so that the reformer temperature is related to the steam-reforming temperature of methane.

Systems with a heated steam reformer (HSR) are feasible also. Catalysts that can be used in heated steam reforming of methanol have already developed; they are also viable for DME. These work at temperatures lower than 300°C, at which methane formation can be avoided. A comparable development would be possible for ethanol. Such a development is probably only possible using low pressures, however. The reforming of ethanol at high pressure makes it necessary to use higher reactor temperatures that promote methane formation. Using hydrocarbons in the steam reformer, methane formation is also to be expected. If methane is formed, the reforming conditions (temperatures) in the reformer have to be adapted to conditions for methane reforming.

Because present anode catalysts are very sensitive to CO poisoning, the hydrogen-rich reformer product has to be scrubbed. High pressures (HP, e.g., 20 bar) in the steam reforming (HSR) of methanol and DME [2,3] make it possible to use metal membranes for scrubbing the hydrogen to obtain a CO-free gas as the fuel for the PEFC. Such a system has a slightly higher efficiency than systems with a shift reactor or with preferential oxidation (of CO), which have to be coupled to the steam reformer as a gas treatment (GT) step.

The net electricity efficiency for this kind of snapshot investigation is derived from fuel-processing and fuel-cell performances, as well as from auxiliary-equipment performances, especially of compressors and expanders, which are necessary for the operation of the fuel-cell system. For different processes and sources, these efficiencies for net electricity generation (NEG) are listed in Table 1. Fig. 2 shows, as an example, a methanol (HSR) powered fuel-cell system at different compressor and expander efficiencies with straight lines indicating the net electrical efficiency including fuel processing and fuel-cell system.

The main losses of electrical and mechanical energy arise from compression for the cathode air, which cannot be completely recovered by expansion of the exhaust. Increasing the efficiencies of the compressor and expansion turbines, one can be used for a decompression step during gas treatment, will lead to noticeably higher system efficiencies (Fig. 2).

5. Process analysis of the direct methanol fuel cell

The direct methanol fuel-cell (DMFC), based on a PEFC, uses methanol directly for electric power generation and promises technical advantages for power trains. A direct methanol fuel-cell system offers higher system effi-

Table 1
System efficiencies of energy-conversion units with fuel cells (PEFC) using different fuels
Explanations: System: HSR: Heated Steam Reformer, Membr.: Gas-Separation Membrane, POR: Partial Oxidation Reformer, PROX: Preferential CO Oxidation, Shift: CO Conversion, Fuel: EtOH: Ethanol, MeOH: Methanol, NG: Natural Gas, Octane: Gasoline as Octane, EtOH: Ethanol, Institution: ANL: Argonne National Laboratory (Il.), BG: British Gas Technology (GB), CJB: Wellman CJB (GB), FZJ: Forschungszentrum Jülich (D), JM: Johnson Matthey (GB).

Reference no.	Institution	Fuel	POR	HSR	Shift/PROX	Membrane	H_2 utilization%	η Cell%	η NEG[a]%
[1]	FZJ	H_2					100	55	47[b]
[4]	FZJ	MeOH		✓		✓	100	55	40[b]
[1]	FZJ	MeOH	✓		✓		91	55	38[b]
[1]	FZJ	MeOH		✓	✓		72	55	39[b]
	FZJ	MeOH	DMFC	Gas.				42	39[c]
	FZJ	MeOH	DMFC	Liqu.				57	50[c]
[5]		MeOH		✓		✓		57	43
[6]	CJB	MeOH		✓	✓		80/90	50	31
[6]	CJB	MeOH		✓		✓	100	50	35
[6]	JM	MeOH	✓		✓		80	50	29
[6]	JM	MeOH	✓		✓		90	50	32
[7]	ANL	MeOH	✓		✓			55	42
[1]	FZJ	EtOH	✓		✓		79	55	37[a]
[1]	FZJ	EtOH		✓	✓		91	55	37[a]
[1]	FZJ	Octane	✓		✓		91	55	37[a]
[5]		Octane	✓		✓			52	32
[1]	FZJ	Diesel	✓		✓		97	55	35[a]
[1]	FZF	Propane	✓		✓		83	55	34[a]
[6]	JM	NG	✓		✓		80	50	27
[6]	BG	NG		✓	✓		80	50	28
[6]	BG	NG		✓	✓		90	50	31
[6]	BG	NG		✓		✓	100	50	24

[a] Net electricity generation.
[b] Air ratio (cathode): 2.5.
[c] Air ratio (cathode): 2.0 without methanol permeation.

ciencies because there is no energy consumption for fuel processing. As a consequence, a significantly smaller system size and lower costs at comparable power densities may be achievable. In principle, there are two different concepts for using methanol directly. The fuel can be delivered to the fuel-cell in a gaseous or liquid form. The actual power densities of a DMFC are clearly lower than those of a conventional hydrogen-fed polymer electrolyte fuel cell. The main problem is that the electrochemical reaction of methanol is kinetically hindered. In addition, methanol permeates through the electrolyte and oxidizes at the cathode. This results in a mixed potential at the cathode. Furthermore, part of the fuel cannot be used for power generation and the efficiency of the system decreases. Methanol crossover is controlled by cell temperature, fuel molarity and operating current. Recently, numerous investigations have addressed the problem of methanol permeation to find a way to reduce it.

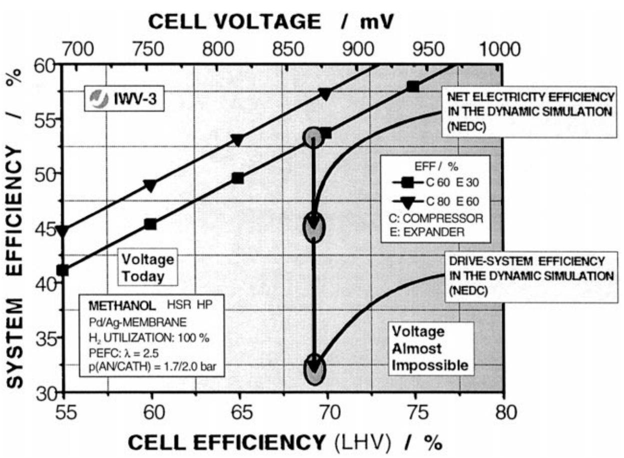

Fig. 2. Process analysis of an indirect methanol fuel cell as well as net and drive-system efficiencies in dynamic simulation (NEDC).

Fig. 3 shows calculated system efficiencies on the basis of thermodynamic engineering calculations for a liquid-fed direct methanol fuel cell system. Using the above-mentioned commercial PRO/II computer program, the fuel cell system can assembled by inserting components for this program in a flow sheet. For the fuel cell itself, in this case the DMFC, it is necessary to develop a special discrete model, which is able to describe the processes taking place in the fuel cell depending on the current/potential characteristics. The simulation model developed enables calculations with and without methanol permeation.

Increasing the cell voltage or fuel cell efficiency generally leads to higher system efficiencies. Calculated system efficiencies greatly depend on the chosen operating conditions. The presented results are based on a stack temperature T_{FC} of 85°C and an operating pressure p_{FC} of 1.75

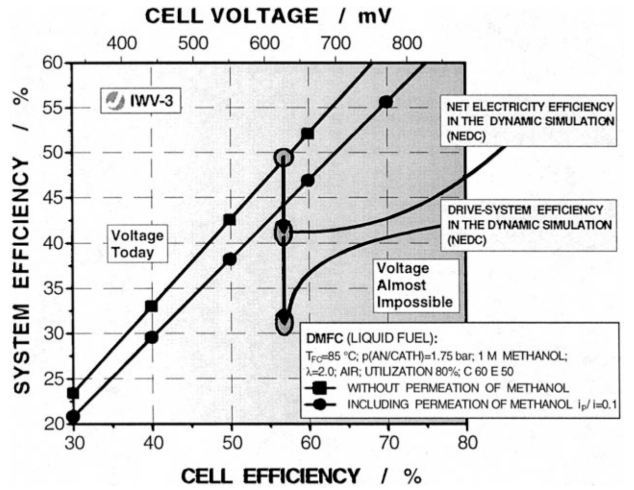

Fig. 3. Process analysis of a direct methanol fuel cell as well as net and drive-system efficiencies in dynamic simulation (NEDC); i_p/i: crossover-density relation.

bar. The concentration is 1 M methanol and the air-to-fuel ratio, $\lambda = 2$. The operating temperature of the catalytic converter is fixed at $T_{cat} = 150°C$. At a fuel cell efficiency of $\eta_{FC} = 50\%$ ($U_{FC} = 550$ mV, related to the lower heating value of liquid methanol (638.5 kJ/mol)), for example, the system efficiency achieves a value of 43% ignoring methanol crossover. The influence of methanol permeation on system efficiency is clearly evident. The crossover density, i_p, is related to the current density, i. The assumption of a value of 0.1 for i_p/i leads to a loss of system efficiency of 5% under the same operating conditions. Typical values for the crossover density, i_p, found in the literature are higher.

For dynamic investigations, a procedure is described for an indirect methanol fuel cell in a following part, for an average fuel cell efficiency of $\eta_{FC} = 0.57$ show the same effects are evident there. The net system efficiency decreases from 50% in the static gunshot calculation to 41%, in the dynamic simulation. The calculated drive-system efficiency in the NEDC attains only values of about 31% (Fig. 3). These results do not consider methanol crossover.

6. Process analysis results

The results derived from process analysis calculations and displayed in Table 1 (FZJ and results from the literature), show the possible efficiencies achievable with the use of different fuels and different means of conversion. On the one hand, they do not include dynamic operation with an electric drive and E-motor and gearbox; on the other hand, they do not consider the technical aspects of the process. Advantages and disadvantages of individual systems for gas production or use of the fuel in combination with a fuel-cell system, have to be determined from experience using a brassboard, a prototype drive or mass-produced vehicles with fuel-cell drives.

In the results displayed for FZJ, losses due to insufficient thermal insulation are neglected. By-products in catalytic reactions are not included in the calculation if poisoning of the anode catalyst is negligible and if there are only traces present. In those cases, the consequences for the respective energy and mass balances are small. These limits mean that, in the present analysis, only determinations of the prospective efficiency for different fuel-cell systems have been carried out.

7. Power-train simulation

With process analysis, it is possible to obtain results, related to the fuel used, which show the total capacity for electricity generation using different systems with fuel cells as the energy converter (Table 1, Figs. 2 and 3). However, these results are valid only in one special state of operation. Then driving a real motor vehicle, there will be permanent changes in the state of operation, which have to correlate with the in respective specific requirements. The demands of one given system will be detected automatically by conducting a standardized driving cycle, for example, in this case, the NEDC (Fig. 4). This cycle is a model for traffic in towns, on roads and on motorways, including acceleration, deceleration and stops. This NEDC allows different vehicle drives to be compared, in this drives of passenger cars.

The Matlab/Simulink simulation software offers a possibility for describing the behaviour of relevant drive components based on their efficiency characteristics and performances. The performance data of a fuel cell system at very low power output largely depends on the energy demand of the peripheral units, which have to operate during the total cycle. Thus, the efficiency of a system with a fuel-cell stack with particularly good cell performance [8] demonstrates its best value after compensating for this energy drain (Fig. 5) at a cell voltage of approximately 700 mV.

In determining the working data for a drive system, the definition of a reference car is very important. In dimen-

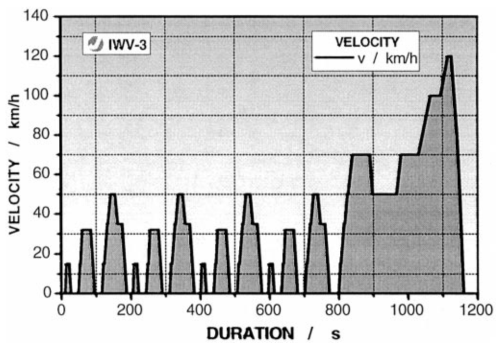

Fig. 4. New European driving cycle (NEDC).

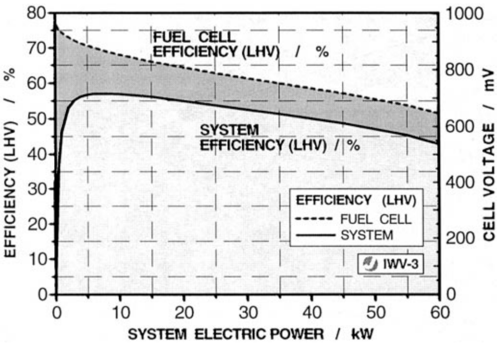

Fig. 5. Net system efficiency at different loads (fuel: hydrogen).

sioning such a motor car, it is necessary to consider the outer parameters of the car as well as drive dynamics, total weight including driver and other loadings such as the fuel tank content. Furthermore, for the determination of the necessary power of the fuel-cell stack, it is important to consider the efficiency of the gear unit, the characteristic of the electric motor and the power less in the cooling blower.

Having, for example, a vehicle with methanol as the fuel, and with steam reforming using HP, it is possible to operate for approximately 80% of the driving cycle with only 5 kW, if the following data of this advanced vehicle can be achieved:

- cross-sectional area, 2 m^2
- drag coefficient, 0.30
- rolling resistance coefficient, 0.008
- total weight, approx. 1200 kg

If the requirements for the vehicle are fixed as

- acceleration from 0 to 100 km/h, 15 s,
- maximum speed, 170 km/h and
- mileage, 500 km

then it is necessary to have a

- mechanical net power at the wheel of, 48 kW

In such a case, an average

- fuel-cell efficiency of approx., 68%

is achievable.

The process analysis, in this case, allows a system efficiency of 53% (Fig. 2). If the peripherals are taken into account, this value would be reduced to approx. 45% net efficiency for electricity generation in the NEDC. During this driving cycle, the efficiency would be decreased even more decreased by the drive train, in particular by the engine and the gear train. In the case described, these derivations lead to an efficiency of approx. 32% at the wheel. This level is valid for an air-compressor efficiency of 60% and an adiabatic efficiency of the expansion turbines of 30%. If it is possible to reduce the parasitic power demand of the peripheral units, the efficiency in the driving cycle would increase accordingly.

8. Overall balances

The balances of FFCs from well to wheel include fuel production and transport to the filling station as well as the use of gasoline for ICEs and methanol or hydrogen for fuel-cell (PEFC) powered drives in passenger cars. These energy and emission balances arise from the KRAKE-FFC (FZJ) calculation model and consider ICE as well as PEFC drives expected for 2005/2010. The calculation includes assumptions for the energy consumption of passenger cars as well as for the specific emissions of ICE. The model then yields the following results: an ICE drive for gasoline from oil with a test drive of 1010 kg and a specific energy consumption at the wheels of 31 MJ/100 km in the NEDC

Table 2
Comparison of FFC: assumption for 2005/2010 (after) KRAKE (FZJ)
Electricity mix of Germany, natural gas mix in Germany, methanol and hydrogen production in Germany

Oil–gasoline ICE	Primary energy (MJ/100 km)	CO (g/100 km)	NO_x (g/100 km)	CH_4 (g/100 km)	VOC (g/100 km)	SO_2 (g/100 km)	PM (g/100 km)	CO_2 (g/100 km)
Gasoline Supply at filling station	18.60	2.5	9.2	14.1	40.5	10.8	2.1	2315
Passenger car. 1010 kg 31 MJ/100 km[a] Emissions: Euro 4	135.80	100	8		10			9780
Balance	154.40	102.5	17.2	14.1	50.5	10.8	2.1	12 095
Natural gas–methanol PEFC								
Methanol supply at filling station	68	6.2	4.7	31	5.1	4.9	0.4	2861
Passenger car. 1153 kg 34 MJ/100 km[a] Emission: FZJ	106	0.1	0.01		0.1		0	7500
Balance	174	6.3	4.7	31	5.1	4.9	0.4	10 361
Natural gas–hydrogen PEFC								
Compressed H_2 supply at filling station	46.9	2.2	4.5	23.6	3.4	3.9	0.3	7390
Passenger car. 1080 kg 33 MJ/100 km[a] Zero Emission	79.8	0	0	0	0	0	0	0
Balance	126.7	2.2	4.5	23.6	3.4	3.9	0.3	7390

[a]At the wheels.

(Table 2, emissions see EURO 4/2005), a PEFC drive for methanol from natural gas with a test drive of 1153 kg and a specific energy consumption at the wheels of 34 MJ/100 km in the NEDC (Table 2) and a PEFC drive for compressed hydrogen from natural gas with a test drive of 1080 kg and a specific energy consumption at the wheels of 33 MJ/100 km in the NEDC (Table 2, zero-emission car). Table 2 shows the results in terms of specific primary energy consumption and specific CO, NO_x, CH_4, NMVOC, SO_2, particle and CO_2 emissions.

In the case of the FFC with an ICE drive, the use of the passenger car contributes considerably to the emission balances, especially for CO, NO_x and CO_2, and also to the energy balance. In the case of the FFC with a PEFC drive and hydrogen or methanol as the fuel, both from natural gas, the dominant contribution to the limited emissions arises from the fuel supply, well-to-filling station. The emission level for passenger cars is zero for hydrogen and near zero for the methanol- powered car with a PEFC power train. For direct comparison of FFCs in terms of specific primary energy consumption and carbon dioxide emissions, and for the chosen boundary conditions, only the PEFC drive based on hydrogen from natural gas can reduce the energy consumption and carbon dioxide emissions compared with the FFC with a gasoline-powered ICE.

9. Conclusions

This comparative study, in terms of energy requirements based on processing analyses and dynamic simulation calculations, yields clear advantages for fuel-cell cars operating on hydrogen even in comparison with the energy demand of a combustion engine (ICE). The assumption of an efficiency rate of 23% for an ICE combustion engine of the future, however, requires a fuel quality that, for the time being, cannot be realized. The comparison also shows that, with on-board reforming, the advantage of fuel-cell cars diminishes particularly if hydrogen is produced from hydrocarbons via autothermal reformers. The same applies to higher weights required for the various units.

While fuel-cell cars operating on hydrogen prove to be zero-emission vehicles, fuel-cell cars operating on methanol offer emission levels considerably lower than the SULEV standard required for CO, NO_x and NMVOC emissions in the American driving cycle and the EURO 4 standard in the European driving cycle. For fuel-cell cars operating on hydrocarbons, this is only partially the case.

In summary, fuel-cell developments for mobile applications are focusing on the following trends and options:

- choosing the ‘‘right’’ fuel,
- proving the feasibility of the new technology, especially in long-time operation,
- achieving the cost reductions necessary from today’s point of view,
- contributing to minimizing energy demand and emissions, and
- implementing the steps necessary to gain access to the market.

The use of hydrogen as a direct fuel for fuel-cell drives appears to be rather a long-term option. Medium-term concepts concentrate on alcohol fuels and gasoline in a competitive situation that, at present, cannot be anticipated. Simpler and more effective fuel-cell drives based on methanol, which require an infrastructure not yet in existence, will compete with more complex fuel-cell drives based on hydrocarbons relying on well-established fuel supply systems, even though present fuel qualities prove insufficient for both fuel-cell drives and advanced combustion engines.

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