

Short communication

## Benchmarking of chemical flowsheeting software in fuel cell applications

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### Abstract

The use of chemical flowsheeting software has become an integral part of the evaluation of the performance of fuel cell systems. There are, however, aspects that have to be kept in mind when comparing the results obtained in different system studies. If care is not taken, the obvious merit of one system over another could later be found to be induced by the software used for the study, more than by a superior systems layout. Some causes of these deviations are discussed based on a comparative system study, which was carried out using three different types of chemical simulation software. It is found that even though there appears to be no differences on an overall level, significant differences are found when examining at a more detailed level. The differences are found to be caused by differing thermodynamic data relating to the steam reforming section of the fuel cell system. Some of the deviations are also believed to be caused by convergence-related issues. © 2001 Elsevier Science B.V. All rights reserved.

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### 1. Introduction

Chemical flowsheeting as a means of performing assessments of chemical process systems has a history that is as old as the concepts of mass and energy balances. At first, the calculations were carried out using only pencil and paper, sometimes assisted by the use of a slide-rule. It comes without saying that the more detailed and complex the system under observation is, the more time-consuming and tedious is the solution of the equations and models necessary to describe the chemical system.

A major change in this methodology was brought about by the introduction of the computer. Now it became much easier and quicker to carry out the calculations needed.

At first the models that were already developed were transferred to the computers as batch-models, where individual models described every unit of a process system, with no interaction between them.

With the evolution of more and more powerful computers, the idea of connecting the different batch models with each

other emerged, thus, allowing model interaction within a simulation. This was the basis for the so-called sequential modular simulators, where data are transferred between the individual models, but they are solved one at a time, in a pre-defined sequence.

The first areas where the computerized flowsheeting techniques were adopted were within the fields of interest of the larger companies within chemical process industries (CPI), who could afford the, at that time, costly computer investments. Today, of course, the development of computers has made it possible to handle these flowsheeting programs on a more or less ordinary desktop computer, making it an everyday tool for most chemical engineers.

It is not at all surprising, therefore, that the fuel cell industry also has adopted the use of flowsheeting as a method for performing system assessments. In many respects, a fuel cell system is nothing but a chemical process plant, combining the fuel cell with many process steps often used in the CPIs.

Many studies have been carried out to predict the performance of fuel cell systems, to mention only a few, those by Malloy, Mäkinen et al. and several EPRI reports [1–7]. These have been carried out either using in-house software

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developed by the fuel cell manufacturers themselves, or by using commercial simulation software available on the market.

When the three authors started discussions about possible co-operation within the area of system studies of molten carbonate fuel cell (MCFC) systems, it was clear that it would be impossible that all three participants should use the same flowsheeting software. This also resulted in recognition of the fact that, if comparisons of future results are to be possible, the tool used in the studies, i.e. the flowsheet simulator, should not introduce differences when using the same input data for a study. If that were to be the case, comparisons would not be worth the effort.

It was this recognition that earlier brought about so-called benchmark calculations in various fields such as nuclear energy [8], CPIs [9] and, later, within electronics industries [10]. The common factor of these works, and others, was to determine a way of comparing software used for different calculation applications, thus, trying to eliminate differences in the results caused by the software itself. As a result of this recognition, it was decided that the parties would carry out a joint benchmark study on a selected MCFC system, thereby establishing possible differences in the simulation results, and the nature of their origin.

The system selected for the study resembles one of the possible system designs considered for the 250 kW natural gas MCFC-system at that time planned to be built by

Netherlands Energy Research Foundation (ECN) and Dutch Fuel Cell Corporation (BCN) [11] by the turn of the century. This layout, which includes external steam reforming of natural gas, was later discarded as being too complicated, resulting in a too costly overall system. A much less complex one involving internal reforming has now replaced it [12]. Within the scope of the present study this is, however, of less importance. Here the main issue is not to establish the best possible system layout, but to clarify whether the use of three different simulation software packages may, or may not, introduce differences into the study results.

The three simulation software packages used for the study were:

- DESIGN-II™ by ChemShare Corp. used by ECN (BCN);
- ASPEN PLUS™ with Model Manager™ used by KTH;
- SPENCE™ by KEMA, used by Vattenfall AB.

## 2. System configuration

The studied system is shown in Fig. 1. It is a 250 kW MCFC plant, which has an external reformer, a heat recovery steam generator and extraction of heat to a district-heating network.

The system has an integrated design showing the following features:

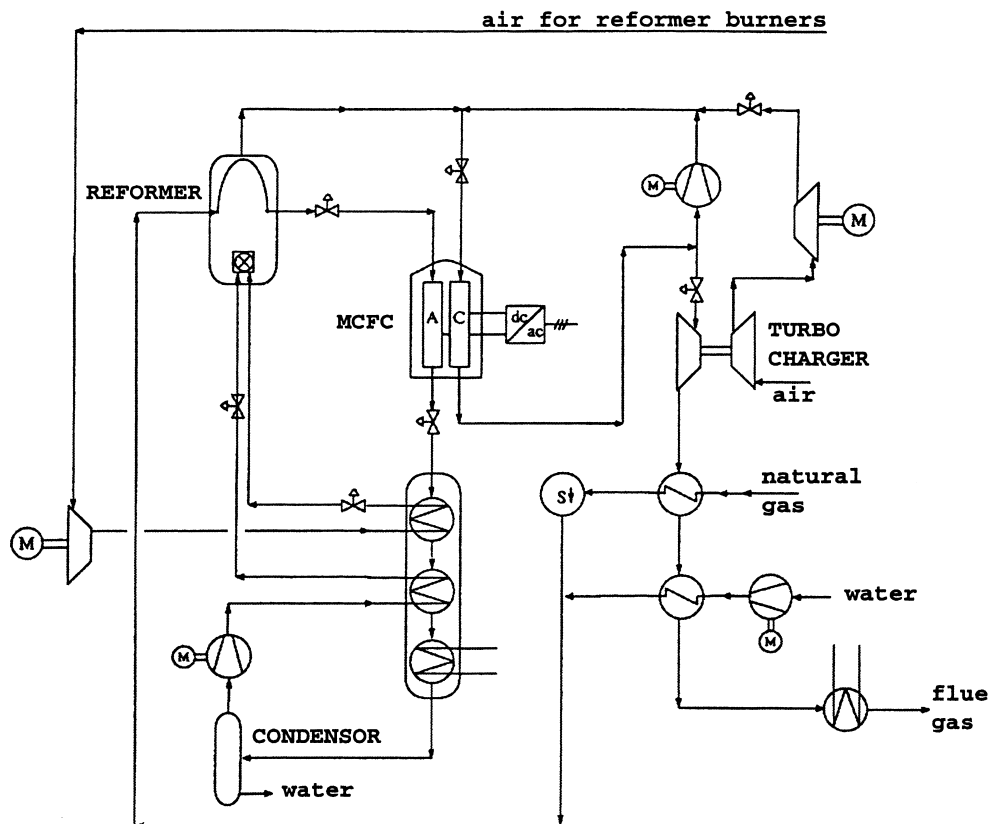


Fig. 1. Schematic flowsheet of the studied 250 kW MCFC co-generation power plant.

- primary fuel used is natural gas,
- CO<sub>2</sub> recycle from anode outlet to cathode inlet, via the reformer burner,
- anode off-gas is used as fuel for the reformer,
- pressurized system, operating at 4 bar at full load,
- steam rejection by condensation from anode off-gas,
- gas cooling, both of anode and cathode off-gases, before the re-circulation blowers.

### 3. Description of main components

Natural gas, after desulphurization, is mixed with steam, which is produced in the heat recovery steam generator. The mixed process gas is fed to the steam reformer, which resembles a heat exchange reformer (HER).

#### 3.1. Reformer

The reformer is modeled to resemble a reformer of the heat exchanger type, as those manufactured by Haldor Topsøe A/S. The layout of their dual stage reformer is shown in Fig. 2.

The only real disadvantage with the Haldor Topsøe reformers is that the fuel used in the reformer burner must

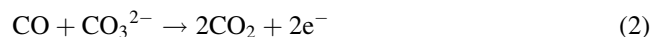
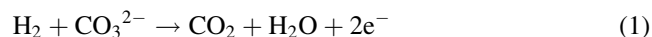
have a high enough heating value to be able to support flame combustion. If this is not the case, the plate type reformer proposed by IHI [14] (Fig. 3), may be considered. Since, this design relies on catalytic combustion of the fuel, the range of heating values allowed for the fuel is much wider, allowing for increased fuel utilization levels and enhanced electrical efficiency.

#### 3.2. Fuel cell

As stated earlier an MCFC stack provides power production with external reforming. The characteristics of the fuel cell are as shown in Table 1.

##### 3.2.1. Fuel cell-anode

At the negative electrode, the anode, the fuel is consumed electrochemically according to reactions (1) and (2).



The fuel component mainly consumed is hydrogen. This is because hydrogen is much more active in electrochemical reactions than carbon monoxide. Since, the anode in an MCFC stack consists of nickel, which is an active catalyst

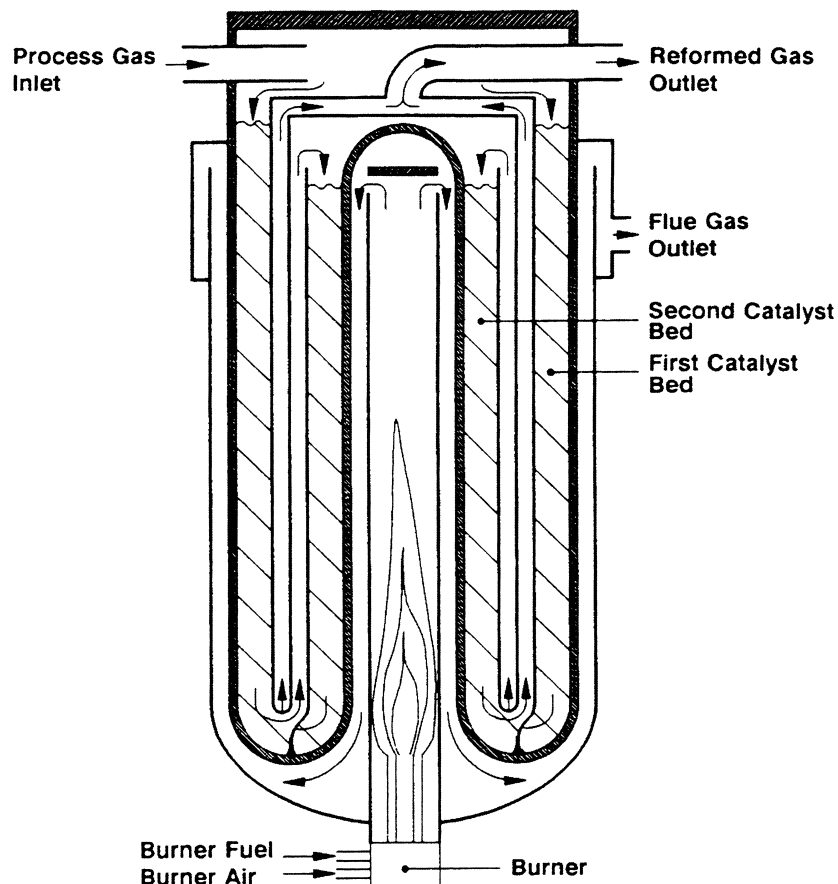


Fig. 2. Schematic drawing of Haldor Topsøe's heat exchange reformer (HER) [13].

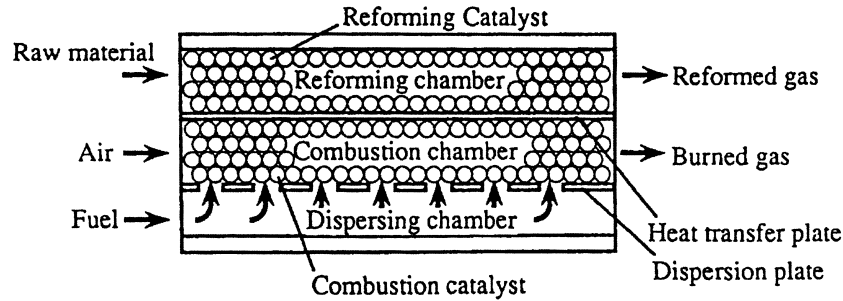


Fig. 3. Plate type reformer proposed by IHI [14].

for the water-gas-shift reaction, most of the carbon monoxide is converted via reaction (3) into hydrogen. The hydrogen is then consumed electrochemically via reaction (1) [15].



### 3.2.2. Anode off-gas recycle loop

Since, the fuel in the anode gas is consumed to more than 70%, the off-gas will contain a large amount of water vapor. Subsequently, the heating value of the anode off-gas has to be increased if it is to be used as a fuel for the heat exchange reformer. This reduction of water content is accomplished by condensing the steam and simultaneously extracting heat for district heating. This also gives the option of recycling the condensed water, thus, providing a system that is self-sufficient in water.

### 3.2.3. Fuel cell-cathode

The feed to the cathode consists of a mixture containing compressed air, exhaust gases from the reformer burners and re-circulated cathode off-gas. The exhaust from the reformer serves as the source of carbon dioxide for the cathode reaction, the air as the oxygen source and the re-circulated cathode gas as a temperature moderator which increases the  $\text{CO}_2$  content and enhances overall oxygen utilization. Waste heat is essentially removed by the oxidant process gas.

### 3.2.4. Heat recovery system

The exhaust gas from the cathode side of the fuel cell is fed to heat recovery steam generators, where steam is produced for the steam reforming process. Other fractions of the exhaust are used for air and natural gas pre-heating.

In addition, heat is, as mentioned above, utilized in a district heating system.

## 4. Simulation models

### 4.1. Fuel cell model

The fuel cell stack is considered to be more or less a black box, which in the simulation models consists of seven different model blocks combined with some FORTRAN in-line programming.

It does not account for details within the cells, i.e. polarization of individual cells or ion transport through the electrolyte matrix. This means that the model (a macro model) is based on fuel utilization and average cell voltage over the cell.

The flow configuration is considered to be co-flow design, where the entering and exiting streams are at temperature equilibrium. This is ensured by heat exchange between the model blocks representing the anode and cathode sides of the fuel cell, combined with cooling via excess cathode gas flow.

Faraday's law, with average cell voltage, fuel utilization and the flow of hydrogen and carbon monoxide entering the anode as inputs, is used to calculate the power production. The cell voltage is predicted using a one-dimensional performance model, and internal losses are accounted for by effective local impedance.

The inlet temperatures of the fuel cell are fixed and by adjusting both re-circulation of cathode off-gas and feed of fresh air, the exit temperature is adjusted to the desired value.

### 4.2. Reformer model

The schematic layout of the simulation model describing the HER is shown in Fig. 4. The heat stream leaving the model symbolizes the heat losses to the surroundings.

#### 4.2.1. The process gas side

The process gas side is simulated by an equilibrium reactor, which is combined with a heater block.

The steam reforming reactions take place in an equilibrium reactor at a constant temperature, the reforming temperature. It is assumed that the reforming reactions, with

Table 1  
Fuel cell characteristics

Parameter	Value
Fuel utilization (%)	75
Fuel cell outlet temperature (°C)	700
Pressurized operation (bar)	4
Average cell voltage (mV)	714
Stack cooling	Cathode gas by recycling
$\text{CO}_2$ -supply	Anode off-gas recycling

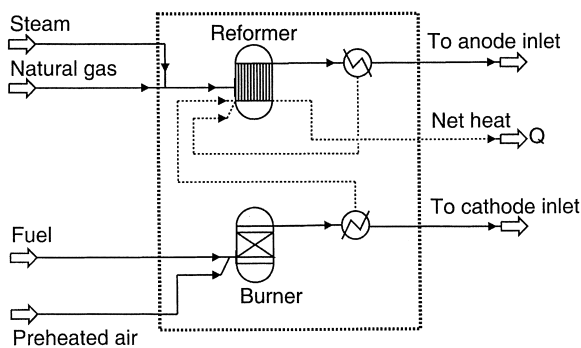
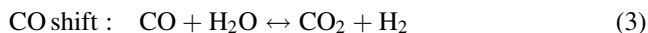
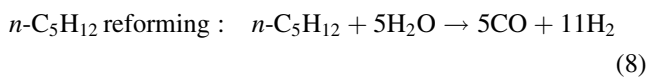
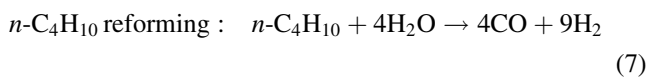
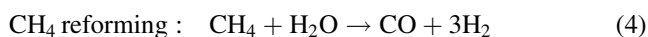


Fig. 4. Layout of the reformer model.

the exception of methane, reach equilibrium. The inability of the methane-reforming reaction to reach equilibrium is accounted for by using a so-called *temperature approach to equilibrium* ( $T_{APP}$ ). This means that the reforming of the higher hydrocarbons is calculated at the reforming temperature, the equilibrium of the methane-reforming reaction is calculated at a temperature deviating from the reforming temperature by a number of degrees Celsius equal to  $T_{APP}$ . Approach temperatures are normally of the magnitude 10–15°C, which means that the equilibrium of the reaction affected is calculated at 10–15°C below the reactor temperature. The magnitude depends on the residence time in the catalyst-bed, steam-to-carbon ratio and catalyst properties.

The following reactions take place in the equilibrium reactor:



All reactions except the water-gas-shift reaction are endothermic, and require the addition of heat. Burning a combustible gas, normally the anode off-gas or natural gas, in the reformer burner produces the heat needed.

#### 4.2.2. Heat exchanger

Since, the reforming temperature and the temperature at which the reformed gas enters the anode compartment of the fuel cell are seldom the same, sensible heat from the reformer product gas can be used for partially heating the reformer, thus, accomplishing also product gas cooling.

#### 4.2.3. The burner side

The burner part of the reformer is modeled as a burner in combination with a heat exchanger. In order to produce the

Table 2  
Steam reforming characteristics

Operation	Pressurized
Steam/carbon ratio	2.5–3.0
Reforming temperature (°C)	815–830
$T_{APP}$ (°C)	–15 for methane
Heat supply	Non-catalytic combustion of anode off-gas

necessary heat for reforming, recycled anode off-gas is used as fuel in the burner. This also leads to an increase in overall system efficiency, eliminating the need for combusting fresh natural gas. One drawback, however, is the need to condense some of the water vapor present in the anode off-gas stream. This separation of water and combustible gas has to be made in order to obtain a gas with a high enough heat content to be burnt in an ordinary burner. If this is not sufficient, reformers applying catalytic combustion may have to be considered. Also, the temperature level is to be sufficiently high, to enable heat transfer towards the reforming process.

In the reformer, the components of the process gas are converted over a nickel-based catalyst according to reactions 3–8.

Since, methane is the dominating hydrocarbon, and its steam reforming is strongly endothermic, the overall heat of reaction will be endothermic, which means that heat must be added in order to keep the reaction going.

Other characteristics of the steam reforming process are shown in Table 2.

## 5. Input data

The input data for the different components (e.g. blower efficiency and fuel cell data) of the system and natural gas composition and flow were supplied by ECN, and are summarized in Tables 3 and 4. Hydrocarbons higher than propane are not included in Table 4, even though the natural gas used in The Netherlands does contain higher alkanes. Nevertheless, their quantities are so small that their influence has not been taken into account.

Table 3  
Input data used in simulations

Equipment	Parameter	Value
Reformer	Temperature (°C)	815
Fuel cell	Cell voltage (mV)	714
	Pressure (bar)	4
	Outlet temperature (°C)	700
Expander	Isentropic efficiency (%)	75
Air blowers	Isentropic efficiency (%)	72
Anode blower	Isentropic efficiency (%)	72
Cathode blower	Isentropic efficiency (%)	72
	Inlet gas temperature (°C)	475
Steam	Temperature (°C)	450

Table 4  
Natural gas composition

Component	%
CH <sub>4</sub>	81.3
C <sub>2</sub> H <sub>6</sub>	2.7
C <sub>3</sub> H <sub>8</sub>	0.4
N <sub>2</sub>	14.5
CO <sub>2</sub>	1.1

## 6. Results

The results of the simulations carried out using the software packages selected for this study appear to be similar at a first glance. This is, however, only true when looking at the overall results concerning total power output or heat generated. At a more detailed level, differences do exist.

In the following sections, we will point out some of these dissimilarities, as well as give an explanation of their origin. The present study is concerned with the question of whether or not differences in the physical data sources could explain the obtained differences.

As discussed above, the reformer can be divided into two sides: the process gas side where the natural gas/steam mixture is reformed and the burner side where anode off-gas is burned with air. Table 5 shows the simulation results for the mixture of natural gas and steam that is fed to the reformer, as well as the gas mixture exiting the reformer after processing.

The deviations in the results are very small, less than 0.5%, except for the methane where the deviations are about 5%. It might be objected that the deviation of the individual methane flow is too small to have any significance. But when doing so, it has to keep in mind that the tolerance for convergence of individual mole flows is 0.0001, which is considerably smaller than the 0.0018 mol/s difference observed between the methane flows. The deviation is not

caused by some difference in the method for equilibrium calculation. Aspen Plus<sup>TM</sup>, Design-II<sup>TM</sup> and Spence<sup>TM</sup> all use an approach based on the minimization of Gibbs free energy to calculate the equilibrium compositions. A reasonable explanation for the deviation in compositions is that the different software packages have different thermodynamical data in their data banks. When the different data bank values are used for equilibrium calculation they cause the difference in composition. In the calculations it is assumed that the reactions take place within the catalyst-bed only, and no further equilibration takes place during the cooling of the gas which has exited the catalyst bed.

When looking at the results for the burner side (Table 6), the difference in temperature of the outlet gases from the reformer is due to less heat needed for the reforming in the Aspen Plus<sup>TM</sup> and Spence<sup>TM</sup> simulations than in the Design-II<sup>TM</sup> case. The cause of this difference is that in the Design-II<sup>TM</sup> case, the heat needed for reforming is calculated as if the produced carbon monoxide is of methane origin only, i.e. the hydrocarbon mixture that is reformed is considered to contain only methane. Since, the reforming reaction is more endothermic for methane than for the higher hydrocarbons, this error results in a higher heat demand than actually necessary.

The composition of the anode off-gas that is fed to the burner varies somewhat between the three software packages.

A difference is the oxygen content of the burner outlet streams, which is slightly lower in the Aspen Plus<sup>TM</sup> and Spence<sup>TM</sup> results. This may most likely be attributed to the difference in reformer methane conversion discussed earlier. The process gas is fed to the anode of the fuel cell, and later the remaining combustibles are fed to the reformer burners. Since methane is inert in the fuel cell reactions, the methane remaining after the reformer will eventually end up in the reformer burners, where it will consume extra oxygen, thereby causing a higher oxygen consumption in the Aspen Plus<sup>TM</sup> and Spence<sup>TM</sup> cases.

Table 5  
Reformer-process gas side

	Inlet			Outlet		
	Aspen Plus	Design-II	Spence	Aspen Plus	Design-II	Spence
Gas composition (mol/s)						
Hydrogen	0.0000	0.0000	0.0000	2.2304	2.2376	2.2400
Methane	0.6707	0.6707	0.6707	0.0361	0.0343	0.0361
Ethane	0.0223	0.0223	0.0223	0.0000	0.0000	0.0000
Propane	0.0033	0.0033	0.0033	0.0000	0.0000	0.0000
Nitrogen	0.1196	0.1196	0.1196	0.1196	0.1196	0.1196
Oxygen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Carbon monoxide	0.0000	0.0000	0.0000	0.4971	0.4972	0.4875
Carbon dioxide	0.0091	0.0091	0.0091	0.2011	0.2028	0.2107
Water	1.8129	1.8129	1.8128	0.9318	0.9283	0.9221
Mole flow (mol/s)	2.6379	2.6379	2.6378	4.0161	4.0197	4.0160
Mass flow (g/s)	47.9868	47.9862	47.9862	47.9868	47.9863	47.9862
Temperature (°C)	449.6241	449.0780	450.00	600.0000	600.0000	600.00
Pressure (bar)	4.5000	4.5000	4.5000	4.0000	4.0000	4.0000
Molar weight (g/mol)	18.1913	18.1911	18.19	11.9486	11.9377	11.95

Table 6  
Reformer–burner side

	Inlet			Outlet		
	Aspen Plus	Design-II	Spence	Aspen Plus	Design-II	Spence
Gas composition (mol/s)						
Hydrogen	0.4262	0.4295	0.4375	0.0000	0.0000	0.0000
Methane	0.0361	0.0343	0.0361	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nitrogen	1.7964	1.7964	1.7963	1.7964	1.7964	1.7963
Oxygen	0.4514	0.4514	0.4514	0.0383	0.0411	0.0383
Carbon monoxide	0.2556	0.2542	0.2443	0.0001	0.0001	0.0000
Carbon dioxide	2.4880	2.4958	2.4995	2.7796	2.7841	2.7799
Water	0.4858	0.4899	0.5050	0.9842	0.9879	1.0147
Mole flow (mol/s)	5.9396	5.9515	5.9701	5.5987	5.6097	5.6291
Mass flow (g/s)	191.6159	191.9702	192.1759	191.6159	191.9705	192.1759
Temperature (°C)	462.1378	462.0980	459.40	639.6795	627.6786	635.80
Pressure (bar)	4.3500	4.3500	4.3500	4.1000	4.1000	4.100
Molar weight (g/mol)	32.2607	32.2557	32.19	34.2248	34.2209	34.14

Also, less methane is available for combustion for Design-II<sup>TM</sup>, than for the other simulation packages, thus, resulting in a slightly lower burner outlet temperature.

### 6.1. Fuel cell

The interesting streams for the fuel cell are its inlet and outlet streams, while the intermediate streams are of minor concern.

As seen in Table 7, somewhat less hydrogen enters the fuel cell for Aspen Plus<sup>TM</sup> and Design-II<sup>TM</sup> than for Spence<sup>TM</sup>. This is probably because of the different software packages having different thermodynamical data, as discussed earlier. Since methane is inert to the anode reactions, there is a higher methane flow in the anode outlet stream as calculated by Aspen Plus<sup>TM</sup>, and Spence<sup>TM</sup> than for Design-II<sup>TM</sup>.

When comparing the carbon dioxide flows at the anode outlet (Table 7), and the burner inlet (Table 6), it can be noted that the amount of carbon dioxide entering the burner is different from the carbon dioxide leaving the anode. This is because some of the carbon dioxide leaving the anode is dissolved in the water removed in the water knock-out drum, thus, being withdrawn from the gas stream fed to the reformer burner (Table 8).

As can be noted, somewhat less oxygen enters the cathode side for Spence<sup>TM</sup> than for Aspen Plus<sup>TM</sup> and Design-II<sup>TM</sup>. The first conclusion that could be drawn, is that less air is fed to the system in the Spence<sup>TM</sup> calculations, than in the other two simulation packages. This is, however, contradicted by the fact that the amount of nitrogen entering the cathode is higher for Spence<sup>TM</sup> than for Aspen Plus<sup>TM</sup> and Design-II<sup>TM</sup>. This fact, together with the use of equal inlet

Table 7  
Fuel cell–anode side

	Inlet			Outlet		
	Aspen Plus	Design-II	Spence	Aspen Plus	Design-II	Spence
Gas composition (mol/s)						
Hydrogen	2.2304	2.2376	2.2400	0.4262	0.4295	0.4375
Methane	0.0361	0.0343	0.0361	0.0361	0.0343	0.0361
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nitrogen	0.1196	0.1196	0.1196	0.1196	0.1196	0.1196
Oxygen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Carbon monoxide	0.4971	0.4972	0.4875	0.2556	0.2542	0.2443
Carbon dioxide	0.2011	0.2028	0.2107	2.4882	2.4969	2.4995
Water	0.9318	0.9283	0.9221	2.7360	2.7364	2.7246
Mole flow (mol/s)	4.0161	4.0197	4.0160	6.0617	6.0708	6.0616
Mass flow (g/s)	47.9868	47.9863	47.9862	170.7419	171.0706	170.7470
Temperature (°C)	600.0000	600.0000	600.00	699.6357	699.6359	700.00
Pressure (bar)	4.0000	4.0000	4.0000	3.8500	3.8500	3.85
Molar weight (g/mol)	11.9486	11.9377	11.95	28.1674	28.1792	28.17

Table 8  
Fuel cell-cathode side

	Inlet			Outlet		
	Aspen Plus	Design-II	Spence	Aspen Plus	Design-II	Spence
Gas composition (mol/s)						
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nitrogen	37.6008	37.6008	38.5437	37.6008	37.6008	38.5437
Oxygen	8.2099	8.2127	6.2684	7.1871	7.1872	5.2456
Carbon monoxide	0.0003	0.0002	0.0000	0.0003	0.0002	0.0000
Carbon dioxide	3.5137	3.5172	3.3799	1.4680	1.4661	1.3343
Water	2.4045	2.4119	4.7488	2.4045	2.4119	4.7488
Mole flow (mol/s)	51.7291	51.7428	52.9409	48.6670	48.6662	49.8724
Mass flow (g/s)	1513.9950	1514.3707	1514.7381	1391.2440	1391.2867	1391.9772
Temperature (°C)	575.0579	575.4371	580.90	700.0000	700.0000	700.00
Pressure (bar)	4.0000	4.0000	4.0000	3.7500	3.7500	3.7500
Molar weight (g/mol)	29.2678	29.2673	28.61	28.5906	28.5884	27.91

information for the three simulation packages, makes the differences most likely attributable to differences in convergence algorithms and initial values used for convergence. This is also believed to be the explanation for both the higher amounts of water entering the cathode in the Spence<sup>TM</sup> case as well as for the higher inlet temperature to the cathode. Both these variables would be influenced by a difference in convergence. Our belief that the differences between Aspen Plus<sup>TM</sup>, Design-II<sup>TM</sup> and Spence<sup>TM</sup> are convergence-related is also supported by the fact that for the Spence<sup>TM</sup> simulation, the initial guess for the cathode inlet temperature is indeed the same as the cathode inlet temperature obtained in the converged Aspen Plus<sup>TM</sup> and Design-II<sup>TM</sup> calculations.

Another significant difference between the three results for the cathode side occurs in the flows of carbon monoxide. The reason for this divergence may be a slightly different composition resulting from the reformer burner.

## 6.2. Rotating equipment

All rotating equipment has ready-made modules in the three simulation packages. Table 9 shows that all three software packages give comparable results, with a consider-

ably large deviation (5%) for the power produced by the expander unit. This rather large deviation could be explained by the fact that the water vapor content and flow of the stream entering the expander as calculated by Spence<sup>TM</sup> is almost twice of that calculated by Aspen Plus<sup>TM</sup> and Design-II<sup>TM</sup>.

It is also important to note that the outlet temperature of the cathode blower deviates by 2.3% for Spence<sup>TM</sup> compared to the other two. A similar deviation in water content and flow is also observed in the stream entering the cathode recycle blower. Both these deviations may well have their origin in the convergence issues already mentioned in the discussion regarding fuel cell results.

## 6.3. Power output and auxiliary power consumption

As shown in Table 10, the results differ only slightly between Aspen Plus<sup>TM</sup> and Design-II<sup>TM</sup> when it comes to produced power, whereas the results obtained by Spence<sup>TM</sup> are about 2% higher. When looking at the system efficiency, the results of Aspen Plus<sup>TM</sup> and Spence<sup>TM</sup> are close, with the Design-II<sup>TM</sup> results some 5% lower.

Table 9  
Results for rotation equipment

Equipment	Power (kW)			Temperature out (°C)		
	Aspen Plus	Design-II	Spence	Aspen Plus	Design-II	Spence
Burner compressor	-13.63	-13.62	-13.62	239.28	238.37	238.60
Cathode compressor	-130.24	-130.15	-130.20	227.09	226.27	226.50
Burner blower	-3.34	-3.34	-3.40	102.92	104.04	104.00
Cathode blower	-24.88	-24.85	-26.47	506.85	506.92	519.90
Cathode expander	156.28	156.00	163.77	507.59	506.8	508.7
Net work	-15.81	-15.96	-9.92			



Table 10  
Overall simulation results

		Aspen Plus	Design-II	Spence
Gross power output ac (kW)		424	424	432
Fuel cell	dc	282	282	282
	ac	268	268	268
Expander		156	156	164
Auxiliary power (kW)		172	172	173
Air compressor for reformer burners		14	14	14
Air compressor for fuel cell cathode		130	130	130
Blower for anode off-gas compression		3	3	3
Cathode re-circulation blower		25	25	26
Net power output (kW)		252	252	258
Heat		266	242	270
O <sub>2</sub> -utilization (%)		12.55	12.5	16.3
CO <sub>2</sub> -utilization (%)		58.5	58.3	60.5
Power efficiency (%)	HHV	39.4	39.40	40.3
	LHV	43.7	43.68	44.7
System efficiency (%)	LHV	89.8	85.6	91.5

## 7. Discussion

As noted earlier, some deviations do exist between the results obtained with the different simulation packages.

When looking at the results on a stream level, it can be noted that a 5% deviation exists for the methane flow exiting the reformer, the results obtained by Design-II<sup>TM</sup> being lower than the flows obtained by Aspen Plus<sup>TM</sup> and Spence<sup>TM</sup>. One might object that since the difference in methane flow between the results generated by Aspen Plus<sup>TM</sup> and Design-II<sup>TM</sup> is only 0.0018 mol/s, this should be neglected. However, when considering the fact that the convergence limit of the programs are 0.0001 mol/s, i.e. 18 times smaller than the flow difference, the reason for neglecting this difference may not be quite as valid.

The original difference in methane flow from the reformer is then transmitted throughout the whole system, first as an inert through the anodes and from there via the reformer burners transferring the disturbance to the cathode side of the system.

This disturbance may also be expected to influence the performance of various types of hardware within the system.

One hypothesis that was put forward to explain the difference in component flows in the system was that they were caused by differences in the parameter values stored in the physical property data banks of the different process simulators. Since the first deviations in flows were noted downstream from the reformer model, it was also expected that the differences in physical data might be centred in the reformer model blocks, i.e. in the data used for methane steam-reforming equilibrium calculations.

With this at hand, the obvious choice was to investigate how an alteration of the  $T_{APP}$  value would influence the methane conversion.

A comparison between the data obtained by Design-II<sup>TM</sup> and Aspen Plus<sup>TM</sup> showed that if the  $T_{APP}$  value used in Aspen Plus<sup>TM</sup> was altered by 2.54°C, i.e. from –15 to

–12.46°C, almost identical results were obtained when comparing the Design-II<sup>TM</sup> and Aspen Plus<sup>TM</sup> gas component flows.

As a further investigation to find out whether the deviations could have their origin in differences in the thermodynamical data, the heat consumption of the reformer model in Design-II<sup>TM</sup> and Aspen Plus<sup>TM</sup> were compared at the same methane conversion. This means that the  $T_{APP}$  used in Aspen Plus<sup>TM</sup> was again adjusted from –15 to –12.46°C. If there would still be a deviation in the heat needed to run the reactions, it could be taken as an indication of differences in the thermodynamical data. When running the simulation, an almost negligible difference in heat consumption of the reformer was observed, thus, giving no indication of whether the basis for differences is caused by different thermodynamical data or not. As a further investigation, the enthalpy and entropy of the streams leaving the reformer were compared, and it was found that the enthalpy values differ by 1.8%, the entropy values associated with the streams exiting the reformer differ by almost 5.9%. This indicates that the difference in equilibrium composition is indeed caused by a difference in the entropy values stored within the physical property data banks of the different software.

Several other reasons for the deviations were also considered. If the mathematical equations describing primarily the equilibrium model of the reformer were to differ, this would influence the conversion of methane through the steam reforming reaction, and thus, influence the exit flow of methane. Since calculation of equilibrium compositions via minimization of Gibbs free energy is considered a standard operation, the only way the equilibrium reactor itself could influence the outcome would be by differing thermodynamical data influencing the energy minimization.

The numerical methods used for calculations and convergence issues might be another source of deviations. If this were the case, we feel that the deviations would not be located to one source, i.e. the reformer, but more evenly

distributed throughout the system, as was noticed for some of the deviations observed for Spence™ regarding the cathode, cathode blower and the expander.

If the descriptions of the unit operation models comprising the overall simulation model differ, it is obvious that this would influence the results. Since all of the equipment except the fuel cell can be considered to be well known and standard, the only possible difference would be in the description of the fuel cell itself. In order to eliminate this risk, the fuel cell was described in the same way in all three studies. Generally, when comparing the calculated merits of different fuel cell systems, the possibility of differing descriptions of the fuel cell itself, and the possible influence on the overall results is an important aspect to take into consideration.

The final source considered possible as an explanation for differences was the use of different sets of equations of state. It is clear to anyone involved with flowsheeting that one of the larger risks of generating “non-realistic results” is the selection of a set of equations of state that is not suitable for the chemical system studied. This is also a risk when comparing results, if the different calculations have been carried out with different equations of state. Even though it was originally our intention to use the same set of equations of state, it was later noticed that the simulations based on the Spence™ software had been carried out with another set of equations of state. Hence, most of the discussion regarding the differences in results has only been considering variations between Aspen Plus™ and Design-II™, somewhat de-emphasising the Spence™ results.

## 8. Conclusions

The dissimilarities present in the thermodynamical data in the physical properties data banks used by the three simulators constitute one explanation of differing results.

The production of heat and electricity shows only small differences between the simulators.

Compositions of some of the material streams differ significantly, but do not influence the overall result to any great extent.

When selecting software for system studies, transparency of data bank values may be as important an issue as those related to the economics of the selected software.

If the results of system studies obtained from different actors in the fuel cell field are to be compared, a thorough comparison should take the following into account before drawing any conclusions concerning different results:

- Has the same simulation software been used? If not, how transparent are the different software packages regarding factors such as thermodynamic data, unit operation models, equations of state used and the fuel cell model used.
- If these transparency criteria are not met, additional calculations on the different systems to be compared,

using the same simulation package, should be made, thereby eliminating “software-related” differences.

- There is an obvious need for validation of commercial process simulators, since otherwise differences in the calculated results between different software packages can be more a result of differences in the software packages themselves, than of differences related to the real process studied.

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