



# Development of an ejector for passive hydrogen recirculation in PEM fuel cell systems by applying 2D CFD simulation

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## Abstract

The anode subsystem is a major energy consumer of polymer-electrolyte-membrane (PEM) fuel cell systems. A passive hydrogen recirculation system, like an ejector, is an excellent solution to maximize hydrogen utilization while maintaining low parasitic losses. However, high development efforts are necessary to maximize the performance of the ejector for the entire operating range. This research paper provides part of a toolchain for ejector development, consisting in particular of a multi-parameter simulation based on rotational symmetric 2D CFD. The 2D CFD greatly helps optimize the design of the ejector, reducing development effort, and increasing accuracy. In addition, the main correlations between thermodynamic states and geometry on the entrainment ratio are evaluated. Subsequently, an ejector is designed for a PEM fuel cell application using 2D CFD and the results show in which operating range a single ejector can be applied. This toolchain enables rapid design and optimization of ejector geometry, saving development time and cost while increasing accuracy and extending the operating range.

**Keywords** PEM fuel cell · Passive anode hydrogen recirculation · Ejector development toolchain · Rotational symmetric 2D CFD · Multi-parameter simulation · Design of experiment DoE

## List of symbols

### Latin letters

$A_i$	Area at position $i$ [m <sup>2</sup> ]
$c_i$	Velocity of mass flow $i$ [m/s]
$c_p$	Specific heat capacity [J/(kg K)]
$d_i$	Diameter of $i$ [mm]
$F$	Faraday's constant = 96,485 [As/mol]
$I$	Fuel cell current [A]
$k$	Kilo = 10 <sup>3</sup> [–]
$l_i$	Length of $i$ [mm]
$M$	Mach number [–]
$M_i$	Molar mass of species $i$ [g/mol]
$N$	Number of cells [–]
$\dot{m}_i$	Mass flow at position $i$ [g/s]
$p_i$	Pressure at position $i$ [Pa]

$R_i$	Gas constant for gas $i$ [kJ/kg K]
$T_i$	Temperature at position $i$ [K]
$z$	Valency, number of electrons per mol in reaction [–]

### Greek letters

$\Delta$	Difference
$\theta$	Angle of diffuser [°]
$\kappa$	Isentropic exponent [–]
$\lambda$	Hydrogen stoichiometric ratio [–]
$\mu_i$	Mass fraction of species $i$ [–]
$\rho_i$	Density at position $i$ [kg/m <sup>3</sup> ]
$\psi_{\max}$	Flow coefficient at critical condition [–]
$\omega$	Entrainment ratio [–]

### Subscripts and superscripts

avg	Average
b	Back
crit	Critical
d	Discharge
diff	Diffuser
eje	Ejector
in	Inlet
FC	Fuel cell
H <sub>2</sub>	Hydrogen

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max	Maximum
min	Minimum
mix	Mixing chamber; mixing
out	Outlet
prim	Primary
sec	Secondary
<i>t</i>	Nozzle throat@@

### Abbreviations

1D, 2D, 3D	One, two and three spatial dimensions
BoP	Balance of plant
CFN	Critical flow nozzle
DoE	Design of experiments
FC	Fuel cell
MEA	Membrane electrode assembly
NXP	Nozzle exit position
OCV	Open-circuit voltage
PEM	Polymer electrolyte membrane or proton exchange membrane
PFSA	Perfluorosulfonic acid
Re	Reynolds number
SIM	Simulation
TS	Timeshare

## 1 Introduction

Greenhouse gases are present in the Earth's atmosphere and trap heat from the sun, increasing the Earth's surface temperature. The amount of greenhouse gases in the atmosphere has increased as a result of human activities like the burning of fossil fuels and deforestation. Using hydrogen as a fuel is one major way to reduce greenhouse gas emissions [1]. PEM electrolysis, a process that uses electricity to convert water into hydrogen and oxygen, can be used to produce hydrogen. When electrolysis is performed with renewable energy, hydrogen can be used as a clean and effective fuel. One application of using hydrogen is by converting the hydrogen back to electricity in PEM fuel cell systems [2]. Since only water is produced when hydrogen is used in fuel cells, it is a cleaner energy source than fossil fuels and can help solve the climate crisis. PEM fuel cell applications in mobility made great development progress in recent years through improvements at the system, subsystem, and component levels [3–16]. However, further improvements are necessary for increasing the attractiveness of fuel cell electric vehicles and stationary applications by reducing development time and costs.

The main component of a PEM fuel cell system is the fuel cell stack which consists of several cells. As the hydrogen is consumed at the active area in the PEM fuel cell, the hydrogen partial pressure at the anode decreases, resulting in a lower hydrogen availability at the anode flow field outlet.

Therefore, more hydrogen needs to be supplied than the fuel cell uses to guarantee that the complete active area receives sufficient hydrogen and maintains a high fuel cell voltage. However, excessive hydrogen needs to be recirculated to maximize hydrogen utilization. The recirculation can either be carried out actively by means of a hydrogen blower or passively by means of an ejector.

The ejector performance highly depends on the geometry and the operating conditions at inlets and outlets. Based on previous work [17], a further toolchain method can be introduced for maximizing performance and accelerating the development of ejectors in PEM fuel cell applications. The development toolchain can be extended by a 2D CFD simulation, in which the ejector flow field is optimized by a rotational symmetric model and design of experiment (DoE) approach (Fig. 1). The main advantage of 2D CFD is that the ejector performance can be predicted faster due to the low computational cost. Moreover, by applying a suitable automated DoE method, a high number of simulation runs can be performed, and the accuracy of the result can be optimized by selecting a suitable cell size.

A preliminary simulation analysis of the ejector has been mainly conducted via the following two simulation strategies:

- Modeling of the ejector by a zero- (0D) or a one-dimensional (1D) simulation model [18–21].
- Application of a commercially available CFD software for two-dimensional (2D) or three-dimensional (3D) simulations.

The difference between the 0D, 1D, 2D, or 3D simulation is the discretization in space. The lower the degree of freedom, the lower the complexity and typically less computational effort is necessary. However, for complex ejector flow field analyses with geometric influences, a 2D CFD model provides more details compared to a 1D model. A 3D CFD

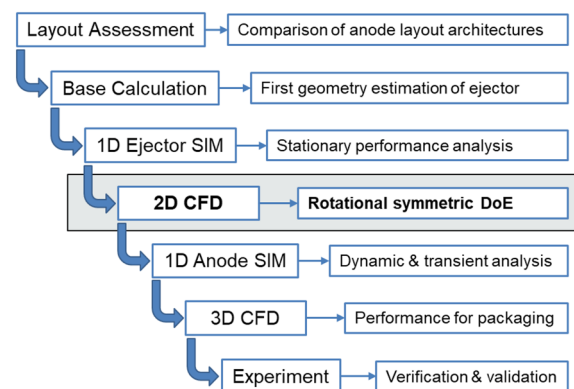
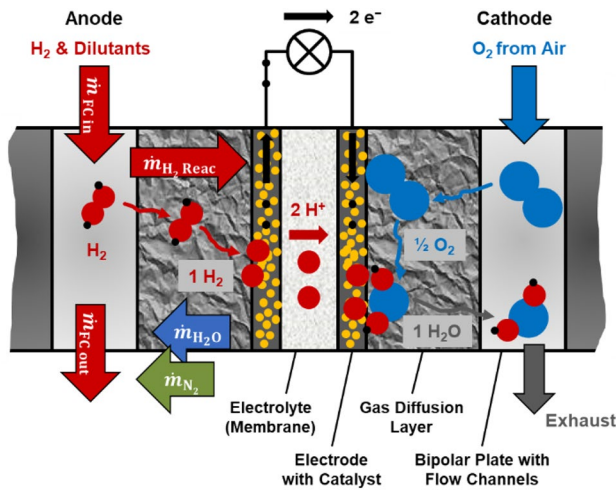


Fig. 1 Toolchain: methods and results ([17], adapted)

**Table 1** Applied 2D and 3D CFD turbulence models for PEM fuel cell applications

Turbulence model	Source
$k$ - $\epsilon$ standard, RNG, or realizable	[23–26]
$k$ - $\omega$ SST	[22, 27–30]

**Fig. 2** Schematic PEM fuel cell (adapted [2])

model provides even more details regarding non-rotational symmetric influences, such as inlet and outlet piping, but the 2D CFD has less computational costs. For example, considering only the rotational symmetric part, if the 3D CFD simulation has 1 cell per degree angle, the 3D CFD model has a 360 times larger mesh than the 2D CFD model, which significantly increases the simulation time.

Table 1 states the most common applied turbulence models for 2D and 3D CFD simulation in the literature for ejectors in PEM fuel cell applications. Large-Eddy simulations are not considered for supersonic ejectors due to the high Reynolds numbers [22].

Before the 2D CFD simulation methodology for a rotational symmetric ejector model is presented in this work, the general boundary conditions of a fuel cell stack have to be analyzed.

### 1.1 PEM fuel cell

The fuel cell consists of the membrane electrode assembly (MEA) which characterizes the electrochemical performance and the bipolar plates which are responsible for the hydrogen and oxygen supply (Fig. 2). The MEA contains the membrane, the catalyst layer on a carbon support layer, and the gas diffusion layer (GDL).

The membrane typically consists of PFSA ionomer (per-fluorosulfonic acid). The membrane has a water uptake capability that enables proton conductivity. The membrane resistance is therefore dependent on the humidity of the membrane and also on its thickness, whereas the membrane thickness greatly influences its mechanical stability [31–33].

The electrodes are highly porous, enabling the delivery of hydrogen and air, electrically conductive, and are in contact with the membrane material. The interface of reactant gas, proton conductive material, and electrically conductive reaction catalyst creates the triple-phase boundary, where the electrochemical reactions take place at the catalyst surface. At the anode, hydrogen is reduced to protons, that pass the membrane to the anode. The dominant proton transport mechanism in sulfonated PFSA membranes is a fast proton hopping from one hydronium ion to the next, described as Grotthuß diffusion [34–36]. At the cathode, the protons are consumed by the formation of water with reduced oxygen. Due to the electrically isolating membrane, the electrons produced at the anode are forced to flow through a circuit, producing an electric current, and subsequently to the cathode, enabling the reduction of oxygen [37, 38].

The bipolar plate provides the required hydrogen or oxygen flow (air) channels and is the main component responsible for the total height of a fuel cell stack. The design and height of the flow channels have a great influence on the media distribution and the pressure drop in the flow field. The gas diffusion layer (GDL) provides an even distribution of flow reactants to the triple-phase boundary layer [39–43].

The hydrogen pressure loss across the inlet and outlet of the bipolar plate is critical for the ejector performance. One fuel cell produces only a limited power output based on the maximum current density and the active area. Therefore, fuel cells are stacked to increase the total power output [44].

### 1.2 Hydrogen supply

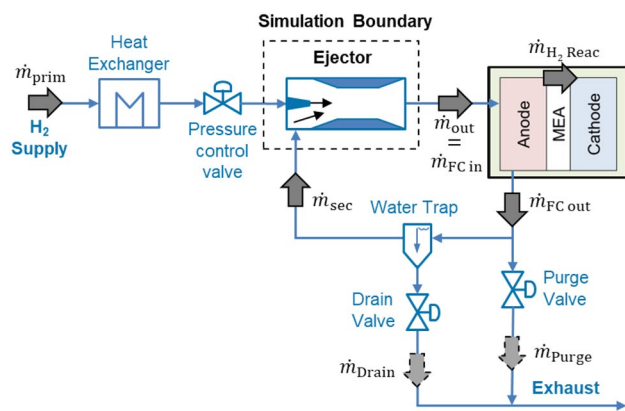
Hydrogen and humidity, as well as impurities, are supplied by the anode inlet ( $\dot{m}_{FC\ in}$ , Fig. 2). As the hydrogen gas flows over the anode, the hydrogen passes through the gas diffusion layer and reacts at the triple-phase boundary ( $\dot{m}_{H_2\ React}$ ).

The theoretical hydrogen consumption by water formation  $m$  of a PEM fuel cell is calculated by Faradays law ( $\dot{m}_{H_2\ React}$ , Eq. 1).  $m$  is directly proportional to the current  $I$  and the numbers of cells  $N$ . Since oxygen is reduced from oxidation state 0 to  $-II$ , the valency  $z$  is 2 (Fig. 3).

Equation 1: Faraday's law [45]

$$\dot{m}_{H_2\ React} = \frac{I \cdot M_{H_2} \cdot N}{z \cdot F} \quad (1)$$

In practice, more hydrogen than the theoretical amount consumed by the reaction is supplied to the fuel cell stack



**Fig. 3** Ejector simulation boundary (adapted [17])

to strictly avoid fuel starvation at the anode catalyst caused by diffusion limitation, delay in hydrogen delivery, pinholes, and competing reactions consuming hydrogen. The ratio between available hydrogen and reacted hydrogen is the stoichiometric ratio  $\lambda$ .

Equation 2: Hydrogen stoichiometric ratio

$$\lambda = \frac{\dot{m}_{\text{H}_2 \text{ FC in}}}{\dot{m}_{\text{H}_2 \text{ Reac}}} \quad (2)$$

The higher stoichiometric ratio means that not all of the hydrogen provided is utilized in the fuel cell. Recirculation is required to recover the excess hydrogen and minimize hydrogen losses.

Dead-end mode operation does not recirculate hydrogen and is not considered in this work because of the higher hydrogen consumption, lower cell voltages, and higher degradation rates compared to recirculation systems [46, 47].

Due to the thin membrane and concentration differences, water back diffusion ( $\dot{m}_{\text{H}_2\text{O}}$ ) and nitrogen crossover ( $\dot{m}_{\text{N}_2}$ ) accumulate and reduce the hydrogen concentration in the fuel cell due to hydrogen recirculation. Therefore, a purge cycle for removing the nitrogen (and gaseous water) is necessary after a certain period to increase the hydrogen concentration and prevent a voltage drop or fuel starvation. Purge cycles result in hydrogen losses, and therefore, a well-designed purge strategy can increase hydrogen utilization while maintaining high cell voltages [48–50].

Liquid water is separated into a water trap in the anode recirculation system and drained periodically. A certain amount of water-level content in the membrane is necessary to keep ionic conductivity high and prevent membrane dry-out (ohmic losses). Generally, the water is produced on the cathode side and humidifies the membrane. However, too much liquid water leads to flooding in the anode and partially blocking the active area [51–54].

To discharge the liquid water from the stack, a higher pressure drop of the fuel cell stack is assumed and the recirculation is designed slightly higher. In case the fuel cell is not supplied with sufficient hydrogen, fuel starvation occurs, the cell voltage decreases locally, and the fuel cell degrades [55, 56].

### 1.3 Degradation caused by hydrogen fuel starvation

A shortage of fuel in the cell not only causes a power drop, but also causes serious degradation of the catalyst layer. The main degradation mechanism occurring in the fuel cell due to fuel starvation is the electrochemical carbon corrosion. Two degradation mechanisms can occur [57–60]:

- Carbon corrosion on the cathode side appears at high cathodic potentials ( $> 0.8$  V) due to a partial/local hydrogen starvation.
- Carbon corrosion on the anode side due to complete hydrogen starvation.

Carbon corrosion is possible due to the presence of platinum at the anode and cathode which lowers the oxidation resistance of carbon. The carbon reacts to  $\text{CO}_2$  at the interface between the platinum and the carbon support layer (Eq. 3). As a result, there is a loss of contact between the platinum and the carbon support layer, followed by decreased catalytic activity and higher activation overvoltages. Additionally, electrode thinning could occur resulting in increased ohmic resistances.

Fuel starvation not only causes a power drop but irreversible degradation of the carbon material in the stack, primarily of the catalyst support. Carbon is not thermodynamically stable at potentials higher than 0.207 V (Eq. 3), but is kinetically inert up to higher potentials, enabling its usage in PEM fuel cells. At very high electrode potentials, carbon corrosion can occur at both electrodes.

The carbon material at the cathode can be oxidized at partial fuel starvation with an in-plane electron transfer, where the cathodic potential is forced to very high values. The carbon material at the anode side is caused by a complete fuel starvation, forcing the anode to produce protons by water splitting and consequently carbon oxidation.

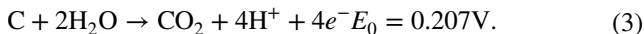
As a consequence, the active area of the triple-phase boundary decreases due to the loss of conductive material, loss of pore structure, and loss of contact with the catalyst and the membrane material. Therefore, a sufficient hydrogen stoichiometry has to be ensured by the hydrogen recirculation system.

Equation 3: Carbon corrosion in PEM FC

**Table 2** Comparison overview ejector and blower

Criteria	Ejector	Blower
Number of components and moving parts	Low +	High –
Weight and volume	Low +	High –
Energy demand	Low +	High –
Production cost	Low +	High –
Setting possibility of the recirculated mass flow	Low –	High +

+ = favorable, – = unfavorable



As a result, the main underlying influencing factor for carbon corrosion is a low hydrogen stoichiometry caused by insufficient hydrogen supply at the anode inlet. Therefore, sufficient hydrogen stoichiometry has to be ensured to mitigate carbon corrosion by the hydrogen recirculation system [61].

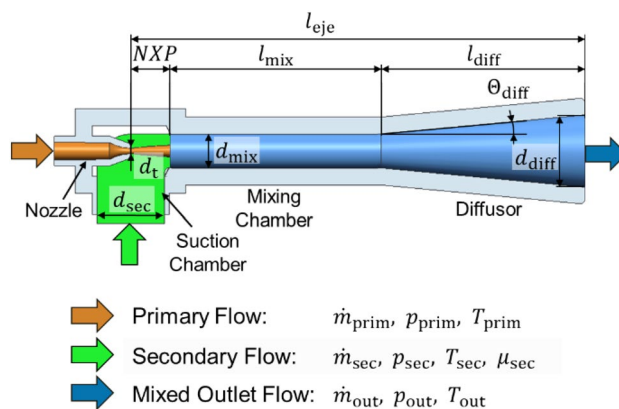
### 1.4 H<sub>2</sub> recirculation

The recirculation can either be carried out actively by means of a hydrogen blower or passively by means of an ejector (Table 2) [17].

Ejectors are generally more compact and reliable than recirculation blowers, because the ejector is a relatively simple component with no moving parts [20]. Additionally, no energy demand is required for operating an ejector except for a pressure regulator [62]. A typical recirculation blower consumes between 400 W and up to 2 kW for automotive applications [63, 64]. In comparison, a pressure control valve typically has less than 20 W, which is necessary for both active and passive recirculation. The recirculation blower has higher weights, and higher costs in production and issues can arise due to corrosion [65].

However, the recirculation blower can provide the appropriate hydrogen mass flow to the fuel cell over a wide range of load points, ensuring that the fuel cell is supplied with the necessary hydrogen under all operating conditions. The ejector’s recirculated mass flow is defined by the geometry and by the thermodynamic states at inlets and outlets. Therefore, the recirculated mass flow needs to be designed specifically for the application and, hence, the setting possibilities of the recirculated mass flow are limited. To guarantee the same reliable hydrogen supply with the ejector but with all other previously mentioned advantages, the ejector flow field needs to be simulated and optimized over the entire operating range.

The main components of the anode path and the ejector with its simulation boundary are illustrated in Fig. 3. The ejector outlet pressure  $p_{out}$  is the fuel cell anode inlet



**Fig. 4** Ejector main geometry (adapted [17])

pressure and the secondary inlet pressure  $p_{sec}$  is the fuel cell anode outlet including the water trap.

The ejector has a primary flow, a secondary flow, and an outlet flow (Fig. 4). The ejector consists of two main investigation areas, the nozzle and the rest of the ejector consisting of a suction chamber, a mixing chamber, and a diffuser.

The nozzle is responsible for the maximum possible hydrogen mass flow supply and the minimum possible hydrogen supply at critical conditions (a sonic condition in the nozzle throat). The suction chamber, mixing chamber, and diffuser define the performance of the ejector.

#### 1.4.1 Nozzle

The hydrogen mass flow control through the nozzle can be applied by the nozzle inlet pressure-based control (pulsed or continuous pressure) or the nozzle throat area control (needle or multi-pipe approach) and combinations of previously named [17]. Additional hydrogen mass flow control applications can be reviewed in [66–71].

The hydrogen mass flow through a nozzle is calculated by the nozzle throat area  $A_t$ , nozzle inlet pressure  $p_{prim}$  and temperature  $T_{prim}$ , the critical flow coefficient  $\psi_{crit H_2}$ , and the discharge coefficient  $c_d$  (Eq. 4). Each parameter and its influences are analyzed below.

Equation 4: Nozzle hydrogen mass flow

$$\dot{m}_{prim} = A_t \cdot p_{prim} \cdot \sqrt{\frac{2}{R_{H_2} \cdot T_{prim}}} \cdot \psi_{crit H_2} \cdot c_d$$

$$A_t = \frac{d_t^2 \cdot \pi}{4}. \tag{4}$$

Generally, the lower the nozzle throat diameter, the higher the performance of the ejector. However, with decreasing



diameter, the nozzle inlet pressure increases quadratic ( $d_t^2 \sim p_{\text{prim}}$ ) [23, 72].

The nozzle inlet temperature depends on the initial temperature of the hydrogen in the storage system and on whether a hydrogen heat exchanger is connected upstream to the nozzle. Typically, a hydrogen heat exchanger is used and the hydrogen at the nozzle inlet has a temperature of 60–70 °C. A higher nozzle inlet temperature also results in a higher mixed gas temperature at the inlet to the fuel cell stack, and no condensation of water can occur (flooding).

The critical flow coefficient for hydrogen  $\psi_{\text{critH}_2}$  depends on the isentropic exponent (Eq. 5), which depends on temperature and pressure at the nozzle throat. The critical pressure and temperature are calculated by an isentropic change of state at nozzle inlet conditions. The critical flow coefficient is calculated by real gas data based on REFPROP [73] and displayed in Fig. 5.

Equation 5: Critical states and flow coefficient for hydrogen

$$p_{\text{crit}} = \left(\frac{2}{\kappa + 1}\right)^{\frac{\kappa}{\kappa - 1}} \cdot p_{\text{prim}}$$

$$T_{\text{crit}} = \frac{2}{\kappa + 1} \cdot T_{\text{prim}}$$

$$\psi_{\text{critH}_2} = \sqrt{\frac{\kappa}{\kappa + 1}} \cdot \left(\frac{2}{\kappa + 1}\right)^{\frac{1}{\kappa - 1}} \tag{5}$$

The critical flow coefficient has a higher dependency on the temperature than on the pressure. The critical flow coefficient influences the total hydrogen mass flow of <0.5%.

In Eq. 4, the discharge coefficient  $c_d$  describes the real mass flow through a nozzle compared to an isentropic nozzle and, therefore, takes the nozzle geometry into account. The discharge coefficient can be expressed as a function of the Reynolds number (Re) [74–78]. A typical hydrogen nozzle for a fuel cell application between 30 and 200 kW has a

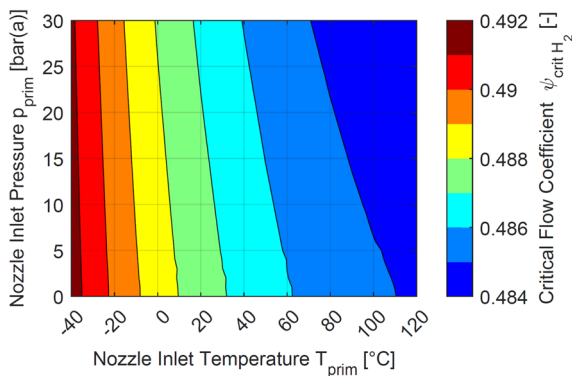


Fig. 5 Critical flow coefficient  $\psi_{\text{critH}_2}$  based on real gas data

throat diameter  $d_t$  between 1 and 3 mm. A Reynolds number range is given in Eq. 6 for typical PEM fuel cell conditions in vehicle applications (nozzle inlet: 3–30 bar(a) and 70 °C).

Equation 6: Reynolds number range hydrogen nozzle

$$Re = \frac{c_{\text{crit}} \cdot d_t}{v_{\text{crit}}} = 4 \cdot 10^4 \text{ to } 10^6 \tag{6}$$

Figure 6 shows two possible nozzle geometries for critical flow throat (CFN) design. The continuous line shows the area for a relative uncertainty of 0.3% with a 95% confidence interval. Both CFNs decrease quickly to lower Reynold values due to the increased friction loss near wall. The discharge coefficient is highly similar comparing hydrogen with nitrogen for Reynolds numbers > 1000 [79], because they have a similar value of isentropic exponent. Both hydrogen and nitrogen are diatomic molecules.

Reynolds number range for typical PEM fuel cell ejectors indicates that the nozzle throat operates mainly in the laminar region. Neglecting the influences of the discharge coefficient can result in a real hydrogen mass flow deviation of up to 4%.

The discharge coefficient and the critical flow coefficient must be taken into account to determine the diameter of the nozzle throat and thus the maximum possible hydrogen supply. In addition, purging, draining, and a certain transient load change safety margin should be considered as well.

### 1.4.2 Suction chamber, mixing chamber, and diffuser

For the performance of the ejector, the suction chamber, the mixing chamber, and the diffuser are responsible.

The suction chamber is responsible for optimal secondary intake flow. Typically, the secondary mass flow enters

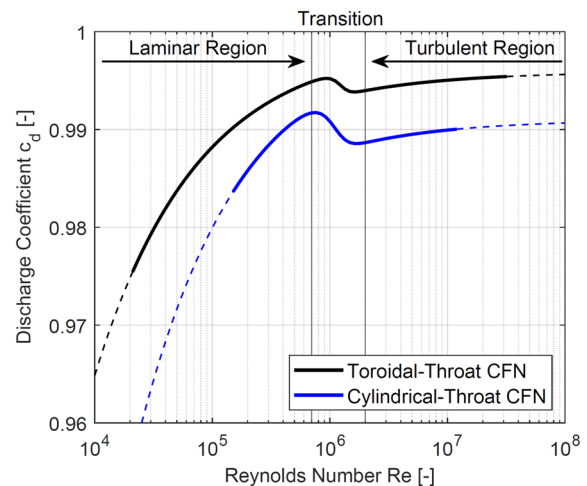


Fig. 6 Discharge coefficient  $c_d$  dependent on turbulence regime and nozzle geometry [77]

on one side of an ejector system. Therefore, non-symmetric flow occurs and may deflect the primary nozzle flow, which decreases performance. If the ejector packaging allows, a rotational symmetric suction chamber is favorable with high secondary inlet cross sections to reduce the incoming velocity. Since a 2D CFD model requires a rotational symmetric axis, the suction chamber must be analyzed in the 3D CFD simulation (Fig. 1). Experience has shown that a minimal suction chamber inlet diameter  $d_{\text{sec}}$  of 20 mm is recommended for fuel cell vehicle applications.

The mixing chamber and diffuser should be highly concentric to the nozzle axis. Often packaging requirements limit the maximum length of the ejector  $l_{\text{eje}}$ . The mixing chamber length and the diffuser length share the maximum available ejector length, since the nozzle and NXP can often be made relatively short. The diffuser outlet should be chosen as big as possible to minimize pressure losses between the ejector outlet and fuel cell stack inlet.

Recommended parameter range [23, 24]:

- Nozzle exit position:  $NXP = 0-4 \cdot d_t$
- Mixing chamber diameter  $d_{\text{mix}} = 2-6 \cdot d_t$ .

## 2 Methodology

First, the boundary conditions of the ejector are described. Then, the trade-off between mesh size, accuracy, and simulation time is explained. Finally, a general optimization study of the entrainment ratio provides details about how to maximize performance. The ejector secondary mass flow is used to calculate the entrainment ratio  $\omega$  of the ejector and further the stoichiometric ratio  $\lambda$  of the fuel cell. Those are the key performance indicators. The following equations are valid for steady-state conditions [17].

Equation 7: Entrainment ratio  $\omega$  and stoichiometric ratio  $\lambda$

$$\omega = \frac{\dot{m}_{\text{sec}}}{\dot{m}_{\text{prim}}}$$

$$\lambda = 1 + \mu_{\text{sec H}_2} \cdot \omega. \quad (7)$$

Generally, the entrainment ratio needs to be maximized, which also maximizes the stoichiometric ratio. Thermodynamic states as well as geometries can be varied to maximize the entrainment ratio.

### 2.1 System-level boundary conditions

Many parameters can be defined before starting the simulation optimization due to the boundary conditions of the anode path. The following boundary conditions are typically given for the hydrogen recirculation system.

Fuel cell stack boundary conditions:

- The fuel cell power request requires a certain hydrogen mass supply through the ejector's nozzle. And the nozzle inlet pressure  $p_{\text{prim}}$  is defined by the hydrogen mass flow.
- The fuel cell inlet pressure and the pressure loss over the stack are given for a certain operating condition by the fuel cell stack manufacturer.
- Water separation efficiency is assumed to be 100% (due to very high separation efficiencies achieved in a previous analysis [80–82]).

Ejector boundary conditions:

- Nozzle throat diameter  $d_t$  should be as small as possible, respecting the maximum available nozzle inlet pressure to maximize performance.
- The diffuser outlet diameter is maximized to the available diameter of the anode FC inlet.
- Ejector length  $l_{\text{eje}}$  is limited according to packaging requirements.

The following parameters are variable according to the preliminary stated boundary conditions:

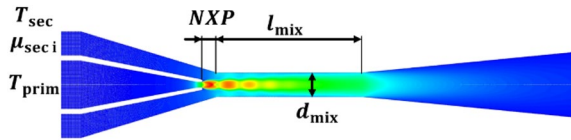
Variable parameters:

- Geometry:
  - o Nozzle exit position:  $NXP$
  - p Mixing chamber length  $l_{\text{mix}}$
  - q Mixing chamber diameter  $d_{\text{mix}}$
- Thermodynamic states:
  - o Primary inlet temperature  $T_{\text{prim}}$
  - p Secondary inlet temperature  $T_{\text{sec}}$
- Secondary inlet mass concentration:  $\mu_{\text{sec } i}$ 
  - o Hydrogen  $\mu_{\text{sec H}_2}$
  - p Nitrogen  $\mu_{\text{sec N}_2}$
  - q Water  $\mu_{\text{sec H}_2\text{O}}$ .

This leads to a multi-parameter CFD simulation system of seven degrees of freedom for a given fuel cell stack load point (Fig. 7). The secondary inlet concentration has two degrees (instead of three), because the third concentration can be calculated according to Eq. 8.

Equation 8: Secondary mass concentration

$$1 = \mu_{\text{sec H}_2} + \mu_{\text{sec N}_2} + \mu_{\text{sec H}_2\text{O}}. \quad (8)$$



**Fig. 7** Exemplary ejector 2D CFD velocity flow field with the six variable parameters

To simulate the multi-parameter model, the following simulation model setup is used (Table 3).

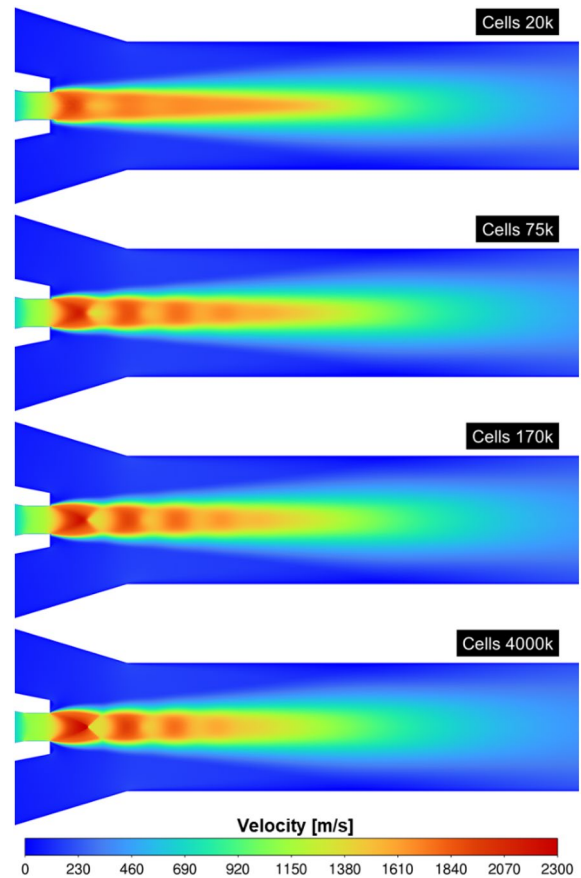
A mesh size analysis is conducted with the previously stated simulation setup.

### 2.2 Mesh analysis, and trade-off between simulation time and accuracy

The mesh size has a significant influence on the simulation time and accuracy. Figure 8 shows the influence on the velocity stream between a mesh size of 20 k, 75 k, 170 k, and 4000 k cells for the same boundary condition. The Mach diamonds are hardly visible for a 20 k mesh size compared to 4000 k.

The Mach diamonds result from the expansion of the nozzle flow into the suction chamber which results in supersonic velocities above 2000 m/s. A difference between the 20 k and 4000 k is that the high gradients of the diamonds are visible with a higher resolution. The higher the mesh size, the higher the velocity which also enhances the entrainment ratio.

Figure 9 compares different mesh sizes and the resulting entrainment ratio and evaluates four of these meshes in detail. The entrainment ratio does not change significantly for very high mesh sizes (> 1000 k). A mesh size of 200 k cells has less than a 1% deviation compared to an “infinite” mesh size. Furthermore, a low mesh size is rather a conservative result compared to a high mesh size. If for example, the cell count is too high (200 k instead of



**Fig. 8** Ejector mesh size influence

80 k), then approximately three times as many simulations can be conducted or the total amount of simulation time can be reduced by approximately 67% while maintaining high accuracy with < 2% deviation.

The simulations are performed on a standard computer (specifications in Table 4). The time durations for the simulations are specified in Fig. 9.

**Table 3** 2D rotational symmetric CFD setup

Simulation tool	Ansys fluent
Turbulence model and setup	<i>k-ε</i> model realizable Enhanced wall treatment Viscous heating Compressibility effects
Material	Ideal gas; ideal-gas-mixing-law
Model interfaces	Primary inlet: mass flow inlet with temperature Secondary inlet: pressure inlet with temperature, H <sub>2</sub> , N <sub>2</sub> and H <sub>2</sub> O concentration Ejector outlet: pressure outlet
Mesh	20–4000 k cells, quadrilateral cells



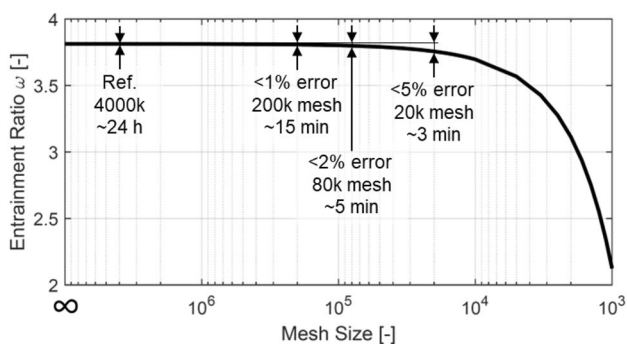


Fig. 9 Trade-off: mesh size, accuracy, and simulation time

Table 4 Computer setup

CPU	Intel(R) Core(TM) i5-8500 3.00 GHz up to 4.10 GHz 6 cores (4 cores allocated for CFD)
RAM	32 GB, DDR4 SDRAM, 2666 MHz

If the same 2D CFD simulation is performed with a 3D CFD model with a cell angle of 3°, the mesh size increases by a factor of 120. This leads to a mesh size of 10 million cells considering a 2D CFD mesh size of 80 k cells. DoE optimization with a mesh size of 10 million is very computationally intensive and is therefore not recommended.

Therefore, the ejector geometry should be developed with 2D CFD instead of 3D CFD due to the high computational effort. In addition, to further minimize the simulation effort, the piping connections to and from the fuel cell and the ejector should be simulated separately by a 3D CFD model. After minimizing the pressure of the piping, the complete 3D CFD should be simulated for validation purposes only.

Depending on the level of result accuracy and number of simulation points, the mesh size is adjusted.

### 2.3 Sensitivity analysis of entrainment ratio

Due to the large number of variable parameters that influence each other, ejector development usually requires many simulations to optimize the performance range. Table 5 shows the parameter variation range for the following simulations. The following figures are displayed with the constant values.

Depending on the number of variable parameters, a strategy for the number of different simulations is required. If a seven-parameter Design of Experiments (DoE) is performed with a full factorial design, the number of simulations for ten variations of each parameter is 10 million, which is neither feasible nor needed. Therefore, the number of simulations should be decreased using sampling techniques. Examples

Table 5 Parameter variation range and constant value

Parameter	Min	Const	Max
$d_{mix}$ [mm]	3	4.3	8
$NXP$ [mm]	0	4	10
$l_{mix}$ [mm]	10	17	30
$T_{prim}$ [K]	273	293	353
$T_{sec}$ [K]	273	343	373
$p_{sec}$ [bar(a)]	1.15	1.18	1.25
$p_{out}$ [bar(a)]	1.30	1.38	1.45
$\mu_{secH_2}$ [%]	0	24	100
$\mu_{secN_2}$ [%]	0	46	50
$\mu_{secH_2O}$ [%]	0	30	50

of DoE sampling designs include Latin Hypercube Sampling Design, Central Composition Design (CCD), or Optimal Space-Filling Design (OSF).

Figure 10 illustrates the entrainment ratio map, which was generated from the 2D CFD simulation results (Latin Hypercube Sampling Design) using the genetic aggregation surface methodology type. The constant values of Table 5 are used for the following figures.

Based on Fig. 10, the mixing chamber diameter has a higher influence on the entrainment ratio compared to the nozzle exit position and mixing chamber length. Since the axis of the entrainment ratio has the same scale, it can be seen that the mixing chamber length has a slightly greater influence than the nozzle exit position. A minimum mixing chamber length is necessary for the exchange of momentum between the primary mass flow and secondary mass flow (blue curve,  $l_{mix} = 10mm$ , Fig. 10).

Figure 11 shows the influence on the entrainment ratio over the primary temperature  $T_{prim}$  and secondary temperature  $T_{sec}$ . The entrainment ratio increases at higher primary temperatures, indicating that the use of a hydrogen heat exchanger upstream of the nozzle inlet is recommended. The entrainment ratio also increases with lower secondary temperatures, due to higher suction density.

Increasing the primary temperature  $T_{prim}$  leads to higher sonic velocities in the nozzle throat, which further increases the impulse of the gas flow and, thus, the higher the entrainment ratio of the ejector (Eq. 9).

Equation 9: Sonic velocity of hydrogen  $c_{crit}$

$$c_{crit} = \sqrt{\kappa \cdot R_{H_2} \cdot T_{crit}} \tag{9}$$

A heat exchanger between the fuel cell anode outlet and the hydrogen nozzle inlet is advantageous. The reduced temperature at the anode outlet increases the nozzle inlet temperature. As it can be seen in Fig. 11, both the lower temperature of the secondary gas and the increased temperature of the nozzle inlet enhance the entrainment ratio.

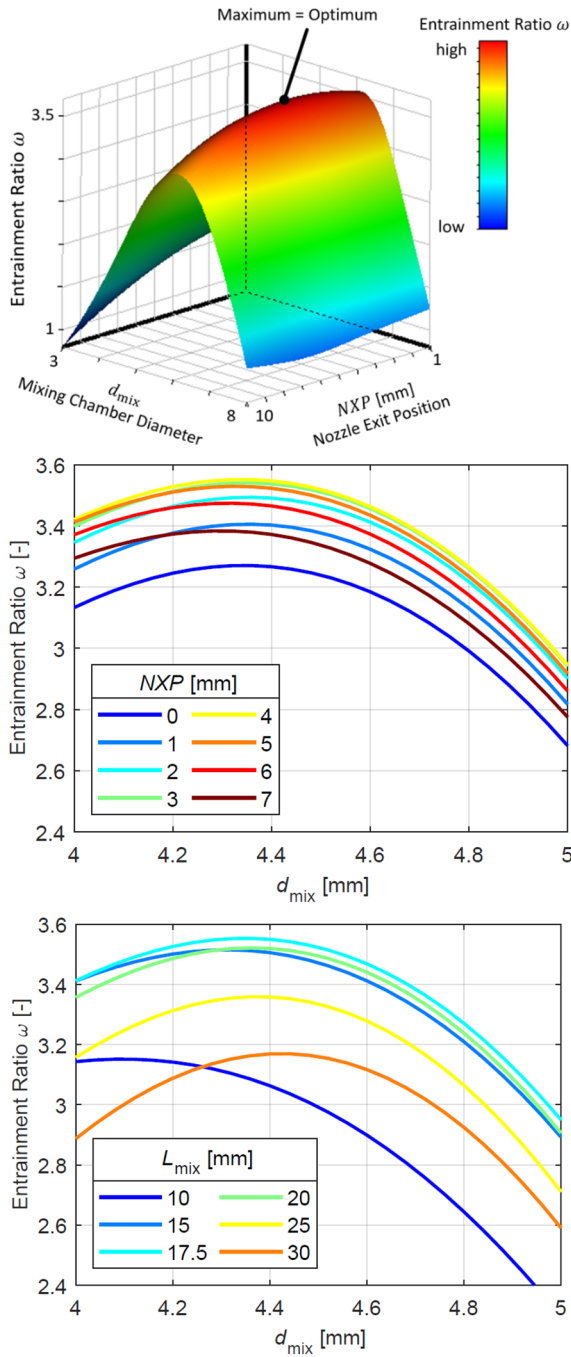


Fig. 10 Geometry correlation on entrainment ratio

The entrainment ratio increases with higher concentrations of nitrogen and water due to the increased molar mass of the mixed gas (Fig. 12). However, even though the entrainment ratio increases, the stoichiometric ratio decreases. The highest stoichiometric ratio can be achieved with 100% hydrogen concentration at the secondary inlet. Typical stoichiometric ratios are between 1.4 at full load and can be as high as 5 at part load.

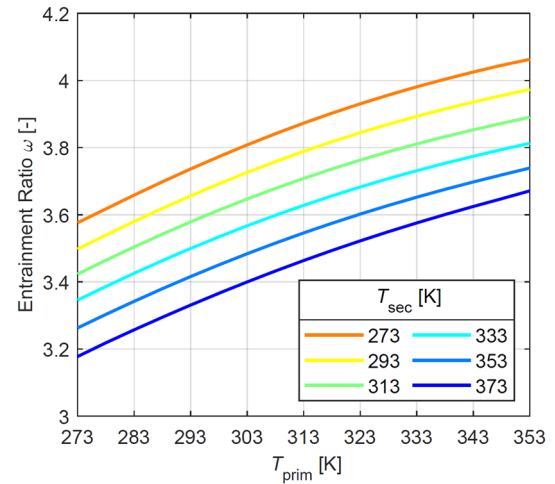


Fig. 11 Temperature sensitivity

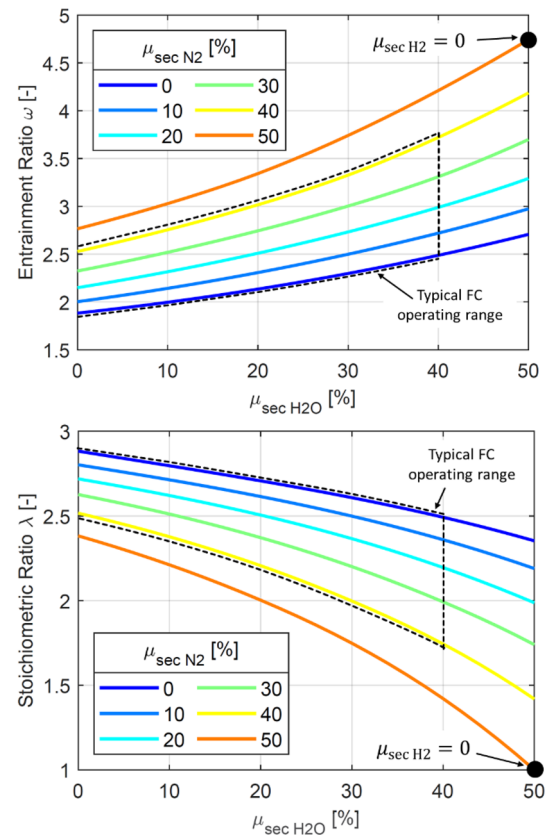


Fig. 12 Secondary mass concentration sensitivity

Figure 13 shows the influence on the sensitivity of the pressures between the secondary inlet and the ejector outlet. These pressures are defined by the system, but additional components in the anode recirculation can introduce additional pressure losses leading to reduced entrainment

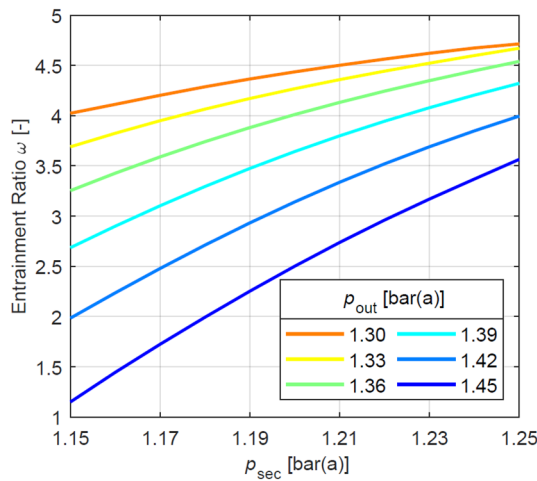


Fig. 13 Pressure sensitivity

ratios. With an additional pressure loss of 0.15 bar, the entrainment ratio can vary up to a factor of 3. As a result, additional pressure loss between stack inlet and outlet has the highest influence on entrainment ratio.

The entrainment ratio dependencies on geometries and thermodynamic states are in line with the literature [21, 83, 84]. The next step describes the results of a single ejector considering FC-specific boundary conditions.

### 3 PEM FC ejector optimization and operating strategy

In this chapter, an ejector for a PEM fuel cell application is designed considering the appropriate boundary conditions.

#### 3.1 Boundary conditions specific fuel cell system

The following boundary conditions are given for the specific PEM fuel cell stack, which need to be satisfied by the ejector application (Table 6). The fuel cell stack’s nominal power rating is 30 kW. The minimum stoichiometric ratio required from the fuel cell increases for lower loads.

Furthermore, the following boundary conditions are given on the anode level.

Boundary conditions:

- Maximum nozzle inlet primary pressure  $p_{\text{prim max}} = 12 \text{ bar}(a)$
- An anode heat exchanger is available to adjust the hydrogen temperature. Primary temperature  $T_{\text{prim}} = 70^\circ\text{C}$
- Secondary temperature  $T_{\text{sec}} = 70^\circ\text{C}$
- Maximum ejector length  $l_{\text{eje}} = 120 \text{ mm}$ .

For the development of the optimized ejector, the following geometric parameters are available for optimization at each load point:

- Mixing chamber diameter  $d_{\text{mix}}$
- Nozzle exit position:  $NXP$
- Mixing chamber length  $l_{\text{mix}}$ .

#### 3.2 Ejector design

During PEM fuel cell operation, the fuel cell operates at different load conditions, and hence, the thermodynamic states of the ejector change and thus the optimal geometry change. The local optima are simulated by the minimum hydrogen mass concentration  $\mu_{\text{sec H}_2\text{min}}$  stated in Table 6, which represents the worst-case stoichiometric ratio. The best-case stoichiometric ratio is 100% hydrogen at the secondary inlet. If the hydrogen concentration falls below the minimum, a purge cycle is required to increase the hydrogen concentration.

Figure 14 shows the ejector entrainment ratio maps for four different load conditions stated in Table 6 at each optimized mixing chamber length (similar to Fig. 10 top). The load point (11%) does not achieve the defined minimum stoichiometric ratio of 5 due to the high-pressure difference between the anode FC inlet and outlet and the high required stoichiometric ratio according to boundary conditions.

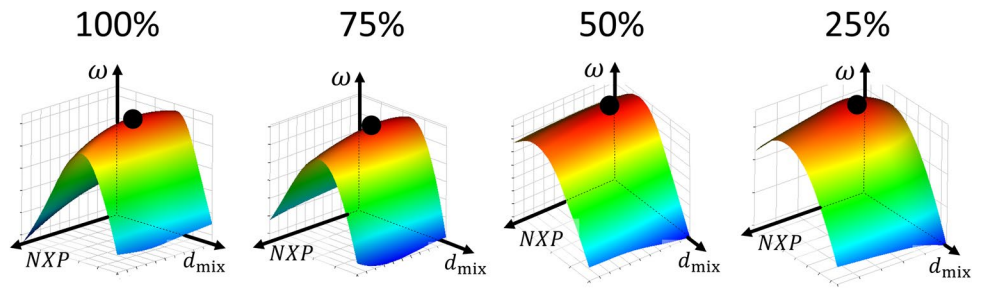
Each load point has an optimum for the ejector geometry to maximize the entrainment ratio and the stoichiometric ratio. The local optimum stoichiometric ratio  $\lambda_{\text{local opt}}$  is calculated by the maximum entrainment ratio according to Eq. 7 (Table 7). If the load point, which corresponds to the nozzle hydrogen mass flow, of the PEM FC stack decreases, then the optimum of the NXP, and mixing chamber diameter and length decrease as well.

The local optimum stoichiometric ratio  $\lambda_{\text{local opt}}$  and the minimum stoichiometric ratio  $\lambda_{\text{min}}$  are displayed in Fig. 15.

Table 6 Fuel cell stack boundary conditions

Load [%]	$\dot{m}_{\text{prim}}$ [g/s]	$\lambda_{\text{min}}$ [–]	$p_{\text{FC in}}$ [bar(a)]	$p_{\text{FC out}}$ [bar(a)]	$\mu_{\text{sec H}_2\text{min}}$ [%]
100	0.63	1.40	1.60	1.38	41
75	0.47	1.53	1.48	1.27	34
50	0.31	1.87	1.38	1.18	24
25	0.15	2.70	1.30	1.12	18
11	0.07	5.00	1.26	1.09	44

**Fig. 14** Entrainment ratio map for each load point (schematic overview)

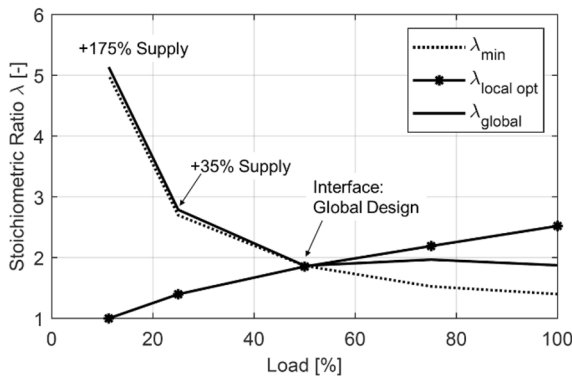


**Table 7** Local optima

Load [%]	$d_{mix\ opt}$ [mm]	$NXP_{opt}$ [mm]	$l_{mix\ opt}$ [mm]	$\lambda_{local\ opt}$ [-]
100	6.1	5.0	24	2.52
75	5.3	4.2	22	2.19
50	4.3	3.7	17	1.85
25	3.3	2.9	9	1.40

**Table 8** Load map

Load [%]	100	75	50	25	11
Timeshare TS [% of total time]	50	15	15	15	5



**Fig. 15** Stoichiometric ratio

The minimum required stoichiometric ratio for mid-to-high load (50% and above) is achieved. The interface between the local optimum and minimum fuel cell stoichiometric ratio is the global design point which is the geometry at 50% load, since it covers the widest operation range.

Each load point is re-simulated with the global design geometry. The stoichiometric ratio with the global design  $\lambda_{global}$  is lower for high loads but still achieved. However, lower loads need an additional operating strategy to fulfill the minimum required stoichiometric ratio.

First, the number of purge cycles is increased for the 11 and 25% load point, which leads to a higher secondary hydrogen concentration and a higher stoichiometric ratio. However, increased purging is not sufficient and additional hydrogen needs to be supplied by the nozzle to increase nozzle flow impulse and recirculation. The additional hydrogen improves recirculation but is lost by purging. Thus, 35% additional hydrogen must be added for the 25% load point and 175% for the 11% load point. The main

effect on the dynamics of the system is that the purge valve is actuated more frequently or, as a second option, the purge valve is actuated continuously in a partial open state.

The load profile of the PEM FC application needs to be considered to calculate the total hydrogen utilization (Table 8). In total, the hydrogen utilization decreases to 97% by this operating strategy considering the load map in Table 8 (Eq. 10). For this application, the additional hydrogen is acceptable due to the very low operating time for the 11% load point.

Equation 10: Hydrogen utilization

$$H_2\text{Utilization} = \frac{\sum_{i=1}^5 \text{Load}_i \cdot TS_i \cdot \dot{m}_{\text{prim act } i}}{\sum_{i=1}^5 \text{Load}_i \cdot TS_i \cdot \dot{m}_{\text{prim } i}} \quad (10)$$

In case the low-load range (11–25%) has a significantly higher timeshare, other operating strategies can be considered. Each of the following systems has better performance over the entire operating range [17]:

- A second low-load ejector in parallel
- A pulsed injector-ejector unit
- A variable nozzle throat area control ejector.

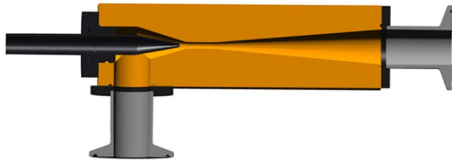
For this application, Table 9 states the final and most important ejector geometries and Fig. 16 displays the final design of the ejector.

The next development toolchain step is the 3D CFD simulation to improve non-rotational symmetric influences based on detailed packaging considerations (cp. Fig. 1). In this publication, geometry optimization using 3D CFD simulation is not discussed in detail, only general findings.

Generally, the performance of the 3D CFD model is highly dependent on the piping. Experience has shown that if the pressure loss in the piping is low, a small loss of

**Table 9** Final ejector geometry

Geometry	Value [mm]
Nozzle throat diameter $d_t$	1.1
Mixing chamber diameter $d_{\text{mix}}$	4.3
Diffuser outlet diameter $d_{\text{diff}}$	22
Nozzle exit position $NXP$	4
Mixing chamber length $l_{\text{mix}}$	17
Diffuser length $l_{\text{diff}}$	99

**Fig. 16** Ejector CAD

entrainment ratio can be expected (<10%). In contrast, fillets on each edge within the ejector enhance flow and increase the entrainment ratio in the same range. Thus, if both pipings are added and fillets are applied, the performance will remain approximately in the same entrainment ratio. To minimize the simulation effort, the piping connections to and from the fuel cell and the ejector should be simulated separately using a 3D CFD model. The entire anode path should only be validated using 3D CFD.

## 4 Conclusion and outlook

The 2D rotational symmetric CFD is explained with a preliminary analysis of the influences on the nozzle hydrogen mass flow, the suction chamber, the mixing chamber, and the diffuser.

The mesh size analysis shows how to minimize computational effort while maintaining high accuracy. A simulation run can take from 3 min to 24 h depending on the mesh size and the necessary accuracy. Furthermore, a smaller mesh size has a lower entrainment ratio, which is a conservative result compared to an extremely high mesh size. By selecting the appropriate mesh size, the simulation time can be reduced by approx. 67% (80 k instead of 200 k), while maintaining high accuracies <2%.

Maximizing the nozzle inlet temperature and minimizing the secondary temperature increase the entrainment ratio. Impurities, such as nitrogen and water, increase the entrainment ratio but decrease the stoichiometric ratio. Generally, the lower the pressure difference between the ejector outlet and the secondary inlet, the higher the entrainment ratio. The mixing chamber diameter has the

biggest influence on performance compared to the nozzle exit position and mixing chamber length.

The ejector geometry should be developed using 2D CFD instead of 3D CFD due to the high computational cost to allow a high number of parameter variations via DoE. The entrainment ratio of the 3D CFD model is dependent on the piping connected between ejector and stack as well as fillets within the ejector. Experience has shown that the piping (additional pressure loss) and the fillet in the ejector (enhanced flow) have an opposite influence on the entrainment ratio and, thus, the entrainment ratio remains in the same range. It is recommended to minimize the pressure losses in the piping in a separate simulation and to use the 3D CFD of the entire anode path only for final validation.

Finally, the ejector design is evaluated from a local analysis to a final ejector design according to the fuel cell stack boundary conditions. A single ejector has a limited operating range, which depends mainly on the nozzle inlet pressure, in this case, 12 bar(a). If an ejector with a larger operating range is required, the nozzle inlet pressure should be increased or other operating concepts, such as a pulsed ejector or a needle ejector, can be used.

Anode recirculation through an ejector instead of a recirculation blower reduces the number of components, weight, moving parts, and power requirements. However, the design of the ejector is critical to maintain the stoichiometric ratio and avoid degradation mechanisms.

This methodology can be applied to a wide range of ejector areas and significantly reduces development efforts in future.

General key findings:

- Maximize nozzle inlet temperature and minimize secondary temperature to maximize entrainment ratio.
- Minimize pressure loss in the anode path and recirculation.
- A small mesh size is a conservative estimation of the entrainment ratio.
- A small mesh size enables a large number of parameter variations over DoE.
- A simple ejector satisfies the stoichiometric ratio in the 50–100% load range for the given fuel cell boundary condition.
- Additional hydrogen is necessary to extend the operating range to lower loads, but results in hydrogen losses.

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## Declarations

**Conflict of interest** The authors declare no competing interests.

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