Definition of validated membrane reactor model for 5KW power output CHP under different natural gas compositions

Definition of validated membrane reactor model for 5 kW power output CHP system under different natural gas composition

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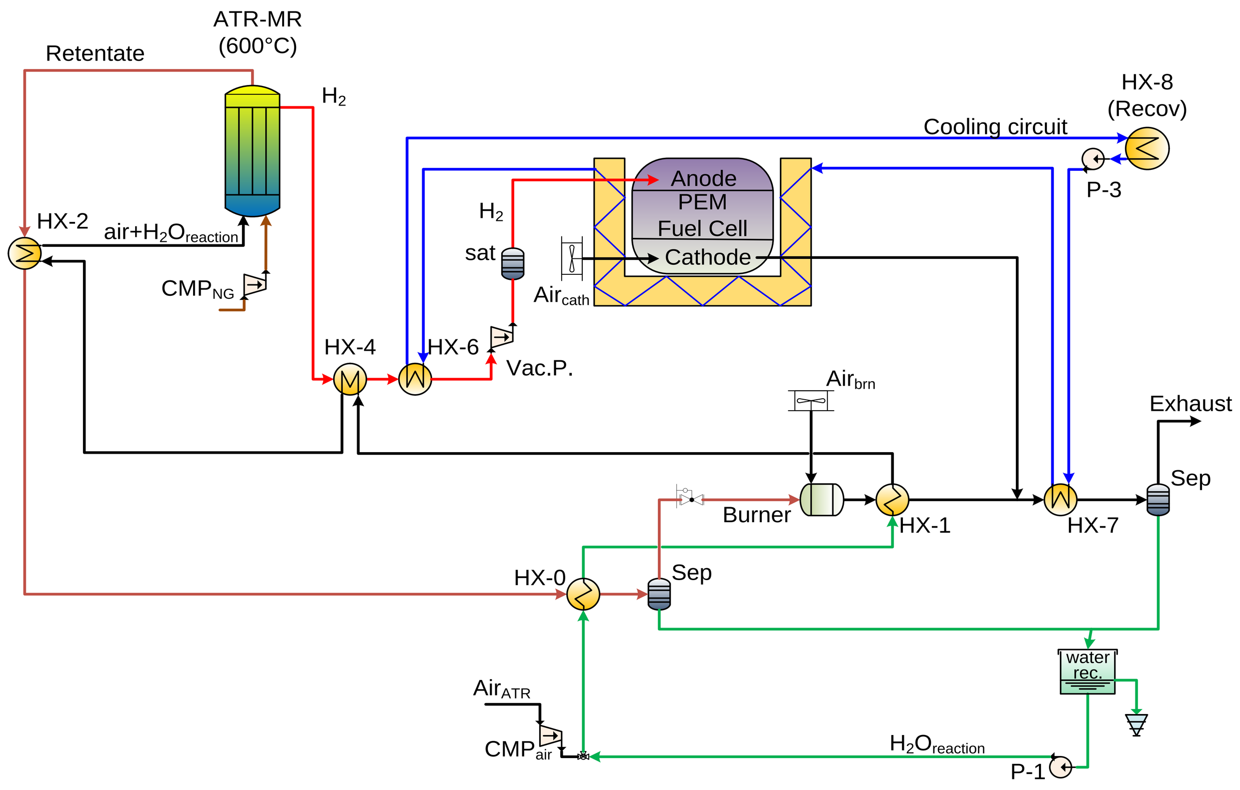
Abstract

In the last years, many studies focused on the adoption of membrane reactor in micro-cogeneration system based on PEM fuel cell thanks to the pure hydrogen production. This work deals with (i) the design of a FBMR flexible towards different NG qualities (ii) and its integration in PEM based systems of 5 kW power output system. Indeed the variation of NG composition has a big impact on the performance of the micro-CHP system and fuel processor life time. Four typical NG compositions from reference European countries are considered in this study 2 different membrane reactor model are compared: the first is a 1D phenomenological model, the latter is inside a model of the overall PEM based micro-CHP in Aspen Plus. Furthermore, since the overall PEM based micro-CHP system is modelled using Aspen Plus®, the phenomenological model is used to validate the fuel processor implemented in the CHP model. In this case, the FBMR is modelled by adapting a series of equlibrium reactors followed by hydrogen extraction.

Micro-CHP Layout flexibility

The micro-CHP system is designed to generate 5 kWel and 6.2 kWth of hot water (where the cooling circuit temperatures are 60/40 °C). At design conditions, the net electric efficiency and the total efficiency are respectively 40.1% and 89.2%. The fuel processor is based on fluidized autothermal membrane reactor (600 °C and 8 bar) fed with NG, producing pure hydrogen flow (@ 0.3 bar) without the use of sweep gas. An air flow, below the stochiometric value, burns a fraction of NG in order to sustain the endothermic SR reactions. From the vacuum pump, the H_2 flux feeds a dead-end LT PEM FC (@ 75 °C) cooled by the water heat recovery loop.

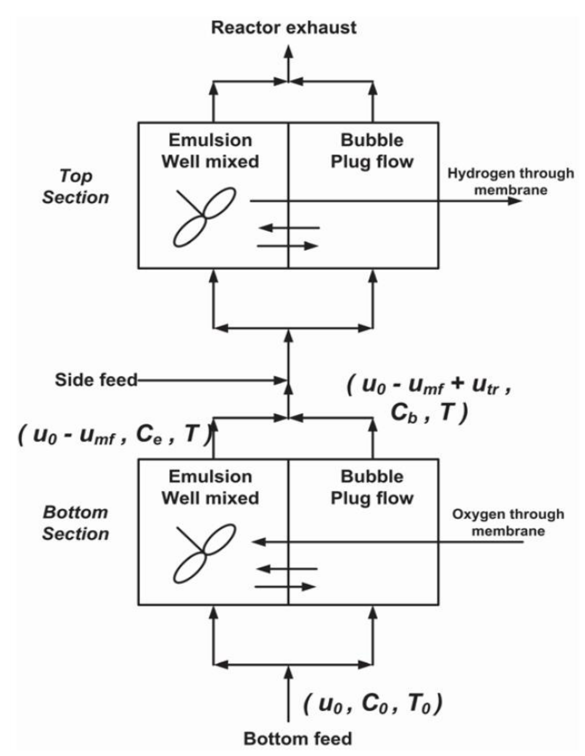


CHP Design & Costraints	
T (°C)	600
P (bar)	8
S/C	2.5
HRF	0.92
P H_2perm (bar)	0.3
P H_2 in FC (bar)	1.2
η_{FC} (%)	60
UA of HX's	cost

After the design of the FBMR and the definition of the main CHP parameters using the UK case (average EU-NG), layout flexibility and different control strategies for the other NG compositions are investigated.

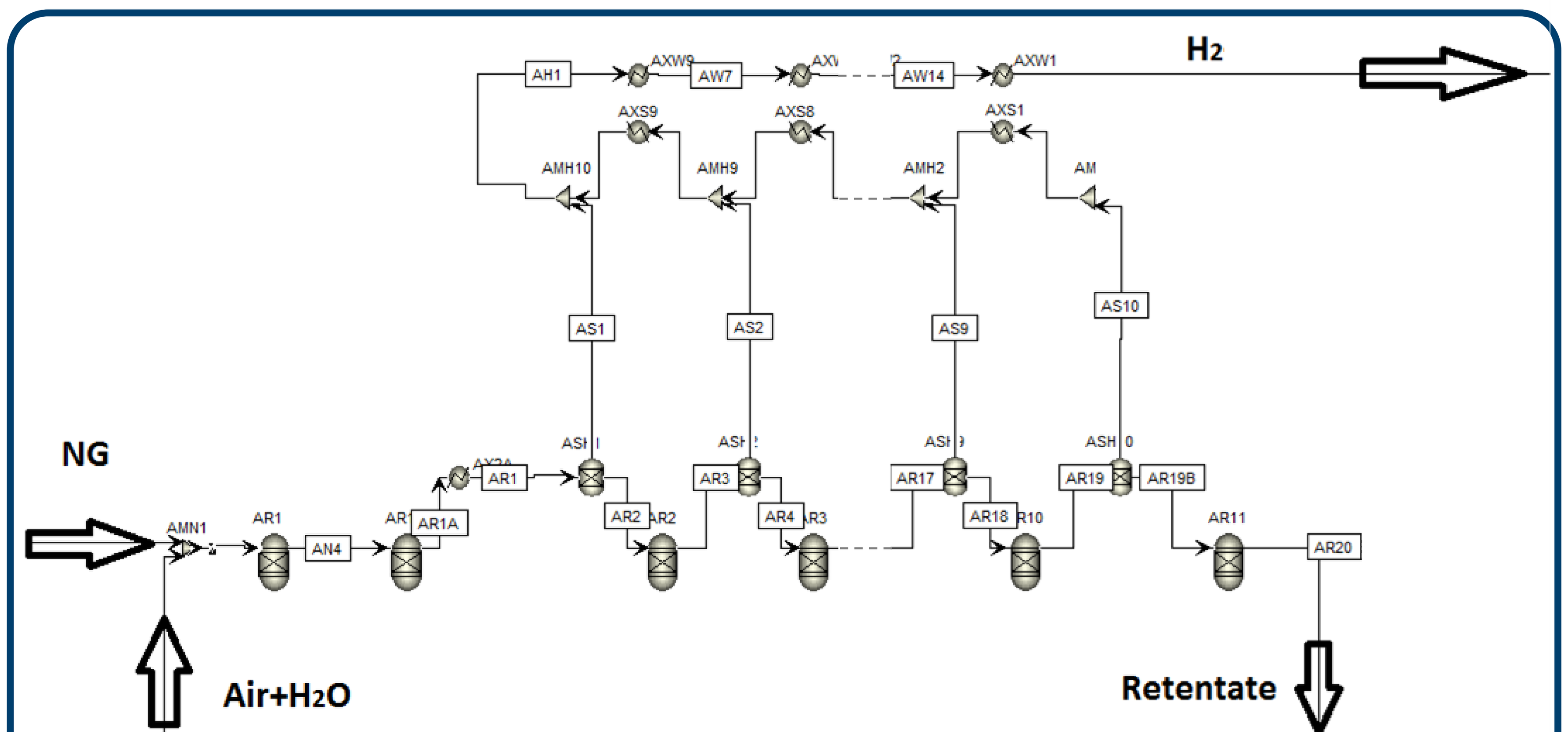
		European NG Qualities			
Species	**u.m.**	**UK**	**IT**	**NL**	**ES**
CH_4	%mol	92.070	99.581	81.23	81.570
C_2H_6	%mol	3.405	0.056	2.85	13.380
C_3H_8	%mol	0.761	0.021	0.37	3.670
n-C_4H_{10}	%mol	0.177	0.002	0.08	0.400
i-C_4H_{10}	%mol	0.140	0.006	0.06	0.290
n-C_5H_{12}	%mol	0.048	-	0.02	-
i-C_5H_{12}	%mol	0.061	0.002	0.02	-
C_{6+}	%mol	0.090	0.007	0.08	-
CO_2	%mol	0.865	0.029	0.89	-
N_2	%mol	2.375	0.296	14.4	0.690
LHV	MJ/kg	46.740	49.730	38.0	48.610
Wobbe index	MJ/Nm³	52.0	53.1	43.6	56.6
H_2 potential	mol H_2/ mol NG	4.07	3.992	3.523	4.656

Membrane Reactor Model (1)



The phenomenomegical 1D membrane reactor model allows the simulation of FBMR for separation of hydrogen from a reacting mix undergoing steam methane reforming (SMR) or autothermal reforming (ATR). The steady state overall (bubble and emulsion phases) component mass conservation equations and the total volume balance (to calculate the excess velocity) have been formulated, taking chemical transformations in the emulsion phase and a net gas production due to the chemical reactions and gas removal via membranes into account.

Membrane Reactor Model (2)



The membrane reactor, implemented in Aspen Plus®, is discretized in a series of 10 reactors and separators. Each reactor is set to equilibrium conversion (SR&WGS reactions + Total Oxidation at the inlet) by Gibbs free energy minimization. In the separators, hydrogen is extracted (infinite perm-selectivity is assumed) according to the permeation expression. In both the models, temperature profile along the reactor bed is uniform both radially and axially.

Results

Performances of the micro-CHP system under the 4 EU-NG qualities are reported in the table. Since the reactor operating pressure is constant for all the cases, the only parameter control is the air flow λ_{ATR}. The NL case has the low electric efficiency due to the large amount of N_2 in the NG: this implies an higher power input and higher auxiliary losses. On the other hand it has the best thermal recovery. The other 3 cases have quite similar performances even if the ES case, with the big amount of hydrocarbons heavier than methane, has the best electric performances.

CHP system results	u.m.	UK	ITA	NL	ES
S/C	-	3.0	3.0	3.0	3.0
NG power input [LHV base]	W	12632	12589	12814	12565
Net AC power output	W	5000	5000	5000	5000
Fuel Cell AC power output	W	6308	6314	6315	6309
Thermal recovery	W	6588	6578	6746	6498
Net electric efficiency	$\%_{LHV}$	39.59	39.72	39.02	39.80
Net thermal efficiency	$\%_{LHV}$	52.16	52.25	52.65	51.71
Total efficiency	$\%_{LHV}$	91.74	91.97	91.67	91.51
λ_{ATR} (air to fuel molar)	-	0.229	0.233	0.234	0.23
Total membrane area	m²	0.114	0.114	0.114	0.114
Hydrogen permeation	Nm³/h	3.59	3.59	3.61	3.57
Hydrogen Recovery Factor	%	92.00	92.00	92.00	92.00
NG compressor	W	150	153	176	129
Air compressor	W	355	354	361	347
Cathode air blower	W	187	187	188	186

The comparison between the two membrane reactor models shows some deviations that are still under investigation. They are principally due to the thermal integration approach, causing a different NG conversion and H_2 permeation flow.

	MR outlet flow (mol/s)			
	UK		ITA	
Species	**Model (1)**	**Model (2)**	**Model (1)**	**Model (2)**
CH_4	0.0024	0.0001	0.0014	3.88E-05
H_2O	0.0176	0.0138	0.0202	0.0142
H_2	0.0013	0.0033	0.0032	0.0025
CO	0.0004	0.0013	0.0009	0.0010
CO_2	0.0132	0.0146	0.0121	0.0151
N_2	0.0281	0.0280	0.0282	0.0280
H_2 perm	0.0360	0.0440	0.0380	0.0440

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