

The Novel Heat Accumulator for the Heating of Electric Vehicles

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Keywords : the needed values of heating power, driving range of the electric vehicles, heat accumulator, the colligative properties of ionic solutions, measurements on the heat accumulator in the real condition

Abstract : This paper deals with the impact of heating on the driving range of electric vehicles (EV-s), as the energy from a car battery is used on both driving and heating of the car. The possible solution is the novel heating device with its own energy source – low pressure heat accumulator. The use of inner heat exchanger in this accumulator makes the design of whole device very easy and with the division of a high - pressure from a low – pressure part increases its safety. With addition of some salts into water, it is possible to decrease the value of inner pressure (vapor pressure) in heat accumulator along with the conservation of good thermophysical properties of the storage medium. In conclusion the measurements on heat accumulator in real conditions are presented

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1 Introduction

The high energy efficiency of electric devices (electric motor + power electronics + battery) in electric vehicles entails the need to find a compensation for large waste heat of ICE. In this case not only new designs of a car heating device can provide satisfactory solution but finding of a novel energy source for heating and so making the whole energy of car battery free for driving (the energy consumption of other electric devices like lights etc. is negligible). Limited capacity of batteries, their longer charging times along with insufficient charging network make from the driving range of EV-s one of the most interesting parameters for customers decision by choice of a new car. So can be appropriate solution a great advantage.

2 The waste heats of the electric vehicles, required heating powers and the decrease of driving range

ICE-s are thanks their low energy efficiency the main heat source in cars. The waste heats of electric engine, power electronics and car battery together are in comparison with ICE negligible. The results from

driving simulation of car ($m_{max} = 1600 \text{ kg}$) according to driving cycle *Artemis Highway 130* show this very clearly (Figure 1). The physical model for simulation with other parameters was made according to ([2], [24]). Values of instant velocities was taken over from ([23]).

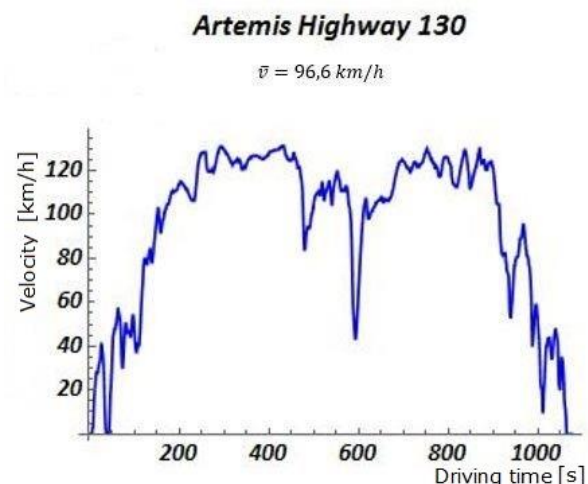


Figure 1 Instant velocities of driving cycle Artemis Highway 130

For calculations of the model was used program *SystemModeller*®. Result of simulation was a set of the values of the effective instant powers needed for car motion. By calculation of waste powers were used constant efficiency values. For electric vehicle $\eta_{EV} = \eta_m * \eta_{batt} * \eta_{povelec} = 0,9^3 = 0,729$, and for ICE $\eta_{benz} = 0,214$. Results are shown on diagram (Figure 2). Average waste power of EV $\bar{Q}_{EV} = 2,5 \text{ kW}$ is much smaller than this of ICE $\bar{Q}_{ICE} = 34 \text{ kW}$

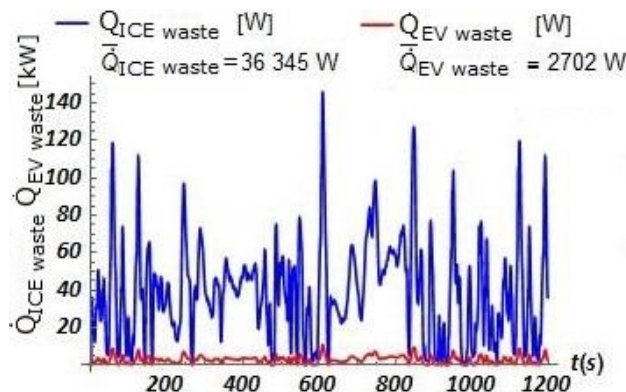


Figure 2 Simulation results – comparison of instant waste powers of ICE (blue) with waste powers of electric vehicles (electric motor + power electronics + Battery, red)

Values of needed heating powers are within the range of 1 kW by ambient temperature of 7 °C up to 5 kW by – 20°C (all with ambient air streaming into car cabin and without solar radiation, figure 3).

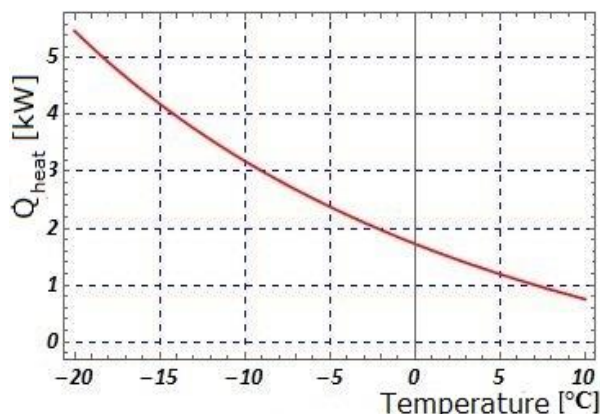


Figure 3 The needed heat powers for heating of cabin air according to ambient temperature

Driving range of some EV-s can decrease by simultaneous consumption of battery energy on driving and heating up to 50% of its initial value how shown on figure 4. This driving range drop was calculated from WLTP (Worldwide Harmonized Light-Duty-Vehicle Test Procedure) - consumption values of Hyundai Ioniq Electro with battery energy capacity of 28 kWh. In real conditions however may be the driving range drop much greater.

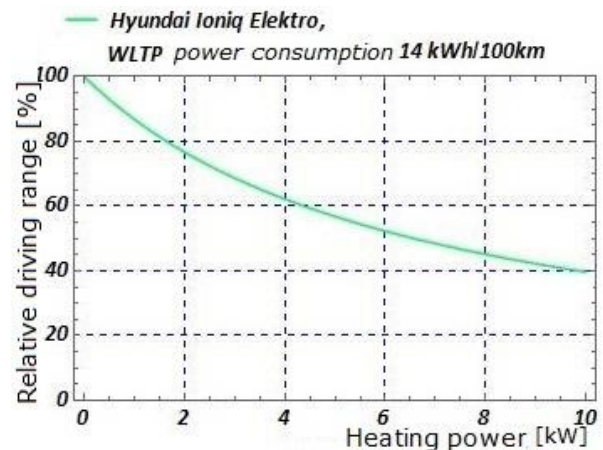


Figure 4 The driving range drop as a function of heating power

3 The design of heat accumulator and the use of colligative properties of ionic solutions

The proposed heat accumulator may be charged from electric network along with car battery. The demanded heating power from accumulator is removed in inner heat exchanger. Heating medium in heating circle may be water or glycol. Inner heater divides the high - pressure part (pressure vessel) from the low - pressure part (heating circle) of heating device. Heating medium gives its warmth on cabin air in outer heat exchanger (Figure 5).

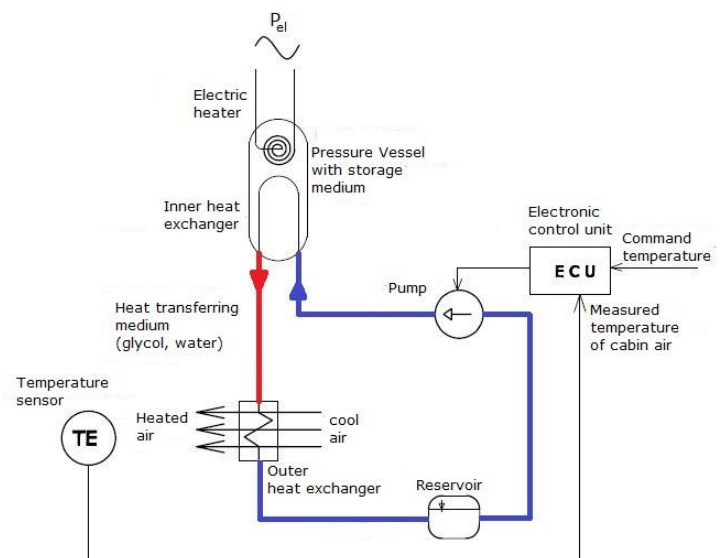


Figure 5 The scheme of the heating device with heat accumulator

As security of passengers is very important, pressure in the heat accumulator must be hold as low as possible. With regard to the DIN EN 13 445 norm is the pressure vessel of heat accumulator a pressure device according to paragraph 3, clause 1.2 . For these vessels holds the diagram on picture 6 good. As can be seen from this diagram, the value of product composed from maximal pressure PS an nominal volume V of the vessel in litres should be smaller or equal to 200 (blue marked area in diagram, category I and II) also $PS * V \leq 200$. Pressure vessels of category I and II need neither outer nor inner periodic strength and other tests. Thus the nominal pressures in accumulator were chosen to fulfil this rule.

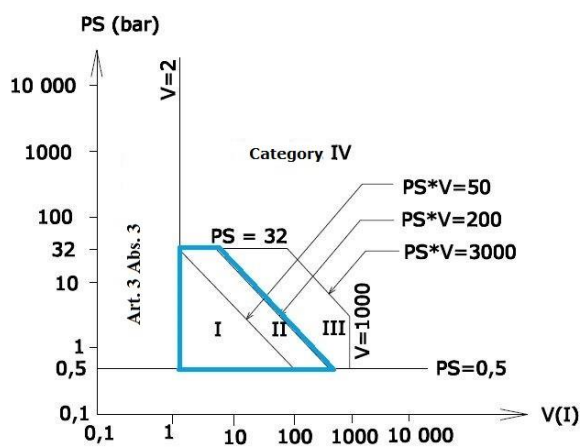


Figure 6 DIN EN 13 445 diagram for pressure devices according to paragraph 3, clause 1.2

But rule $PS * V \leq 200$ influences nominal amount of energy in accumulator as well. Energy in accumulator can be calculated with equation (1) :

$$Q = (m_{med} * \bar{c}_{p,riem} * \Delta T) / 3600 \text{ [kWh]} \quad (1)$$

Where :

m_{med} –

the weight of storage medium in accumulator

$\bar{c}_{average}$

– average specific thermal capacity of storage medium

ΔT – temperature difference

The nominal energies, pressures and temperatures in the accumulator by using of water as storage medium and validity of $PS * V \leq 200$ rule are (Table 1, Figure 7) :

Table 1 Volumes, energies, temperatures and pressures in heat accumulator

$V[l]$	$Q[kWh]$	$t[^\circ C]$	$p[bar]$
10	1,4	210	20
15	1,7	190	12,6
20	2,0	180	10

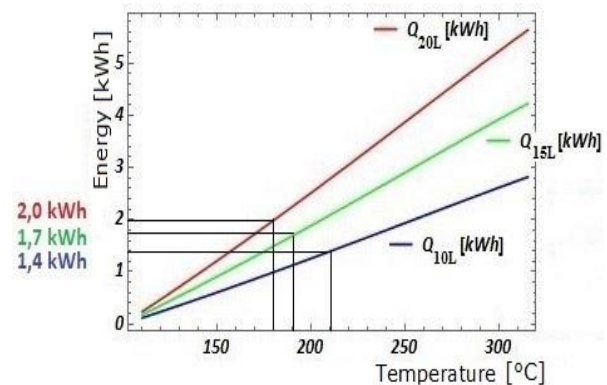


Figure 7 The nominal energies in heat accumulator by fulfillment of the $PS*V \leq 200$ rule, storage medium pure water

One of the possibilities how to increase the energy in the accumulator by validity of the $PS * V \leq 200$ rule is using of colligative properties of the ionic water - salt solutions. One of colligative properties is vapor pressure drop. But the thermodynamic properties, mainly specific thermal capacity and density, what are important parameters for quantum of energy, change by addition of salt into water as well . To do the use of salt solutions purposeful, the storable energy in accumulator have to be higher than these of water.

The fulfillment or failure of this condition is shown on two salt solutions $MgCl_2$ (magnesium chloride) and $CaCl_2$ (calcium chloride) with concentration range (mass concentration) between 30 up to 50 %, resp. 55 % in case of calcium chloride. Water solutions of these salts have much higher pressure drop as other chlorides ($NaCl$, KCl) and their solubility is much better as well. But it must be noted on this place that the state of art knowledges about vapor pressures of ionic solutions as well as their thermodynamic properties at high temperatures ($t_{sol} > 100^\circ C$) are not well known as in case of pure water and unlike water, for salt solutions we have not international respected data set. Thus the thermodynamic - colligative data used in this work were collected from many articles and tables ([29] up to [38]) as well as our own measurements. The vapor pressure drops of $MgCl_2$ solutions are steeper than these of $CaCl_2$ solutions on same concentrations (Table 2, Figure 8).

Table 2 Vapor pressures of $CaCl_2$ and $MgCl_2$ solutions

$t[^\circ C]$	$p_{water} [bar]$	$p_{30\%}^{CaCl_2} [bar]$	$p_{30\%}^{MgCl_2} [bar]$	$p_{50\%}^{CaCl_2} [bar]$	$p_{50\%}^{MgCl_2} [bar]$
150	4,761	3,5	2,59	1,95	0,86
300	85,877	61,1	53,3	41	27,2

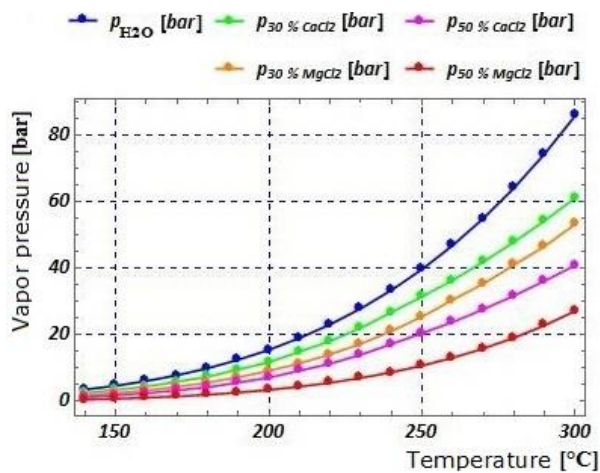


Figure 8 The vapor pressure drop of CaCl_2 and MgCl_2 water solutions in comparison with the vapor pressure of pure water (blue)

Specific thermal capacities of CaCl_2 and MgCl_2 in high temperatures area ($t_{\text{sol}} > 100^\circ\text{C}$) at same concentrations differ not so much as in case of vapor pressures. Their values depend mainly from mass concentration and temperature (Table 3, Figure 9).

Table 3 Specific thermal capacities of CaCl_2 and MgCl_2 solutions at high temperatures

$t [^\circ\text{C}]$	c_{water} [kJ/kgK]	$c_{30\%}^{\text{CaCl}_2}$ [kJ/kgK]	$c_{30\%}^{\text{MgCl}_2}$ [kJ/kgK]	$c_{50\%}^{\text{CaCl}_2}$ [kJ/kgK]	$c_{50\%}^{\text{MgCl}_2}$ [kJ/kgK]
100	4,217	2,7	2,68	2,06	1,68
300	5,752	3,8	3,83	2,86	2,95

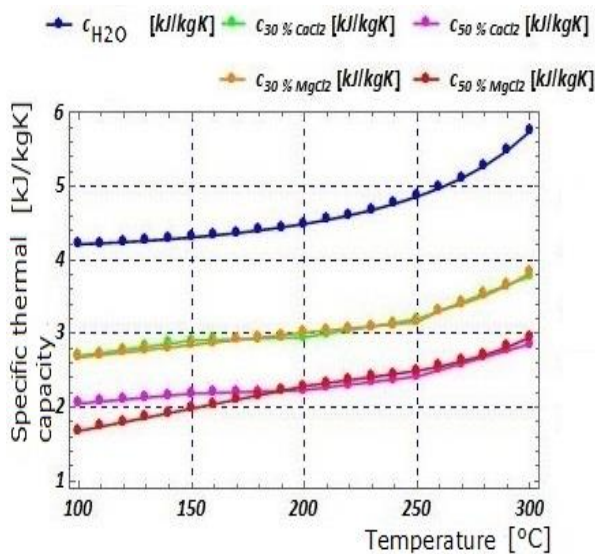


Figure 9 The drop of specific thermal capacities of CaCl_2 and MgCl_2 solutions at high temperatures in comparison with water (blue)

Densities of CaCl_2 and MgCl_2 solutions increase with increasing mass concentration. Their density at boiling point temperature and 50% concentration is approximately equal – around 1500 kg/m^3 , what is about 50% more than in case of pure water.

Energies in accumulator by fulfillment of $PS \cdot V \leq 200$ rule are higher than these of water in used concentration range only in case of MgCl_2 solution (Figure 10). Energy capacity of 10 l accumulator, filled with 15 kg of 50 % MgCl_2 solution is 1,7 kWh what is about 21% more than in case of pure water ($Q_{\text{vody}}^{10\text{L}} = 1,4 \text{ kWh}$).

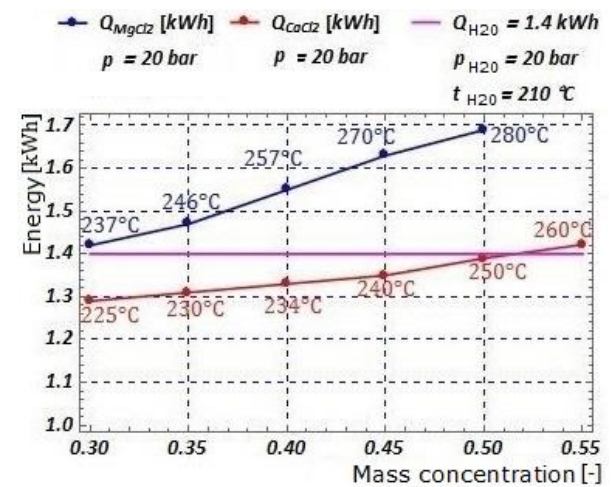


Figure 10 The comparison of energies of CaCl_2 and MgCl_2 water solutions with the energy of pure water

Another possibility how to store more heat energy in accumulator is division of one big volume V into smaller – elementary volumes V_{elem} . So can be nominal pressure PS in this elementary volumes higher ($PS \cdot V_{\text{elem}} \leq 200, V_{\text{elem}} \leq V, V = \sum V_{\text{elem}}$). Thus the sum of energies in elementary volumes is higher than energy in one big volume. The use of inner heat exchanger makes this concept easy.

As mentioned above, colligative – thermophysical properties of ionic solutions at high temperatures are not well known. Research of these properties can bring interesting results and not only these of binary solutions but solutions of water and mixture of many salts.

Essential for the use of heat accumulator is its ability to hold inner temperature as long as possible, also good thermal insulation. High demands fulfill the evacuation of inner pressure vessel also the use outer housing (Figure 11).

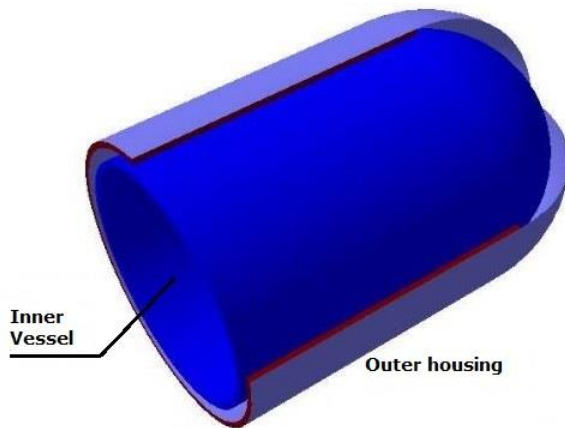


Figure 11 The design of thermal insulation for the heat accumulator

For example, waste heats of 10l accumulator with total area of $0,27m^2$, the gap between inner vessel and outer housing $\delta = 1cm$ and area of outer housing $0,31m^2$ by using of the evacuation range from 15 W (emissivity 0,02 of silvered areas) up to 123 W (emissivity 0,14 of glazed metal plate [15]). Thus times in which the storage medium in the accumulator cool down to the half of its initial teperature (in our case from $240^{\circ}C$ to $120^{\circ}C$) ranges from eight days for silvered areas up to one day for glazed steel (Figure 12). In reality are cooling times shorter due to thermal loses in the area of outlet pipes. But with appropriate design arrangements can the real cooling times approximate to ideal values.

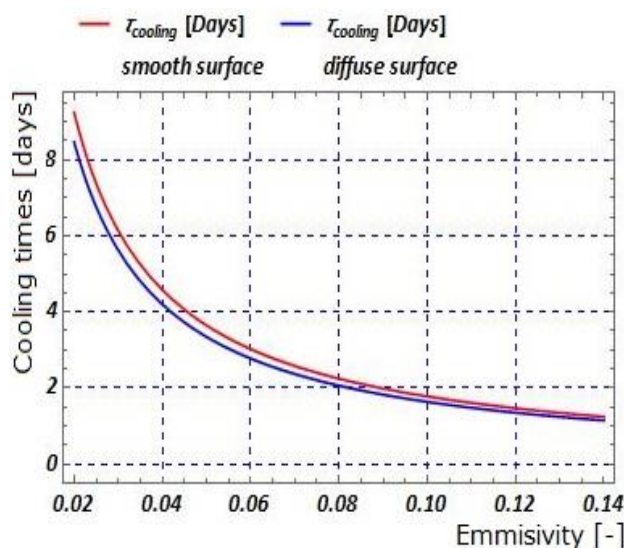


Figure 12 Ideal cooling times of the evacuated heat accumulator on the half of its initial temperature ($t_{ini} = 240^{\circ}C$) for various materials/surfaces ($\epsilon = 0,02$ silvered surfaces $\div$ 0,14 glazed steel)

4 The use of heat accumulator in real weather conditions – measurements of inner temperature and heating power

The inner temperature of storage medium in the accumulator is key parameter for determination of its actual resp. remaining energy Q_{rest} as well as consumed energy Q_{cons} . By current measurement of operational times of heating device we can calculate its average power $\bar{Q}_{aver}$ as well. Our experimental heat accumulator (Figure 13) had been not evacuated. It was insulated with rockwool. Thus its waste heats were much higher than by evacuation of accumulator. But thanks its position during measurements in rear space of car (Škoda Fabia) contributed its waste heats to heating of cabin air as well. Thus it could be considered as an ideal heat accumulator without heat losses.



Figure 13 Tthe experimental heating device in rear space of car

Testing driving route led from Stupava to the centre of Bratislava – bus station Mlynské Nivy (Figure 14). This route was chosen because it represents very good everyday driving to work, school etc. from surrounding country to the city centre. Time duration of this route is in ideal case between 23 and 26 minutes but in reality it is strong influenced by actual traffic situation. So can be driving time longer than one hour especially in traffic peaks.

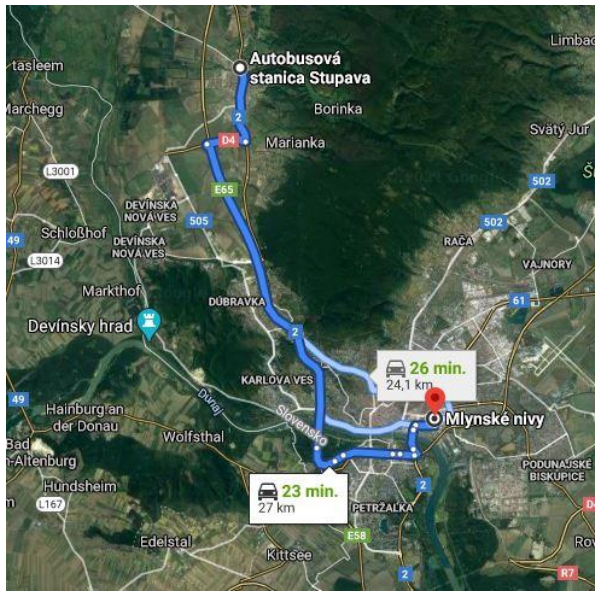


Figure 14 The route of measurement drivings

Accumulator with volume of 10l was filled with 15 kg of 50% $MgCl_2$ solution. Inner temperature on beginning of measurements was always $240^{\circ}C$ ($Q_{240^{\circ}C} \cong 1,22kWh, p = 8,8 bar$). Temperature sensor was placed direct in solution. Precision of temperature measurements was $\pm 1^{\circ}C$. The time duration of driving was measured as well in order to calculate average heating power. The average temperature of cabin air was adjusted constantly on $20^{\circ}C$. Its temperature sensor was attached on rear side of driver's seat at height of his head. The car was not thermal preconditioned at the beginning of measurements thus its initial temperature was always equal to ambient temperature. Measurements was done mostly evenings or by cloudy weather in order to eliminate the influence of sunlight. Main objective of this measurements was to prove its ability to heat and hold cabin air on demanded temperature during whole driving. Accumulator can be considered as discharged when its inner temperature drop to $100^{\circ}C$. The results of measurements are in table 4 and at the Figure 15 :

Table 4 (in two parts) : Measurement results, ($Q_{init} = Q_{240^{\circ}C} \cong 1,22kWh$)

Date	Beginnin g [hod]	End [hod]	Total time [min]	t_{okolia} [$^{\circ}C$]
11.02. 2021	16:35	17:17	42	- 10
12.02.	17:10	17:49	39	- 10
13.02.	17:04	17:45	41	- 7
14.02.	17:22	18:02	40	- 8
15.02.	16:44	17:22	38	0
20.02.	16:06	16:46	40	+ 5
21.02.	16:10	16:48	38	+ 2
28.02.	16:29	17:06	37	+ 8
09.03.	17:40	18:21	41	+ 1

Date	t_{accum}^{end} [$^{\circ}C$]	Q_{rest} [Wh]	Q_{rest}^{relat} [%]	$\bar{Q}_{aver}$ [W]
11.02. 2021	100,1	0	0	1742
12.02.	108,6	82	6,8	1749
13.02.	118,1	173,3	14,2	1532
14.02.	112,1	116	9,5	1656
15.02.	152	498	40,8	1140
20.02.	171,1	681	55,8	808
21.02.	162,3	597	48,9	983
28.02.	187,1	834	68,4	625
09.03.	149,1	470	38,6	1097

Where :

t_{accum}^{end} – temperature in accumulator at the end of driving

Q_{rest} – remaining energy at the end of driving (useful energy drops at $100^{\circ}C$ practically to zero)

$\bar{Q}_{aver}$ – average heating power

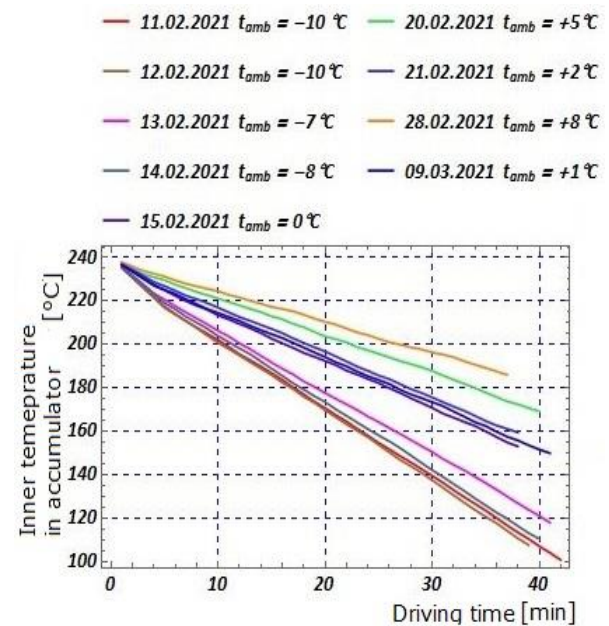


Figure 15 Inner temperatures in accumulator during the test drivings

As the results show could heat accumulator heated cabin air during driving in all cases. By lower ambient temperatures between $-10^{\circ}C$ and $-7^{\circ}C$, drop the useful energy in accumulator at the end of driving practically to zero. By ambient temperature between $0^{\circ}C$ and $8^{\circ}C$ remained in accumulator at the end of driving from 38,6 % up to 68,4 % of useful energy.

5 Conclusion

On the basis of performed measurements may be testified that the designed device proved very good by the practical use. Thus it is significant to investigate more the colligative – thermophysical properties of ionic solutions at high temperatures as well as to improve the design of heat accumulator and its connection into heating of cabin air in electric vehicles.

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Industrial-Scale Hydrogen Production Plant Modelling

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Abstract : Considering the process characteristics, hydrogen production via steam methane reforming is a vital part of oil refinery not just in terms of materials, but of energy integration as well. This work extends the mathematical model describing hydrogen production by ATE (Approach to Equilibrium) parameters implemented within the chemical reactors' models. Equations for ATE parameter prediction, i.e. mass flow of process feed (natural gas) and reaction temperature, were formulated. Verification of the whole model as well as of its parameters was performed using process data from a real hydrogen plant. The extended mathematical model is suitable for the evaluation of the influence of increased hydrogen content in natural gas on plant's material and energy efficiency, as renewable hydrogen injection and co-transport in natural gas pipelines in future is proposed by the European Union as a means of decreasing carbon dioxide emissions.

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1 Introduction

Nowadays, 63% of global demand for hydrogen [1] is used in chemical and petrochemical industry, where ammonia production is the largest consumer, followed by methanol production [2]. Moreover, hydrogen demand for ammonia and methanol production is expected to increase due to economic and population growth [3]. Refineries represent the second largest consumer of hydrogen with 30% market share [3] using hydrogen for hydro-processing of crude oil and petroleum products, which involves removal of impurities (sulphur, nitrogen...), as well as the production of lighter and more valuable fuels and materials [4].

Hydrogen production can be achieved in several ways: from fossil fuels, water electrolysis, biomass-based or biological production [5]. Natural gas steam reforming constitutes 48% of world's hydrogen production [5]. As it produces significant amounts of carbon emissions, there is a need to look for more environmentally friendly ways of production such as gasification of waste fuels [5,6] or usage of bioethanol instead of methane [7]. Another approach is focused on

enhancing the efficiency of natural gas steam reforming and carbon dioxide capture [8-10].

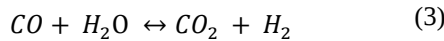
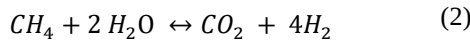
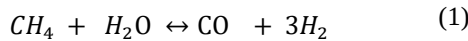
Within the plan of the European Union (EU) to cut down carbon emissions, enrichment of natural gas with hydrogen produced by water electrolysis, using electrical energy from renewable sources, has been considered [11]. One of the goals set in this plan is to reach 10% hydrogen content in the natural gas pipelines until 2030 [12], as this can be achieved without the need for significant investments to existing infrastructure. Thus the increased interest in the influence of hydrogen presence on flame characteristics [13], leakage of hydrogen in pipelines [14], their embrittlement [15], etc.. However, the impact of hydrogen presence in natural gas on hydrogen production by natural gas steam reforming remains unexplored.

The aim of this work is to extend the existing mathematical model of hydrogen production, based on material and energetic balances, by calculation of chemical equilibrium in chemical reactors [16] to evaluate the impact of hydrogen content in natural gas on hydrogen production efficiency of steam reforming. The Approach to Equilibrium (ATE) was chosen as a suitable way to assess real operation of chemical reactors, i.e. the deviation of the real composition of

outflow reaction mixture from its equilibrium composition. This approximation adjusts the calculation of system temperature on which the value of equilibrium constant is dependent. This simplification allows summing up the influence of various catalyst-, material- and process-related aspects on equilibrium, hence the composition of reaction mixture, by a single parameter value. Approaching the chemical equilibrium in the chemical reactor is dependent on factors such as reaction time and temperature, which were subjected to closer examination.

2 Mathematical model

Steam reforming chemistry is based on chemical equations (1), (2) and (3). Hydrogen yield depends on reaction temperature, pressure, ratio of steam and hydrocarbons in the reaction mixture, and ratio of hydrocarbons and hydrogen in the reaction mixture.



Design of the examined hydrogen plant is outlined in Figure 1. To preheated natural gas, high-pressure superheated steam is added in the mass ratio of approximately 1:3.5. This mixture is then preheated again and passed through pipes of a reforming reactor filled with Ni-containing catalyst. Temperature in this reactor is above 800°C, which favours reactions (1) and (2). Reaction mixture leaving the reforming reactor is cooled down in a steam generator to below 400°C and continues to a high-temperature shift (HTS) reactor filled with Fe-based catalyst, selective towards reaction (3) only. Under these conditions, carbon monoxide is transformed (shifted) to carbon dioxide and hydrogen. At the outlet of the HTS reactor, another steam generator is located followed by a series of heat exchangers, so the reaction mixture cools down to 40°C, as required for the Pressure Swing Adsorption (PSA) process. In PSA, pure hydrogen (over 99.9 % vol.) is separated from the reaction mixture, while the offgas from this process is burned in the reformer furnace as the main fuel, together with natural gas as the supplementary fuel.

Mathematical model of the plant is based on the solution of material and energy balances. As chemical equilibrium constants of reactions (1), (2) and (3) serve as a base for the reactors' material balances, equilibrium composition was calculated from equations (4) and (5) while equilibrium constants were calculated from equations of polynomial interpolation curves. Polynomial coefficients were evaluated from equations (6) and (7) using temperature dependent heat capacity,

formation enthalpies and entropies, in the temperature interval of (700 - 900) °C. The obtained coefficients of polynomial equation (8) are shown in Table 1.

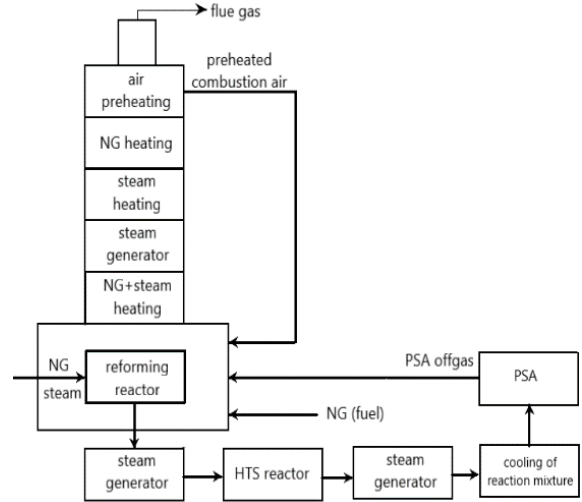


Figure 1 Scheme of steam methane reforming (SMR) hydrogen plant. HTS = high-temperature shift, NG = natural gas

$$K_a = \left(\frac{p}{p^\theta}\right)^{\Delta_v} \left(\frac{1}{\sum \dot{n}_i}\right)^{\Delta_v} \prod_{i=1}^I (\dot{n}_i)^{v_i} \quad (4)$$

$$\dot{n}_i = \dot{n}_{0,i} + \sum_{j=1}^J v_{ji} \xi_j \quad (5)$$

$$\Delta_r G = \Delta_r H - T \Delta_r S \quad (6)$$

$$\Delta_r G = RT \ln K_a \quad (7)$$

$$K_a = a(T - 273,15)^5 + b(T - 273,15)^4 + c(T - 273,15)^3 + d(T - 273,15)^2 + e(T - 273,15) + f \quad (8)$$

Higher hydrocarbons (C2+) present in natural gas were assumed to react quantitatively in the reforming reactor during reaction mixture heating, in accordance with their preferred reactions. Selection of the preferred reaction was based on the value of the corresponding equilibrium constant. Equilibrium constants were compared at 500°C, as this was the design temperature of the reaction mixture entering the reforming reactor. Reactions of higher hydrocarbons with the highest value of equilibrium constant are summarised in Table 2.

Steam production was also calculated. As it results from Figure 1, steam production takes place in convective section of the furnace of the reforming reactor and in steam generators placed before and after the HTS reactor. Heat flux was obtained using design temperatures, calculated composition of reaction

mixture and heat capacity in the form of polynomial coefficients. Enthalpy of water steam was taken from the h-s diagram.

Table 1 Coefficients of polynomial equation (8) describing equilibrium constant dependence on temperature for chemical reactions (1), (2) and (3)

	a (10 ⁻¹²)	b (10 ⁻⁹)	c (10 ⁻⁶)	d (10 ⁻³)	e	f
(1)	1.62	-5.18	6.61	-4.21	1.33	167
(2)	0.79	-2.47	3.10	-1.94	6.07	75.5
(3)	0.00	6.41	-0.14	1.13	-4.18	595

Table 2 Preferable reactions of higher hydrocarbons – stoichiometric coefficients of reactants and products

v	H ₂ O	CO	CO ₂	H ₂	CH ₄
C ₂ H ₆	-2	0	1	3	1
C ₃ H ₈	-3	2	1	7	0
C ₄ H ₁₀	-2	0	1	1	3
C ₅ H ₁₂	-2	0	1	0	4

3 Approach to Equilibrium

To assess the influence of uneven heat and mass transfer, uneven velocity profiles and mixing intensity, distribution of catalyst, etc., parameter Approach to Equilibrium (ATE) was employed. It was assumed that the above factors can be summed up by the change of equilibrium composition of the reaction mixture. As the deviation from chemical equilibrium is mainly determined by the reaction temperature, ATE value was added to the measured reaction temperature. Equilibrium constant for reactions (1) to (3) was calculated with the help of modified polynomial interpolation curves equations as shown in equation (9).

$$K_a = a(T - 273.15 - ATE)^5 + b(T - 273.15 - ATE)^4 + c(T - 273.15 - ATE)^3 + d(T - 273.15 - ATE)^2 + e(T - 273.15 - ATE) + f \quad (9)$$

The value of this parameter was first calculated from design data. Considering the design feed and comparing the calculated and designed composition of the reaction

mixture leaving the reforming reactor, ATE values for reactions (1) and (2) were calculated to obtain results as close to the design data as possible. Similarly, ATE value for reaction (3) was calculated by comparing calculated and design composition of the reaction mixture leaving the HTS reactor. The obtained composition of dry reaction mixture is provided in Table 3. These values are related to the ATE values given in Table 4. Difference of calculated and designed water steam production was below 1%.

The initial ATE values, valid for design conditions, were adjusted in accordance with the real reaction temperature in the chemical reactor and real mass flow of processed natural gas, equation (10), to achieve higher difference from the equilibrium composition due to reduced reaction rate as a result of lower reaction temperature. Similarly, higher mass flow of reaction mixture means shorter reaction time, thus higher difference from equilibrium composition can be expected.

Table 3 Comparison of design and calculated composition of dry reaction mixture
HTS = High-temperature shift

Mole %	Outlet/reforming reactor		Outlet/HTS reactor	
	design data	calc. data	design data	calc. data
H ₂	71.57	71.51	71.57	71.51
CO	12.39	12.45	12.39	12.45
CO ₂	8.54	8.56	8.54	8.56
N ₂	0.23	0.23	0.23	0.23
CH ₄	7.27	7.26	7.27	7.26

Table 4 Calculated approach to equilibrium (ATE) values for design data

ATE(1)	13.8
ATE(2)	16.8
ATE(3)	1.7

$$ATE = ATE_0 \frac{\dot{m}_{NG} T_0}{\dot{m}_{NG,0} T} \quad (10)$$

4 Results and Discussion

Hydrogen production plant operation data comprising nine months of operation were used for model verification. The data included mass flow of natural gas, steam mass flow, mass flow of recirculated hydrogen used for natural gas desulphurisation, combustion air mass flow and temperatures of reaction mixture leaving the reforming reactor and the high temperature shift reactor. Average composition of natural gas during the considered period was adopted [17]. Data measured during plant outage, as well as data measured during co-processing of refinery off-gases for hydrogen production were discarded.

Rates of reactions (1) and (2) were calculated by iteration, so the composition complied with equation (4), where equilibrium constant was obtained by equation (9). As the initial value for the iteration, ATE value adjusted by equation (10) was used. Calculated methane content of the reaction mixture leaving the reforming reactor was compared with the measured one and ATE parameter values for reactions (1) and (2) were iterated to minimise the difference between calculated and measured methane content.

Similarly, calculated carbon monoxide content of the reaction mixture leaving the high temperature shift reactor was compared with the measured one and ATE value of reaction (3) was iterated to minimise the difference.

This approach provided three ATE values daily for the data set; these values were further examined to determine their dependence on reaction temperature and natural gas mass flow, resulting in equation (11). ATE for reaction (1) is presented as an example.

$$ATE = a + b \dot{m}_{NG} + c T_R \quad (11)$$

Figure 2 provides the course of average daily temperatures measured in the reforming reactor and corresponding ATE values of reaction (1) for 145 days, followed by the outage of the steam reforming plant.

Equation (11) was used to predict ATE values. For this application, parameters of equation (11) were iterated to obtain predicted ATE values with the lowest sum of the squares of the deviations from calculated ATE values.

Comparison of calculated and predicted values of the ATE parameter of reaction (1) is shown in Figure 3.

As it can be seen in Figure 3, prediction of ATE values based on the values of natural gas mass flow and reaction temperature provides ATE values sufficiently close to the calculated ones. However, mass flow of natural gas and reaction temperature are not the only factors affecting the composition of the reaction mixture at the reactor outlet. Catalyst aging was also considered,

but this approach was later dismissed due to the lack of relevant data on the catalyst age.

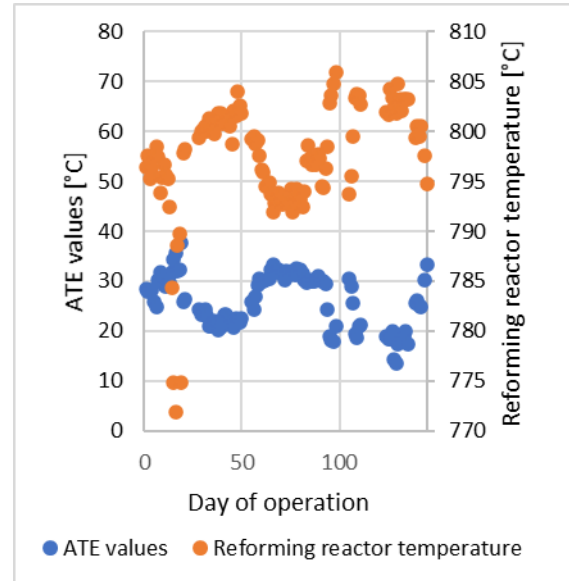


Figure 2 Average daily values of reaction temperature and calculated approach to equilibrium (ATE) value during plant operation

This approach was applied for each ATE parameter and the values of this parameter in equation (11) for reactions (1) and (2) are summarised in Table 5.

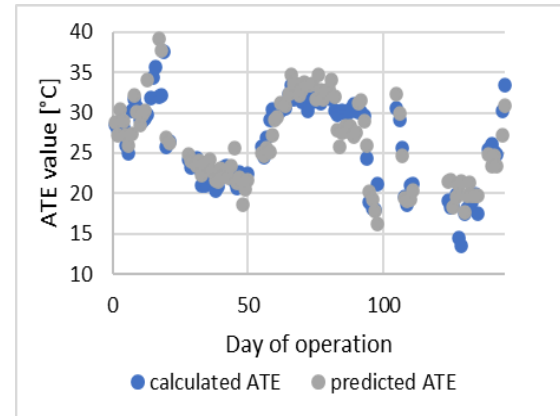


Figure 3 Comparison of calculated and predicted ATE values for reaction (1)

Table 5 Parameters of equation (11) for reactions (1) and (2)

	a [K]	b [10^{-3} K.h/kg]	c [-]
ATE of reaction (1)	1102.81	0.38	-1.35
ATE of reaction (2)	0.00	-1.81	0.05

To evaluate the dependence of reaction (3) on reaction temperature inside the reforming reactor (as this temperature determines the composition of the reaction mixture at the inlet of the HTS reactor), its ATE value was obtained using equation (12), parameters of this equation are provided in Table 6.

$$ATE = a + b \dot{m}_{NG} + c T_R + d T_{HTS} \quad (12)$$

Table 6 Parameters of equation (12)

a [K]	b [10^{-12} K.h/kg]	c [-]	d [-]
0.00	8.75	0.17	0.40

Equations (11) and (12) were included in the mathematical model and methane content of the reaction mixture at the outlet of the reforming reactor and carbon monoxide content at the outlet of the HTS reactor were determined.

Figure 4 shows the comparison of measured and calculated methane content of dry reaction mixture at the outlet of the reforming reactor. Calculated data were obtained using the original equation (6) and equation (11), for ATE parameters prediction.

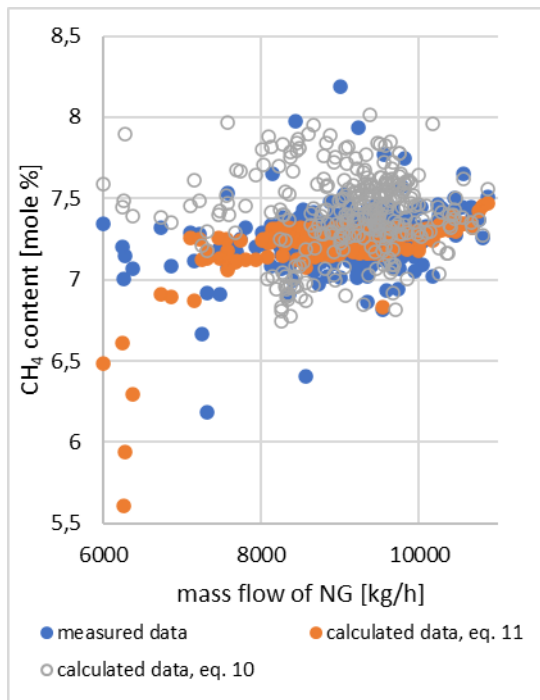


Figure 4 Comparison of measured and calculated methane content of dry reaction mixture at the outlet of the reforming reactor

As it can be seen in Figure 4, equation (11) results in smaller differences between measured and calculated data than equation (6). Despite the mismatch of some experimental data, it can be assumed that equation (11)

is capable of reliable prediction of ATE values used for the determination of the reaction mixture composition. Its use is limited to values of natural gas mass flow for hydrogen production in the range of 8 to 10 tons per hour. Mass flow below 8 tons per hour occurs only seldom. Thus, their impact on the overall accuracy of the model is negligible.

Similar comparison was performed to demonstrate applicability of equation (12) for the prediction of ATE value of reaction (3). Comparison of measured and calculated carbon monoxide content of dry reaction mixture at the outlet of the HTS reactor is shown in Figure 5.

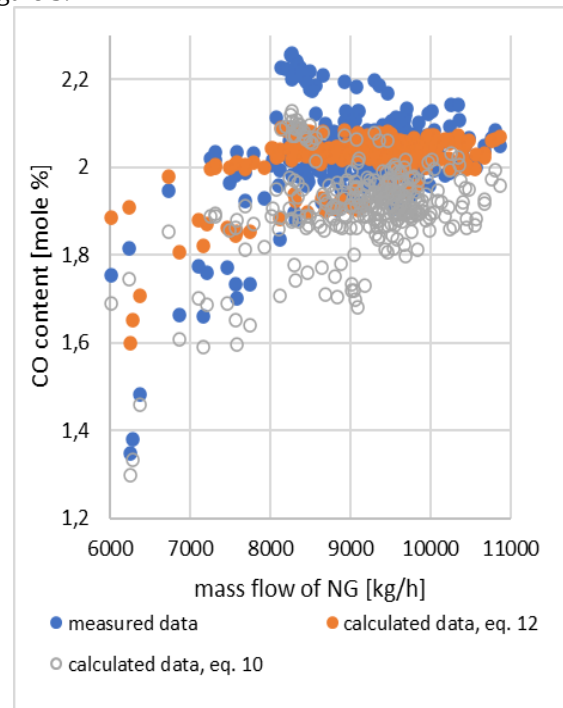
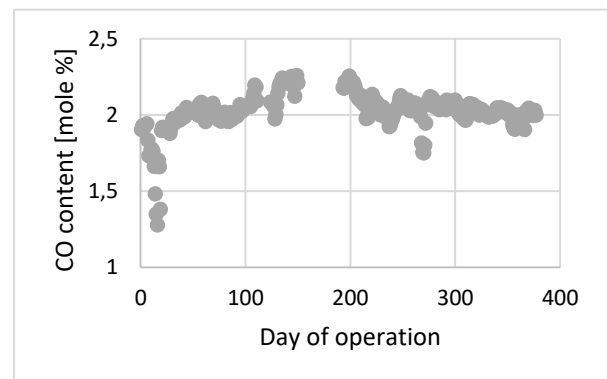


Figure 5 Comparison of measured and calculated carbon monoxide content of dry reaction mixture at the outlet of the HTS reactor

Figure 6 Measured carbon monoxide content at the outlet of the HTS reactor



Following the results shown in Figure 5, it is obvious that equation (12) accurately describes the composition of the reaction mixture at the outlet of the HTS reactor.

Figure 6 shows values of measured carbon monoxide content at the outlet of the HTS reactor. Similarly as in Figure 4, not all measured data were closely followed by the calculated ones. Inaccuracy is eminent for carbon monoxide content above 2.2 mole %, appearing shortly before the outage and a few days after the unit's repeated start of operation (Figure 6). As such high carbon monoxide content seldom occurs, sufficient model accuracy can be declared.

5 Conclusions

The aim of this work was to extend the existing mathematical model of industrial-scale hydrogen production plant by equations able to predict ATE parameters. The use of predicted ATE values in the plant model yielded outlet data in compliance with the measured ones. As these data are fundamental for reliable estimation of reaction mixture composition at the outlet of chemical reactors used for hydrogen production, they are also vital for the modelling of the whole process. On the other hand, this model is not suitable for the description of process behaviour before or after the plant outage. The presented mathematical model is applicable for the prediction of steady state process changes resulting from the higher hydrogen content in natural gas. Non-negligible differences of model results and measured data are visible shortly before and after the plant outage and can be attributed to unsteady state operation. Further model extension will be pursued in our future work.

Nomenclature

a, b, c, d, e, f : Coefficients of model equations
 ATE: Approach to equilibrium
 i : i -th component
 I : Number of elements in the system
 j : j -th chemical reaction
 J : Number of chemical reactions in the system
 K_a : Chemical equilibrium constant
 $\dot{m}$: Mass flow (kg.s^{-1})
 $\dot{n}$: Molar flow (kg.s^{-1})
 p : Pressure (Pa)
 R : Universal gas constant
 T : Temperature (K)
 ν : Stoichiometric coefficient
 ξ : Reaction rate (mol.s^{-1})
 $\Delta_r G$: Gibbs reaction energy (J)
 $\Delta_r H$: Reaction enthalpy (J)
 $\Delta_r S$: Reaction entropy ($J.K^{-1}$)

Indices:

RM: Reaction mixture
 NG: Natural gas
 HTS: High Temperature Shift (reactor)
 0: Initial (state, value)

θ : Standard (thermodynamic state)

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Determination of Pressure Loss of Silencers Used in Air Conditioning

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Abstract : When designing air conditioning systems, it is necessary to pay attention to the level of noise generated during the operation of such a system. Each of the components of the air conditioning system either absorbs or generates noise. Noise in pipes and fittings can be reduced to the required level by dimensioning the pipes. However, noise generated by the fan itself must be eliminated in another way. To eliminate fan noise, silencers are used in the duct just behind the air handling unit. For the correct design of the silencer, it is necessary to pay attention not only to its acoustic attenuation, but also to the pressure loss. If the pressure drop of the muffler is too high, noise will occur directly in the muffler. The pressure losses of the dampers are determined mainly experimentally. Based on the performed measurement, a CFD model of the selected damper was constructed, where the influence of various parameters on the value of the pressure loss of the selected damper was investigated.

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1 Introduction

At present, great emphasis is placed on reducing the noise associated with the operation of air conditioning systems, so components are built into the pipeline network, the task of which is to dampen and absorb this noise. However, for the correct design of the system, it is necessary to know the pressure loss of individual components of the pipeline network. In the practical design of a silencer, the pressure drop of this component is often forgotten and only its acoustic attenuation of the sound is evaluated. Today, an integral part of various measurements and experiments is a computational model constructed using CFD methods. The created computational model must be verified by measurement. This proven model can greatly facilitate further experiments, as it can be used to solve similar tasks.

2 Silencers in air conditioning

Air conditioning systems must meet strict hygiene standards that set maximum values noise in the room. Therefore, it is necessary to eliminate noise and vibration propagating from sources to other structures. The devices must be equipped with various dampers, inserts, etc., as the partial natural noise attenuation in the pipes and fittings is not sufficient [1-3]. In addition to noise attenuation using various elements used to attenuate noise, it is also possible to use the so-called passive elements. These are divided into the following categories:

- Reduction of the source - the value of the acoustic noise of the fan depends on the fan speed, therefore it is necessary to design the fan correctly,
- Disposition - it is necessary to pay attention to the distribution of individual noise sources,

- Sound insulation - by stripping the equipment and improving the acoustic properties of structures that separate noise sources from protected areas,
- Sound absorption - materials with good absorption properties, used as e.g. tiles or anti-vibration coatings increase the absorption of the structure. [4-8]

2.1 Modeled silencer

A link silencer was selected as the model damper. This type of shock absorber is one of the most commonly used shock absorbers in air conditioning. This type of silencer consists of a set mounted in a square pipe. The individual scenery consists of a sheet metal frame into which mineral wool wrapped in fabric is inserted. According to Gebauer [7], it is possible to regulate the acoustic performance of the system muffler by changing the number and dimensions of mounted scenes. A joint damper was selected as the model damper. This type of shock absorber is one of the most commonly used shock absorbers in air conditioning. This type of silencer consists of a set mounted in a square pipe. The individual scenery consists of a sheet metal frame into which mineral wool wrapped in fabric is inserted. According to Gebauer [7], it is possible to regulate the acoustic performance of the system muffler by changing the number and dimensions of mounted scenes.

The designed silencer consists of six backdrops. The dimensions of the damper are shown in Fig. 1. The spacing between the individual flanges is 66 mm, the spacing between the outer walls of the pipe and the flaps being 33 mm.

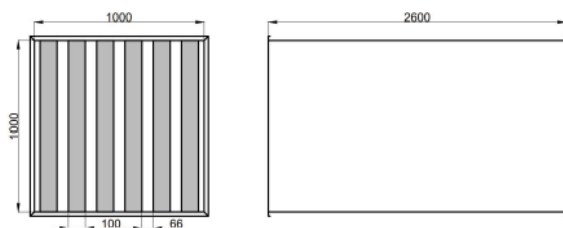


Figure 1 Cross section of modeled silencer

Each of the fitted links will be attached to the duct with rivets. The dimensions of the slide are shown in Fig. 2.

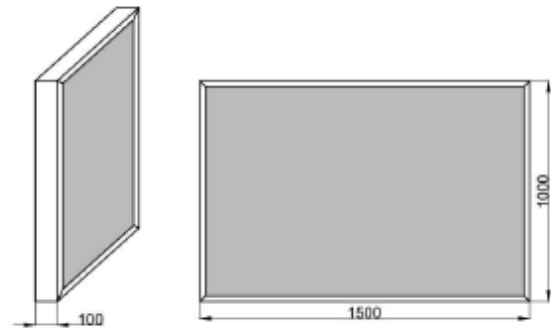


Figure 2 Backdrop inserted in silencer

3 CFD model

Based on the actual model damper, a CFD model was constructed using Ansys Fluent. To use numerical methods to calculate the pressure drop, it was necessary to construct a three-dimensional model of the real damper on which the measurement was performed. The geometry (see Figure 3) was made using Ansys Design Modeler software.

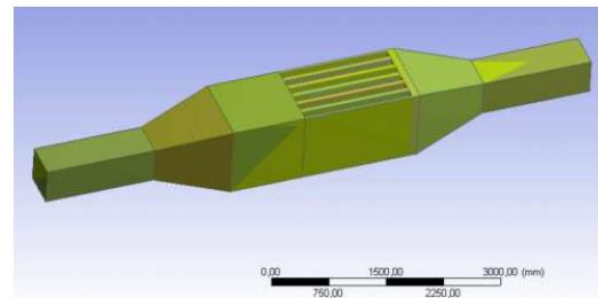


Figure 3 Geometry of modeled silencer

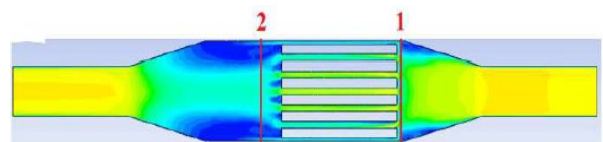


Figure 4 Velocity field in the cross section of the damper

In the model, a boundary condition was used for air entry into the duct (speed-inlet), where the air speed was entered according to the measured values. Next, a wall boundary condition was used to define the slides inserted into the channel. The resulting pressure difference consisted of subtracting the average value from planes 1 and 2, as shown in Figure 4.

According to Lenhard [11] the calculation model k- ϵ Realizable was chosen for the calculation, using the boundary conditions same as those measured during the measurement. The resulting value of the pressure drop and the local pressure drop coefficient are given in Table 1.

Table 1 Pressure loss values calculated by CFD

Volume flow	Δp [Pa]	ξ
3960	5,0	6,7
4366	6,0	6,7
4770	7,1	6,7
5172	8,2	6,6
5549	9,5	6,6
5972	10,9	6,6
6370	12,3	6,6
6700	13,4	6,4
7187	15,5	6,4
7562	17,7	6,5
7939	18,8	6,5

4 Experiment

The measurement was performed on a real silencer, constructed according to Fig. 6. The experiment consisted of measuring pressure drop, temperature, and flow rate using an ALMEMO 2690-8 measuring device. The flow rate was also measured using a Wilson grid with an Airflow PTSXR-K pressure transducer, to increase the measurement accuracy. The individual measuring instruments were connected as shown in the diagram in Figure 5.

Individual measurements were performed for different volume flow values. The flow control was performed using a frequency converter. The measurement started at a frequency of 20 Hz, which we gradually increased by 2 Hz up to 40 Hz.

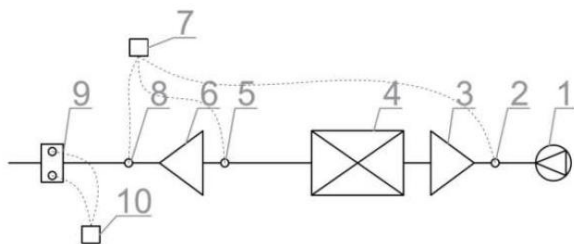


Figure 5 Measurement scheme (1-fan, 2-connection pressure measuring point, 3-pipe transition, 4-silencer, 5-connection point pressure measuring, 6-pipe transition, 7-measuring device ALMEMO 2690-8, 8-measuring measuring point speed, 9-Wilson grid, 10-pressure transmitter PTSXR-K)

The measurement of the pressure difference was performed according to Figure 5 in points 2 and 5. The resulting velocity was determined as the arithmetic

mean of the Wilson grid measurement and the average value determined by the ALMEMO velocity probe. Based on the resulting velocity, we determined the volume flow passing through the damper.

The results of individual measurements of the resulting pressure loss and the coefficient of local pressure losses are given in Table 2.

Table 2 Pressure loss values measured

Volume flow	Δp [Pa]	ξ
3960	4,5	6,2
4366	5,1	5,8
4770	6,5	6,2
5172	9	7,2
5549	10,2	8,9
5972	11,2	8,9
6370	13,2	8,9
6700	15,4	8,9
7187	16,6	6,9
7562	18,3	6,9
7939	21,9	7,5
Arithmetic mean		7,48

5 Discussion

Based on the performed measurement, mathematical model and CFD, we compared the individual values of pressure losses with the values of these losses calculated using the constructed mathematical model and at the same time with the calculation program for the design of silencers from Technov. A comparison of the resulting values can be found in the graph in Figure 6.

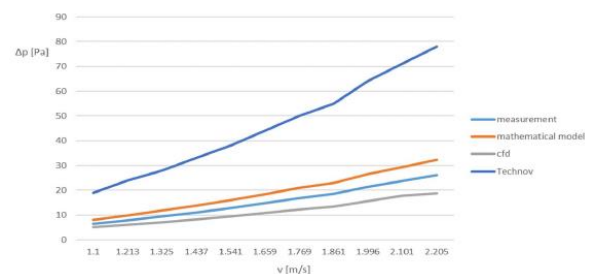


Figure 6 Comparison of achieved results

The above graph shows that the calculated and measured pressure loss values for the model silencer differ slightly. The largest deviation from the measured value is achieved by the calculation program of Technov. Based on this deviation, we can conclude that the program does not report the pressure drop correctly. The difference between the values in the mathematical

model and the measurement can be caused mainly by determining the coefficient of local pressure loss using the coefficients given in Chapter 3. In the mentioned literature, the application of the given graphs for use in air conditioning is not precisely determined.

6 Conclusion

The aim of this work was to verify the accuracy of the design program of slide silencers from Technov using CFD methods. In order to achieve the goal of the work, a mathematical model was made, which was constructed on the basis of available literature, but its accuracy is not sufficient.

The CFD model was constructed using the k-ε Realizable calculation model, which showed the most accurate results for the given application and at the same time the time required for the calculation was significantly shorter than with other models. However, for thorough verification of the model by experimental, it is necessary to perform measurements for other dimensions of link dampers. However, we were not allowed to experiment further in the current situation.

The result of the work is the finding that the application used for the application of silencers from the company Technov does not show the pressure losses of the link silencers correctly, but with a significant deviation from the measured value.

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