Use of methanol based syngas for waste heat recovery in vehicles

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1 Introduction

Electrification and hydrogen economy are touted as two alternatives to decarbonize transport sector. However, it is important to have a sustainable transition from oil and gas economy to these alternatives. Methanol, a liquid fuel with lowest carbon to hydrogen ratio can assist this transition. Methanol is a colorless, water soluble liquid with a mild alcoholic odour. Containing only one carbon atom, methanol is the simplest of all alcohols. During the world war era, synthetic methanol produced from coal was blended with gasoline as a fuel. Methanol-gasoline blends were used by Volkswagen and had shown significant improvement in cars performance. During 1990s, different technological advances were achieved and this reduced the emission problems and at the same time, decreased interest in methanol based fuels. Today, methanol is mainly used as a primary feedstock for the chemical industry with an approximate 70 million ton market per year . This clearly shows it has all the necessary infrastructure in place [1].

Methanol is a hydrocarbon which can be produced from numerous sources like syn-gas, oxidative conversion of methane and reductive hydrogenative conversion of carbon dioxide (CO_2). The chemical recycling of excess CO_2 would also help to mitigate the climate changes caused by use of fossil fuels [2]. The properties of methanol, ethanol and gasoline are provided in Table 1.1 [3].

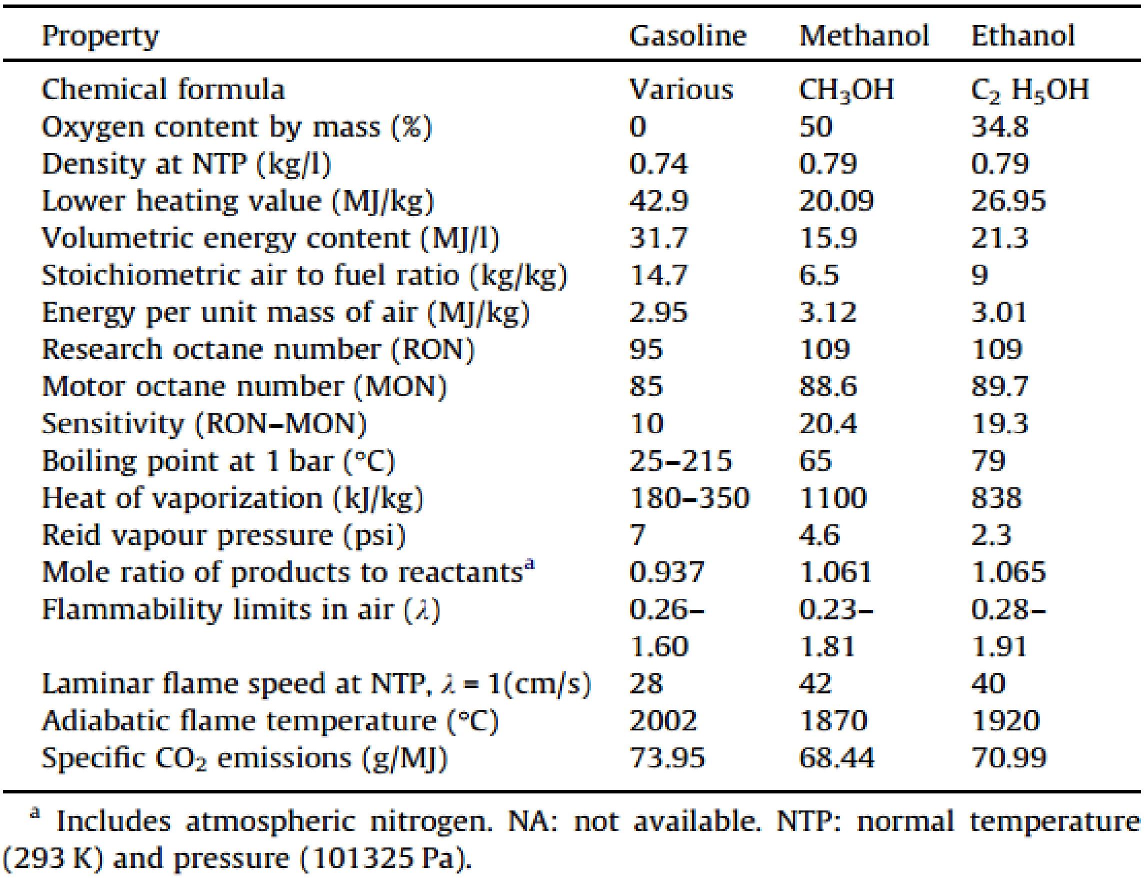
An unique advantage offered by methanol is thermo-chemical recuperation. Methanol can be decomposed to form hydrogen (H_2) and carbon monoxide (CO). The overall reaction is shown in equation 1.1 [4]. This mixture of gases is called a syngas (H_2 + CO). The heat content of syngas is 20.7 % more per unit mass than methanol. Even though ethanol can be converted to syngas, the C-C bond present requires higher dissociation energy.

$$CH_3OH \rightarrow 2H_2 \ + \ CO \qquad \Delta H^0_{298} \ = \ 90.7 \ kJ/mol \tag{1}$$

In an internal combustion engine, about 70 % of total energy is lost as low grade waste heat in coolant and high grade waste heat in exhaust gases. This energy can be used for splitting methanol in to H_2 and CO.

The present study is aimed at computationally evaluating the concept of a vehicle with methanol/ syngas as fuel with an onboard methanol splitter, henceforth called methanol thermo chemical recuperator (M-TCR). This study attempts to provide an overview about a fuel that has potential to supplant gasoline in the future. Methanol has an advantage of having the lowest carbon to hydrogen ratio for any liquid fuel. This helps in low carbon emissions. Furthermore, the increase in energy content of the fuel by splitting of methanol using exhaust waste heat increases overall efficiency of the engine. Hence, methanol can be seen as an unique and prominent answer to the conundrum of fuel crisis, low carbon emissions and increasing overall engine efficiency.

Table 1: Properties of Methanol, Ethanol and Gasoline



Property	Gasoline	Methanol	Ethanol
Chemical formula	Various	CH_3OH	$C_2\,H_5OH$
Oxygen content by mass (%)	0	50	34.8
Density at NTP (kg/l)	0.74	0.79	0.79
Lower heating value (MJ/kg)	42.9	20.09	26.95
Volumetric energy content (MJ/l)	31.7	15.9	21.3
Stoichiometric air to fuel ratio (kg/kg)	14.7	6.5	9
Energy per unit mass of air (MJ/kg)	2.95	3.12	3.01
Research octane number (RON)	95	109	109
Motor octane number (MON)	85	88.6	89.7
Sensitivity (RON–MON)	10	20.4	19.3
Boiling point at 1 bar (°C)	25–215	65	79
Heat of vaporization (kJ/kg)	180–350	1100	838
Reid vapour pressure (psi)	7	4.6	2.3
Mole ratio of products to reactants[a]	0.937	1.061	1.065
Flammability limits in air (λ)	0.26–1.60	0.23–1.81	0.28–1.91
Laminar flame speed at NTP, $\lambda = 1$(cm/s)	28	42	40
Adiabatic flame temperature (°C)	2002	1870	1920
Specific CO_2 emissions (g/MJ)	73.95	68.44	70.99

[a] Includes atmospheric nitrogen. NA: not available. NTP: normal temperature (293 K) and pressure (101325 Pa).

2 Setup

The first step was to design the setup. The amount of heat recoverable in M-TCR is limited due to the catalytic converter light off temperature. It was found that considerable amount of waste heat was used in the phase change process. Therefore, it was decided to pre-vaporize methanol and a separate phase change heat exchanger was placed after the catalytic converter. The setup used for the present study is shown in figure below.

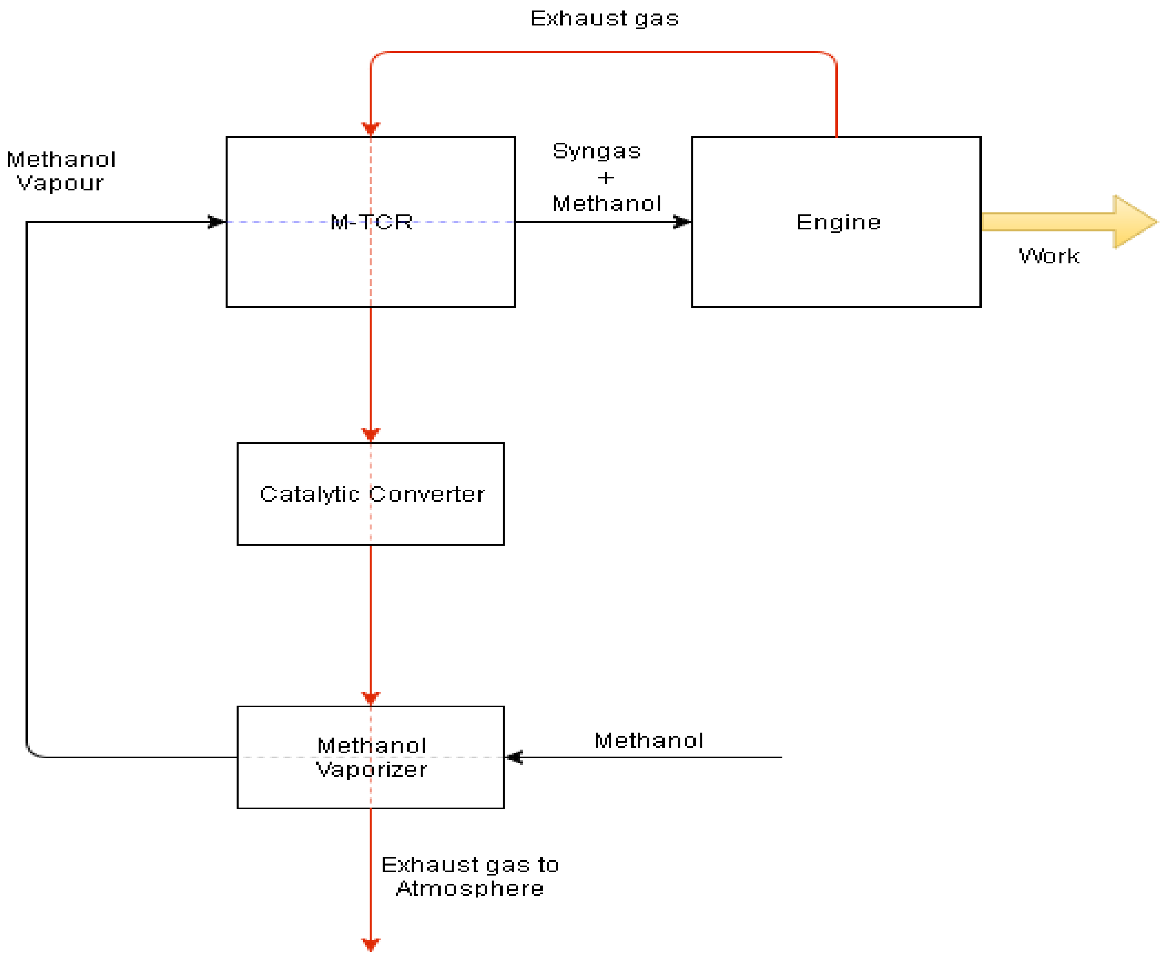


Figure 1: Schematic diagram of the system with pre-vaporizer

3 Methodology

The fundamental concept of this study is based on the endothermic reaction of methanol into a mixture of hydrogen and carbon monoxide. The reaction has been earlier illustrated. The comparison of lower heating values is provided in table below.

Table 2: Comparison of combustion properties of two fuels used in the study

Fuel	**Lower Heating value(kJ/kg)**	**Octane Rating (RON)**	**Laminar flame speed (m/s)(ϕ =1)**	**Source**
Methanol	19930	109	0.42	[3] [5]
Syngas	24063	$>$ 130 (H_2), 106 (CO)	2 (H_2), 0.16 (CO)	[6] [7] [8]

Firstly, a fuel-air standard Otto cycle simulation is run on MATLAB with methanol as fuel and the exhaust gas temperature is obtained. When the temperature is found to be sufficient, feasibility of this concept is checked by doing an analysis on a virtual engine test bench built on AVL Boost. After the feasibility is verified, engine maps of BSFC, exhaust gas temperature, emissions of CO, HC and NOx are obtained for different fuel blends from AVL BOOST.

In the next step, M-TCR model is built based on first law of thermodynamics with certain assumptions. The engine duty cycles for different driving conditions were obtained from previous studies. A tool is built on MATLAB integrating the engine maps and the M-TCR model.

Depending on the type of duty cycle, the engine spends significant amount of time under idle (no load) and fuel cut-off conditions. Hence, it is necessary to consider these states while building the tool. The tool reads the torque and engine speed value and determines the domain it is operating in and directly provides results in the idle and fuel cut-off domain. However, if it is under load, the tool reads the conversion rate from M-TCR and decides the blend to be used and provides the results for the chosen blend from the engine map for the required torque and speed demand obtained from engine duty cycle data.

Power integrator tool is used to compare the performance of a vehicle with and without M-TCR fueled with methanol for certain engine duty cycles obtained from real-world driving. This comparison demonstrates the practicality of this concept. Figure below provides an overview of how the tool developed using MATLAB works.

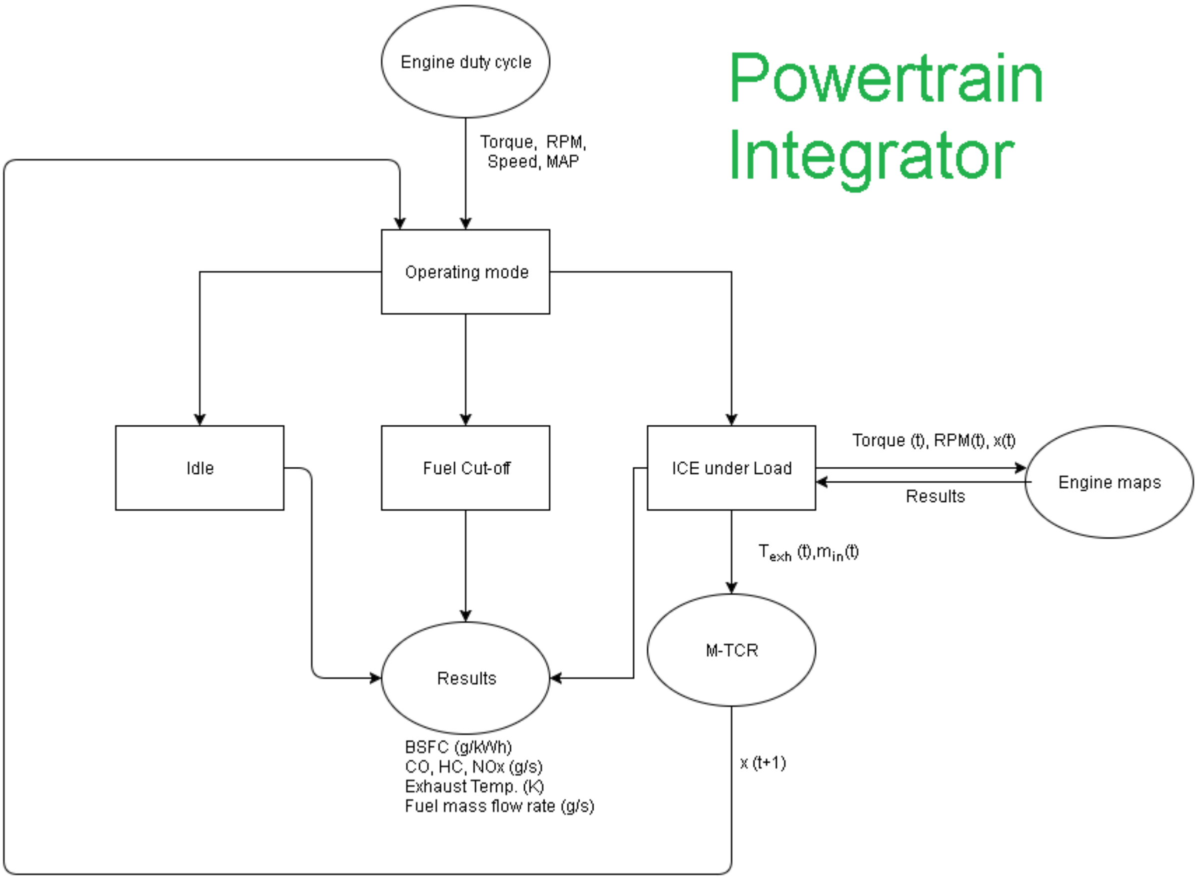


Figure 2: Powertrain Integrator schematic

4 Results & Discussions

In the present investigation, the results are obtained for three real world driving conditions. To check feasibility of the proposed concept on a engine, simulations are carried out using different blends of methanol and syngas (0, 25, 50, 75, 100 % by volume of methanol represented by M0, M25, M50, M75 ans M100 respectively) on AVL Boost. Engine performance and emissions maps are built at constant throttle positions. These maps are used to obtain results for different driving conditions.

Engine duty cycles for three driving conditions are analyzed. The three conditions and their characteristics are provided in table below [9].

Table 3: Average speed and power of the vehicle during three driving conditions under study

Cycle	Distance (km)	Avg. Speed (km/h)	Avg. Power (kW)
Highway	9.65	98.96	23.22
Sub-Urban	24.08	43.32	10.99
Urban	8.69	24.06	8.63

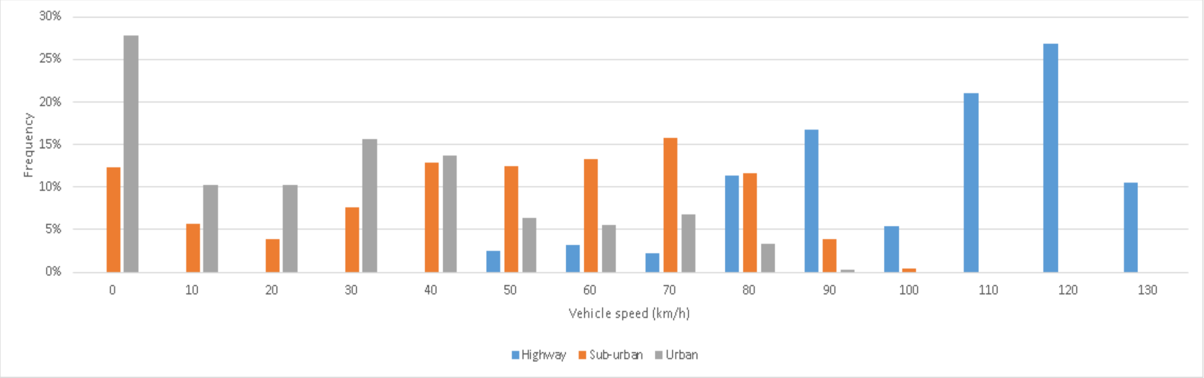


Figure 3: Histogram of vehicle speed for the three driving conditions considered

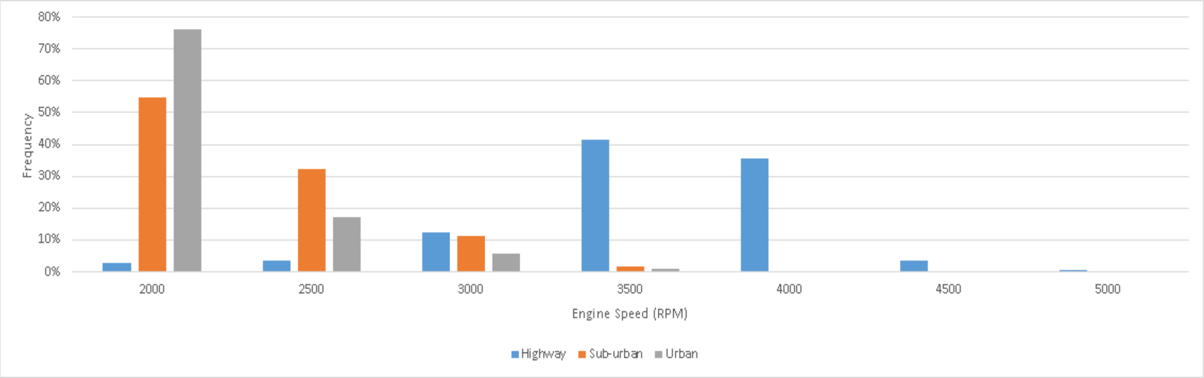


Figure 4: Histogram of engine speed for the three driving conditions considered

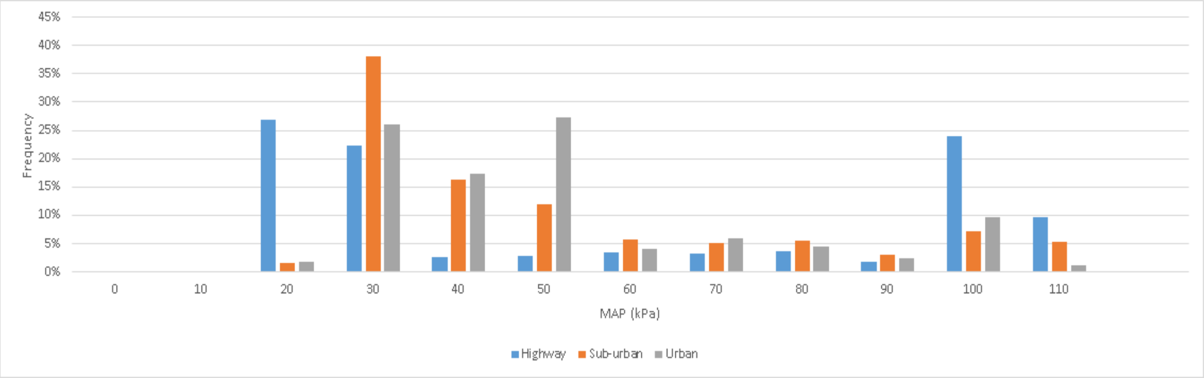


Figure 5: Histogram of MAP for the three driving conditions considered

From histograms above, it is observed that the vehicle is at higher speed at highway conditions and the speed under these conditions is never below 40 km/h. On the contrary, the vehicle is at a speed less than 40 km/h for more than 75 % of the time in urban driving conditions. Similar observations can be made in engine speed. During urban driving, engine operates at lower RPM most of the duration whereas in highway conditions, the engine operates at higher RPM for londer duration. It is interesting to note that MAP never goes below 10 kPa in all three driving conditions. From these histograms, it can be obeserved that the three cycles considered for the study are contrasting and therefore, these driving conditions test the robustness of M-TCR system.

To analyse the behaviour of the system in these three conditions, methanol is used as fuel with an onboard generator in a fictional vehicle and the results are shown figures below. The emissions provided are engine-out emissions and will require exhaust gas after-treatment to meet emission regulations.

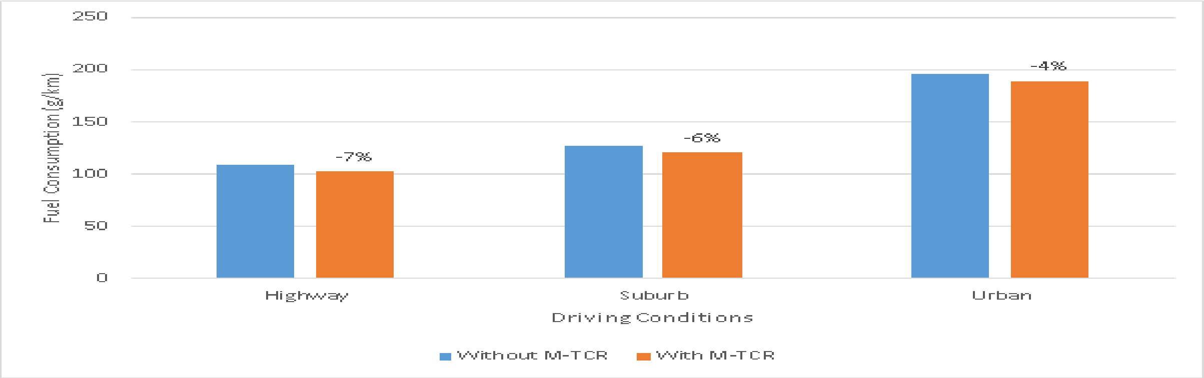


Figure 6: Fuel consumption for three driving conditions with and without M-TCR (The number on the bar graphs denote the % change)

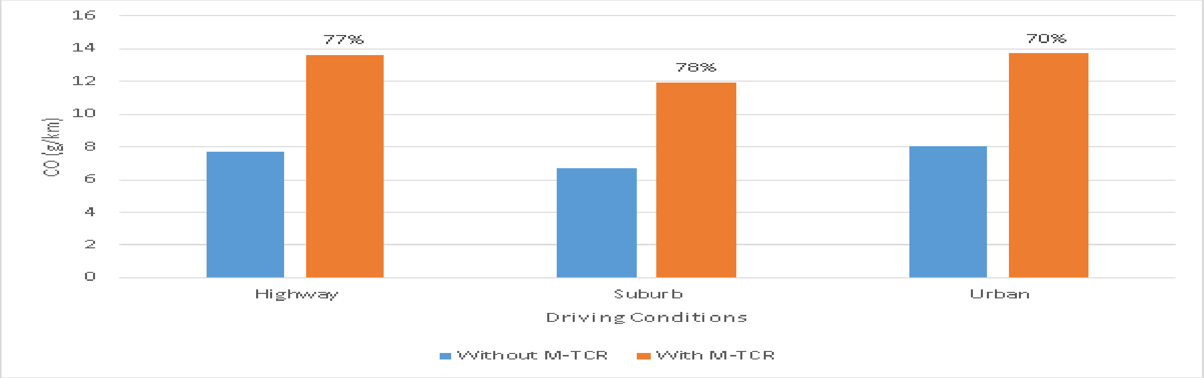


Figure 7: CO emissions for three driving conditions with and without M-TCR (The number on the bar graphs denote the % change)

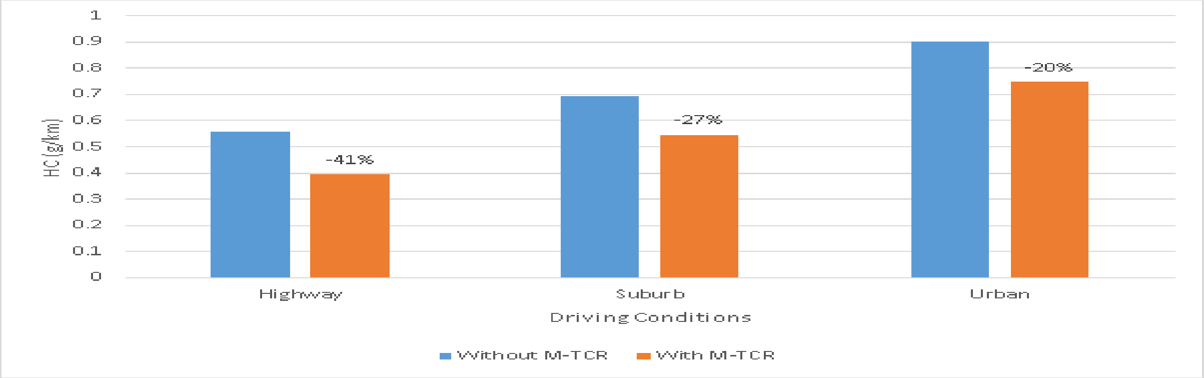


Figure 8: HC emissions for three driving conditions with and without M-TCR (The number on the bar graphs denote the % change)

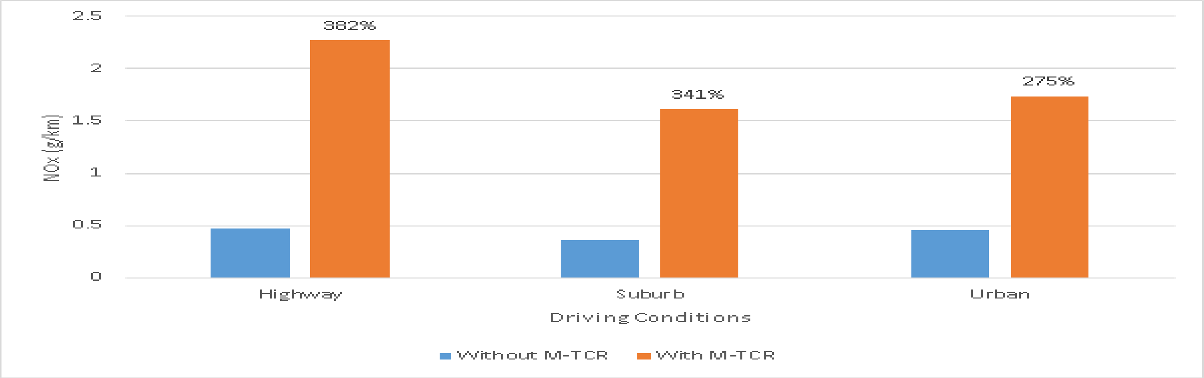


Figure 9: NOx emissions for three driving conditions with and without M-TCR (The number on the bar graphs denote the % change)

From the above figures, it is clear that M-TCR system increases energy efficiency. The fuel savings is about 7 g/km in each driving conditions which roughly translates to 139.51 kJ/km of energy savings. CO emissions are higher with M-TCR as the engine is running at stoichiometric conditions and the amount of CO in the fuel is higher in the vehicle with M-TCR. So, higher CO in case of vehicle with M-TCR is analogous to higher unburned hydrocarbons in case of engine running on gasoline under stoichimetric conditions. HC emissions are lower in case of vehicle with M-TCR due to lower H-C bonds in the fuel compared to the vehicle running on pure methanol. NOx emissions are higher due to higher combustion temperatures in case of vehicle with M-TCR. Even though engine-out exhaust gas emissions are higher in case of vehicle with onboard M-TCR, this can be easily treated using three way catalysts. Average BSFC for the whole and average conversion rate under three driving conditions is provided in the table below. Average BSFC is calculated from the total fuel consumed and overall power demand of the whole cycle.

Table 4: Average BSFC and average conversion rate under different driving conditions

Driving conditions	Avg. BSFC (g/kWh)	Avg. Conversion Rate (%)
Highway	437	77
Sub-urban	475	59
Urban	527	45

The average conversion rate is calculated by the ratio of mass of syngas used to the mass of fuel used in each driving condition. The average BSFC is the highest and the conversion rate is the lowest in case of urban driving conditions and vice versa in highway conditions. This effect is due to different conversion rates and driving conditions. The conversion is higher in highway condition and the driving is more consistent. Hence, these two effects add up in reducing the fuel consumed per unit energy. The vehicle spends considerable amount of time in idle conditions where the fuel consumption per unit energy is very high. On the other hand, the vehicle spends a lot of time in fuel cut-off mode in highway conditions, leading to a lesser fuel consumption per unit energy. Fluctuation between these modes changes the matrix temperature leading to different conversion rates. A histogram of % of time spent in the three operating modes for different driving conditions is provided in the figure below.

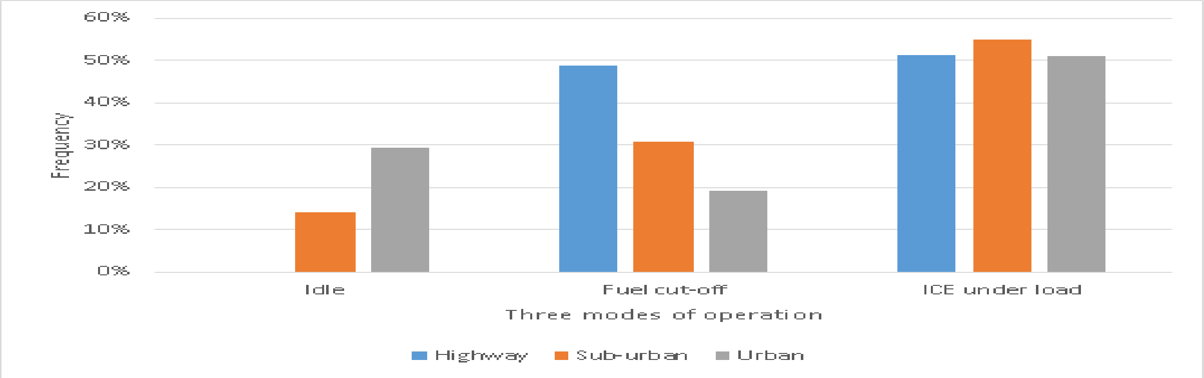


Figure 10: Percentage of time spent in three modes of operation for three driving conditions

From this figure, it is clear that the efficiency of the system drops significantly when the engine operates in idle mode. Similarly, fuel consumption is lower when there is increase in the time spent on fuel cut-off mode.

5 Conclusions

Methanol has a unique property of thermo chemical recuperation. The present study exploits this property using the exhaust waste heat from an internal combustion engine for the endothermic reaction and evaluates its feasibility and utility in real world applications.

The following conclusions can be made from the present investigation:

- There is sufficient heat in the exhaust to convert methanol into a mixture of two moles of hydrogen and one mole carbon monoxide (a syngas). This syngas has about 20 % more energy content per unit mass compared to pure methanol.
- Eventhough the syngas has higher energy content, it displaces some amount of intake air and hence the power output is lower per unit volume of charge compared to pure methanol. However, the amount of fuel required to produce unit energy is lower for syngas compared to methanol.
- Due to the limitation on the amount of heat that can be recovered before the catalytic converter, the design of the whole system has a prominent role in increasing the overall efficiency of the system. A system with methanol pre-vaporizer increases overall efficiency due to higher conversion rates.
- For a given load, BSFC and HC emissions are lower for M0 compared to M100. But, the CO and NOx emissions show the opposite trend. Similarly, for a given speed, BSCO and BSNOx are higher for M0 than M100 and BSHC is lower for M0 than M100.
- The simulations have been performed for three driving conditions (Highway, Sub-urban and Urban). The average BSFC is lower for highway conditions compared to the other two conditions due to the absence of idling and half of the time spent on fuel cut-off mode. Due to lower fluctuations in average M-TCR matrix temperature, the conversion rate is higher in this driving condition compared to other two conditions. It is also discovered that using a exhaust gas bypass during idling and fuel cut-off conditions prevents the cooling of M-TCR matrix (exhaust gas temperature is lower than the matrix temperature).
- The overall energy efficiency increases with the use of M-TCR system. Due to the lower amount of fuel burnt, CO_2 emissions are lower. However, with the M-TCR system NOx and CO emissions increase. Hence, a catalytic converter is essential to meet the stringent emission reduction norms. Another way to circumvent this issue is to use ultra lean mixtures in the engine. The presence of hydrogen in the fuel after conversion provides wider flammability range and may even support qualitative governing in the future.

Summarizing, the proposed concept of onboard M-TCR and its utility has shown feasibility in an automotive vehicle.

References

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