

Modeling Internal Combustion Engine with Thermo-Chemical Recuperation of the Waste Heat by Methanol Steam Reforming

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ABSTRACT

This paper describes a model for the simulation of the joint operation of internal combustion engine (ICE) with methanol reformer when the ICE is fed by the methanol steam reforming (SRM) products and the energy of the exhaust gases is utilized to sustain endothermic SRM reactions. This approach enables ICE feeding by a gaseous fuel with very favorable properties, thus leading to increase in the overall energy efficiency of the vehicle and emissions reduction.

Previous modeling attempts were focused either on the performance of ICE fueled with SRM products or on the reforming process simulation and reactor design. It is clear that the engine performance is affected by the composition of the reforming products and the reforming products are affected by the exhaust gas temperature, composition and flow rate. Due to the tight interrelations between the two main parts of the considered ICE-reformer system, it is desirable to create a single model that simulates joint operation of the ICE and the SRM reactor. Such a model is built with the GT-Power software. It employs published catalytic reactions kinetics. The reformer model is validated using experimental results from a small scale model reactor.

The developed model can be used for the performance optimization of the whole ICE - reformer system including design of the reactor. Simulations with a reformer bed geometry of counter current, multiple tubes performed using the developed model show that heat-transfer is limiting the reformer size, requiring 1.5 m² for complete methanol conversion in lean operation of a 75 kW ICE. Moreover the model can be applied to predict a transient behavior of the system owing to the time dependent approach implemented in the reformer and engine calculations.

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INTRODUCTION

Internal combustion engine is the main power plant in most of the modern transportation systems. As such, it is responsible for a substantial part of petroleum fuel consumption as well as environmental pollution. This fact together with a need for a dramatic greenhouse gas emissions reduction provides a powerful incentive to design energy efficient vehicles operated with alternative fuels. This approach can reduce the economic dependence on expensive oil, contribute significantly to climate change mitigation and decrease the global pollution [1].

Since about 30% of the fuel's energy is wasted along with the hot exhaust gases, utilizing a part of this energy is one of the promising methods of engine efficiency improvement. The most common way of waste heat recovery is turbo-charging. Another way - is by using the energy of exhaust gases to promote endothermic reactions of fuel reforming. This method is frequently called thermo-chemical recuperation (TCR) [2]. TCR can be more profitable than turbo-charging because its

energy transfer is not bounded by isentropic expansion. The idea of TCR through methanol decomposition or reforming is not new and has been investigated in the last few decades. Pettersson et al [3] summed most of the research conducted up to the early 90's. Finegold et al [4] and Takayuki et al [5] had even built cars with on-board methanol decomposition reporting up to 40% increase in efficiency compared to a same type gasoline operated vehicle. Brinkman and Stebar [6] pointed out that a major contribution to the efficiency increase is due to the favorable properties of the decomposition products such as higher flame speed and octane number, wider flammability limits etc. compared to gasoline. The main problems reported in these preceding studies are backfire, coke formation on the reformer, cold start difficulties, lower maximum power due to reduced air charging, formaldehyde formation (in the cases of liquid methanol burning) and pre-ignition.

Research groups from MIT, AVL and MONSANTO [7, 8, 9, 10] overcame some of these drawbacks by feeding the ICE with low temperature ethanol reformat consisted of equal molar fractions of hydrogen, CO and methane. Their studies show brake thermal efficiency (BTE) improvement of 10-17% and 20-25% compared to an ICE fed with E85 and gasoline, respectively. Tartakovsky et al [11, 12] proposed a hybrid direct injection (DI) ICE-methanol steam reforming system (shown in fig. 1) as another way of solving these problems. The paper explores this scheme.

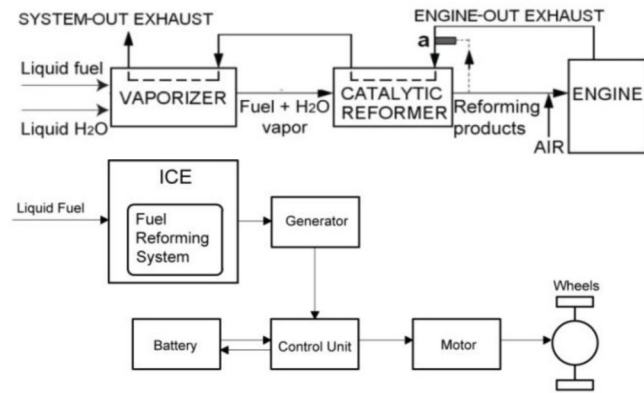


Figure 1. Vehicle hybrid propulsion system (bottom) with onboard fuel reforming (top).

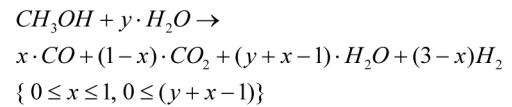
The battery of the hybrid system can be used as an energy source for cold start; SRM is less sensitive to coke formation than methanol decomposition; and the DI method can allow increase in the ICE maximum power output and deal with pre-ignition problems. In a further investigation [13] they performed simulation and performance comparison of an ICE fed with different reforming products. The reforming products compositions used in [13] were derived from equilibrium calculations that were empirically corrected in case of methanol steam reforming. No assessments were made about availability of the energy required to sustain the considered reforming processes. It is clear that the engine performance is affected by the composition of the reforming products and the reforming products are affected by the exhaust gas temperature, composition and flow rate. Due to the tight interrelations between the two main parts of the considered ICE-reformer system, it is desirable to create a single model that simulates their joint operation.

Such a model can be used for determining the required properties of the reformer and its design. It can provide a tool for optimizing the design and operation parameters of the ICE-reformer system. Further on, this model can be applied to shed a light on the complicated transient behavior of the system. The importance of the model is that it provides a rather simplified way of exploring any ICE-reformer system by using the GT-Power software, and thus can help other research groups working on other TCR schemes.

In the current work the GT-Power based ICE model described in [13] is applied to simulate joint operation of direct-injection ICE with SRM reactor. It was applied to provide preliminary considerations on design requirement for the reformer.

STEAM TO METHANOL RATIO SETUP

There is a general consensus that the most active and selective catalysts for the endothermic SRM reaction are CuO/ZnO/Al₂O₃ based catalysts [14], hence the same type of catalyst was chosen for our simulations. The steam to methanol (or S/M) molar ratio in the reformer feed is an important parameter for its operation. Specifically, S/M ratios lower than 1 can provoke coke formation and deactivation of the catalyst and may also result in slower reaction rates. Due to these problems, most of the SRM research is focused on S/M ratios greater than 1 and we have used this limit in our work, as well. Choi and Stenger [15] found that at S/M ratios higher than 0.76 the products of SRM can be considered to be limited to CO, CO₂, H₂O and H₂. For a given reformer size, the highest possible methanol conversion is an important condition for achievement of better efficiency and emissions reduction benefits. Thus, reforming conditions enabling maximal methanol conversion should be realized. Taking this into account, the following overall reforming reaction is preferred:



(1)

where x is often referred to as CO selectivity factor [16].

This equation shows that the only factor affecting the lower heating value (LHV) of the reforming products is x and that the LHV of the mixture is rising linearly along with x . Higher S/M ratios lead to decrease of CO formation [17] and hence reduce the heating value of the SRM products. Furthermore the heat required for the evaporation of the added water will demand a larger heat transfer area between the exhaust gases and the fuel mixture at the evaporator. Agarwal [18] suggest that increasing S/M to 1.4 might increase the SRM reaction rate, thus enabling to downsize the reformer, but experiments made by Santacesaria [19] agree with his findings only at low temperatures (lower than 180 °C). Observations made by Lee et al [20] totally contradict these findings. Taking this information into account, it seems that for an ICE-SRM system the preferable S/M ratio should lie between 1 and 1.4. All the simulation results presented in this work were performed for S/M ratio of 1.

REFORMER MODELING

The GT-Suite package provides tools for modeling heat exchangers and chemical reactions. Chemical reactions are modeled through the use of "Global-Reactions" template and are usually used to simulate chemical reactions in the exhaust aftertreatment systems. There are also

exchanger modeling. However, the “Global-Reactions” template cannot be used within one of the heat exchanger templates and GT-Suite does not have a built-in template for modeling a heat exchanger-reactor. Although GT-Power can cooperate with other modeling applications, it is clear that a solution within the program is superior in terms of computation time, model complexity and flexibility. Therefore, it was decided to develop a physical model that can be applied within the GT-Power software.

Physical Model

A 1-D homogeneous reformer model (i.e., ignoring interphase and intraphase concentration and temperature gradients) of a packed bed reactor (PBR) is considered. This type of reactor is very common for SRM, and enables changing the catalyst type and pellets size. Also, radial gradients are assumed to be negligible [21]. Moreover, combining the solid and gas phases into a pseudo-homogenous medium model makes possible a reasonable approximation of both flow and heat equations under low Mach and Reynolds numbers [22, 23, 24, 25]. It is not yet clear whether the total SRM reaction is better described by methanol decomposition ($\text{CH}_3\text{OH} \rightarrow \text{CO} + 2\text{H}_2$) followed by water gas shift (WGS) ($\text{H}_2\text{O} + \text{CO} \rightarrow \text{CO}_2 + \text{H}_2$) [14] or by direct SRM followed by reverse WGS (r-WGS) [16, 17]. If an empiric power law rate equation is used instead of a full kinetic derived schemes, either of the proposed paths can be chosen since they are linearly dependent. This approach leads to a set of 4 equations derived from the mass and energy conservation laws.

Mass conservation equations:

$$A_t \cdot \varepsilon \cdot \frac{\partial C_{\text{CH}_3\text{OH}}}{\partial t} = -\frac{\partial F_{\text{CH}_3\text{OH}}}{\partial z} - A_t \cdot \varepsilon \cdot r_1 \cdot \rho_{\text{cat}} \quad (2)$$

$$A_t \cdot \varepsilon \cdot \frac{\partial C_{\text{CO}_2}}{\partial t} = -\frac{\partial F_{\text{CO}_2}}{\partial z} + A_t \cdot \varepsilon \cdot (r_1 - r_2) \rho_{\text{cat}} \quad (3)$$

Energy conservation equations for counter current flow:

$$A_t \cdot \rho_{\text{eff}} \cdot C_{p_{\text{eff}}} \cdot \frac{\partial T_{\text{eff}}}{\partial t} = \left(-\frac{\partial \left(\sum_{i=1}^5 C_{p_i} \cdot F_i \cdot T_m \right)}{\partial z} + A_t \cdot k_{\text{eff}} \frac{\partial^2 T_{\text{eff}}}{\partial z^2} + A_t \cdot (\Delta H_1 \cdot r_1 + \Delta H_2 \cdot r_2) \rho_{\text{cat}} + U \cdot P \cdot (T_{\text{exh}} - T_{\text{eff}}) \right) \quad (4)$$

$$A_s \cdot \rho_{\text{exh}} \cdot C_{p_{\text{exh}}} \cdot \frac{\partial T_{\text{exh}}}{\partial t} = \left(-\frac{\partial (C_{p_{\text{exh}}} \cdot F_{\text{exh}} \cdot T_{\text{exh}})}{\partial z} + A_s \cdot k_{\text{exh}} \frac{\partial^2 T_{\text{exh}}}{\partial z^2} - U \cdot P \cdot (T_{\text{exh}} - T_{\text{eff}}) \right) \quad (5)$$

Where:

C_i -Molar density of species i ; F_i -Molar flow rate of species i ; A_t -Cross sectional area of the PBR; ε -Porosity of the PBR; ρ_i -Density of species i ; C_{p_i} -Constant pressure molar heat capacity of species i ; A_s -Cross sectional area of the exhaust gas flow; U -Overall heat transfer coefficient; P -Wetted perimeter between exhaust gas and reforming products; T_i -Temperature of species i ; k_i -Heat conductance of species i ; z -Length coordinate along the PBR axis; r_1 -SRM reaction rate per unit of catalyst load. r_2 -RWGS reaction rate per unit of catalyst load; ΔH_1 -SRM heat of reaction; ΔH_2 -RWGS heat of reaction. Subscript: *eff*-Effective property of the pseudo-homogenous medium; *exh*-Exhaust gases; *cat*-Catalyst;

The boundary conditions are the properties of the exhaust gas and the evaporated water-methanol mixture at the entrance to the reformer.

Reaction Kinetics

Many reaction rate expressions have been proposed for r_1 and r_2 . Each of them was derived from a different experimental setup, operating conditions and catalyst types. In some of the provided reaction rates, diffusion limitations are already incorporated, in some effectiveness factor should be applied and others use temperature related polynomial to extend the limits of their expressions. Therefore, it is critical to be careful in choosing the right reaction rate and, if possible, to make experiments and derive relevant and more accurate rate expressions. Empirical reaction rate is usually the Arrhenius type expression of the form:

$$r = k_1 \cdot f_1(T, P) \cdot \exp\left(\frac{-E_{a,1}}{R \cdot T}\right) \cdot \prod P_i^{S_{i,1}} - k_{-1} \cdot f_{-1}(T, P) \cdot \exp\left(\frac{-E_{a,-1}}{R \cdot T}\right) \cdot \prod P_i^{S_{i,-1}} \quad (6)$$

k_i -Pre-exponential rate constant; E_a -Activation energy; R -Universal gas constant; T -Temperature; P_i -Partial pressure of species i ; S_i -The reaction order related to species i ;

We incorporate two reactions: the practically irreversible SRM (at 1 bar) and the reversible r-WGS. The SRM is described by the power law reaction rate expression based on Purnama's [16] for a $\text{CuO}/\text{ZnO}/\text{Al}_2\text{O}_3$ catalyst, in temperatures above 230 °C:

$$r_1 = 1.95 \cdot 10^5 \cdot \exp\left(\frac{-76[\text{kJ/mol}]}{R \cdot T}\right) P_{\text{H}_2\text{O}}^{0.4} \cdot P_{\text{CH}_3\text{OH}}^{0.6} \left[\frac{\text{mol}}{\text{s} \cdot \text{g}_{\text{cat}}}\right] \quad (7)$$