ChE 345

Process Control, Modeling and Simulation

Final Project

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Modeling Efficiency of a Catalytic Convertor in a Diesel Engine

U.S. patent 9533295-B2 is focused around different composition and arrangements of zeolites in a catalytic converter for a light duty-engine (see **Figure 6**). The standard structures of zeolites tested in this patent include, Beta (see **Figure 1**), MWW (See **Figure 2**), and ZSM-5. These are all different base structures to which a silica powder is applied. The silica serves as the support structure for a palladium-platinum catalyst. Although some tests included silica with aluminum dissolved interstitially (at around .01%), these tests were excluded from the model as they caused inconsistencies and overcomplicated the transfer function derived for this model. The objective of the catalytic converter is to reduce the emission of Hydrocarbons, CO, and NOx by converting them into N2, CO2, and H2O. According to Table 3 in the patent, the Beta zeolite formation with no Al present was most effective in converting the target emissions to less-toxic components.

To approximate a model for the conversion efficiency of any given arrangement of zeolite and catalyst support structure, the team used the data provided in the patent and made some approximations. The data found in Table 3 the patent (**Figure 9**) in gave some insight at a reasonable target range of efficiencies for catalytic converters, and ultimately a target of 56.9% conversion was selected for the model (See **Figures 4&5, 2A**). The derived transfer function used to describe the conversion is a second order function, with numerator dynamics. In the model, there are two states of operation: when the engine is on, and when the engine is turned off. Since the catalytic converter is a passive system and requires no independent power, conversion is 0% when the engine is off, and follows the derived function when turned on. The team assumes a second order function, beyond what the provided data shows, because the team assumes the volumetric flow of exhaust out of the engine exponentially increases from when it is turned on. This means during the first few seconds or milliseconds of operation, there is relatively low emissions for what the converter is designed for, and all operational sites on the converter are active and ready to convert. This yields a short spike in conversion efficiency quickly followed by a non-oscillating approach to steady state. The team used a non-oscillatory approach to steady state because although it creates a slower response time for the model, the time lost is negligible due to inconsistent emissions output of the engine. We assume variable emissions out of the engine due to fluctuating piston firing temperatures, as well as changes on volumetric flow, both characteristics of common engines that negate the need for rapid response in the converter model.

In addition to zeolite configuration efficiency, the team modeled the effect of temperature on conversion efficiency. That patent states that the nominal operating temperature for the catalytic converter is approximately 750*C, which the team used as the target temperature for maximum steady state conversion efficiency. The gain of the transfer function was considered an exponential function of temperature, allowing us to model the change in concentration versus temperature as well as time. The team concluded that conversion efficiency would be directly proportional to changes in temperature outside of a +- 5% range of steady state temperature range.

The main controlled variable is the Temperature, assumed to be the result of greater airflow to the converter. Disturbances in temperature are modelled as step and ramp functions representing uncontrollable changes to the environment, which may be sensed with simple temperature sensors found in heat alarms. A second disturbance is introduced at t = 25 where a portion of the catalyst is deemed inactive, Airflow and, therefore, Temperature are adjusted accordingly.

Consequently, in order to maintain nominal operating temperatures, two PID controllers were added to the model. The controller''s output controls were temperature and conversion efficiency. The controller examined the difference between the output temperature or conversion and the ideal, and they would activate to stabilize it. The controllers physically controls the temperature of the converter If the cause of change in efficiency was temperature related, for instance if the vehicle entered a climate of extreme heat, the PID controllers approximated an air-cooling system that activates to cool down the catalytic converter. **Figure 7** shows the model that was developed in Matlab with both an uncontrolled and a controlled model.

In the example run of the model, the engine is first turned on a t=2, activating the second order zeolite efficiency function, and simultaneously temperature begins to rise in the catalytic converter exponentially. Temperature and zeolite efficiency both reach their respective steady states, and emissions conversion efficiency approaches 56.9% at around 3Tau. The vehicle then undergoes an engine failure where the temperature of the converter to rise above nominal operating range. The PID controller (which approximates an air cooling system) is activated immediately, resolving the difference between the ideal. The temperature is then lowered via a ramp function which brings the system back to nominal range. Steady state is maintained for a short while, then the model exemplifies a rock hitting the converter damaging it. In the process some of the Pt catalyst is lost and no longer usable. This is represented in the model with another step down disturbance that eventually returns a new steady state value of reduced catalyst availability of 54.2%. **Figure 8** shows the plot of conversion versus time, where the yellow line represents the conversion without Control and the purple line represents the controlled conversion.

The team's model provides an acceptable level of safety, in this case towards the environment. In an ideal situation, there would be 100% conversion of emissions at all times of operation, but current designs do not allow for this.Therefore the next best option is to keep the converter running at the maximum efficiency possible which is around 56.9%. Temperature is controlled in this example because an overheating engine or converter is potentially dangerous for the operator of the car.

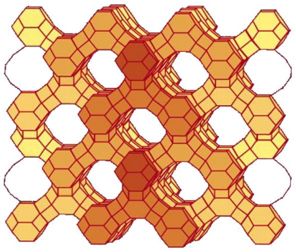

Figure 1 (Beta Structure)

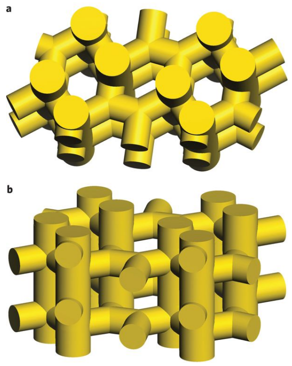

Figure 2 (MWW structure)

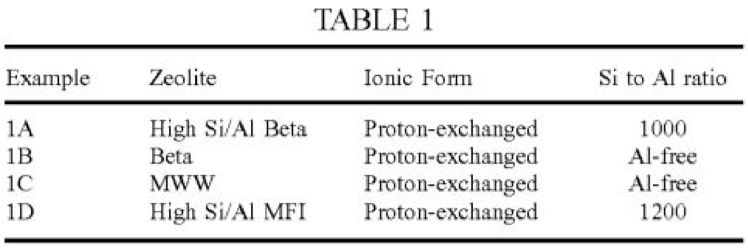

TABLE 1

Example	Zeolite	Ionic Form	Si to Al ratio
1A	High Si/Al Beta	Proton-exchanged	1000
1B	Beta	Proton-exchanged	Al-free
1C	MWW	Proton-exchanged	Al-free
1D	High Si/Al MFI	Proton-exchanged	1200

Figure 3

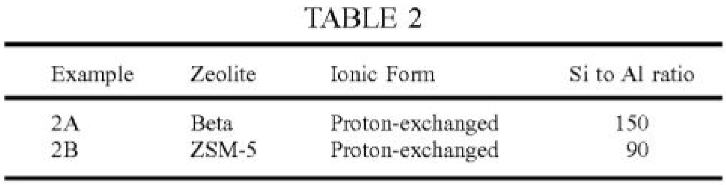

TABLE 2

Example	Zeolite	Ionic Form	Si to Al ratio
2A	Beta	Proton-exchanged	150
2B	ZSM-5	Proton-exchanged	90

Figure 4

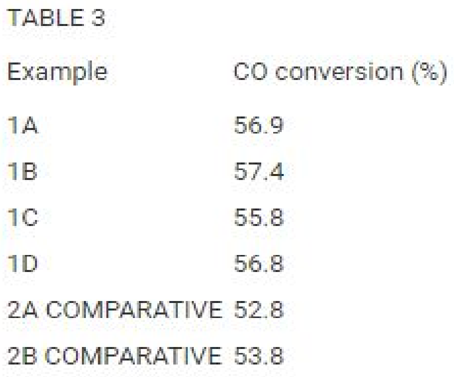

TABLE 3

Example	CO conversion (%)
1A	56.9
1B	57.4
1C	55.8
1D	56.8
2A COMPARATIVE	52.8
2B COMPARATIVE	53.8

Figure 5

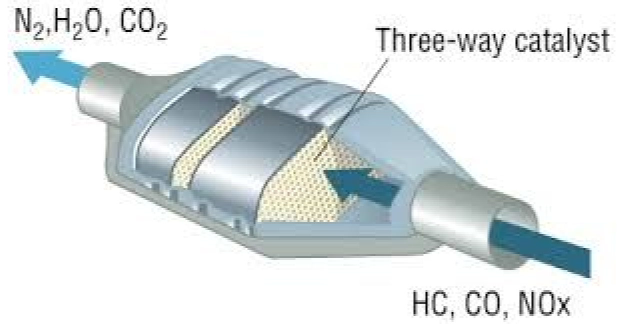

Figure 6

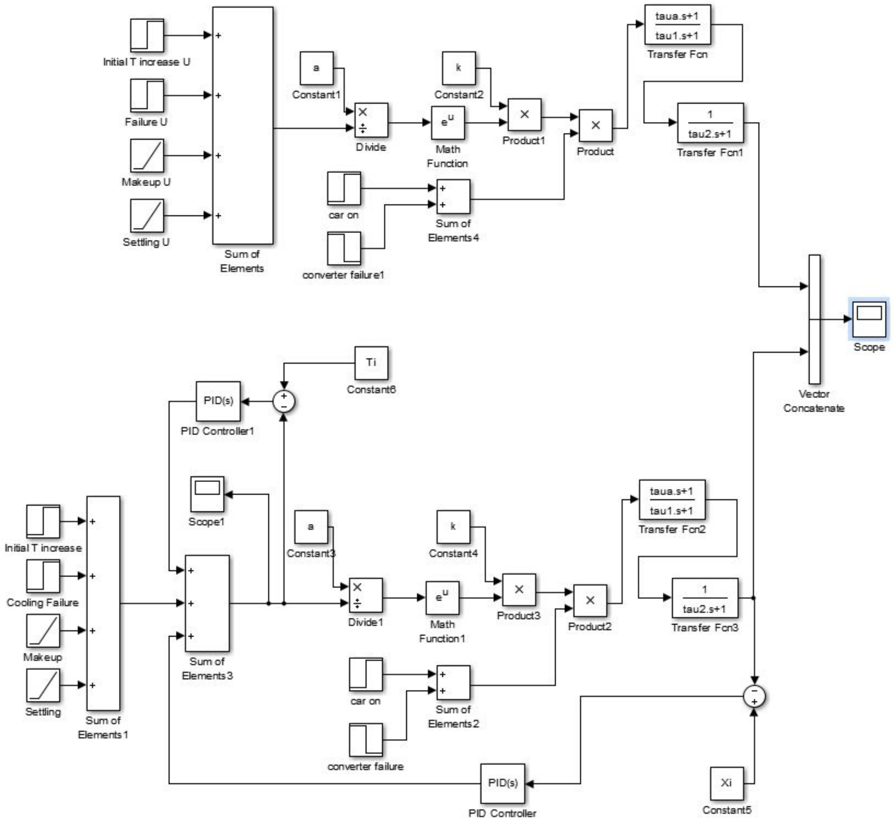

Figure 7

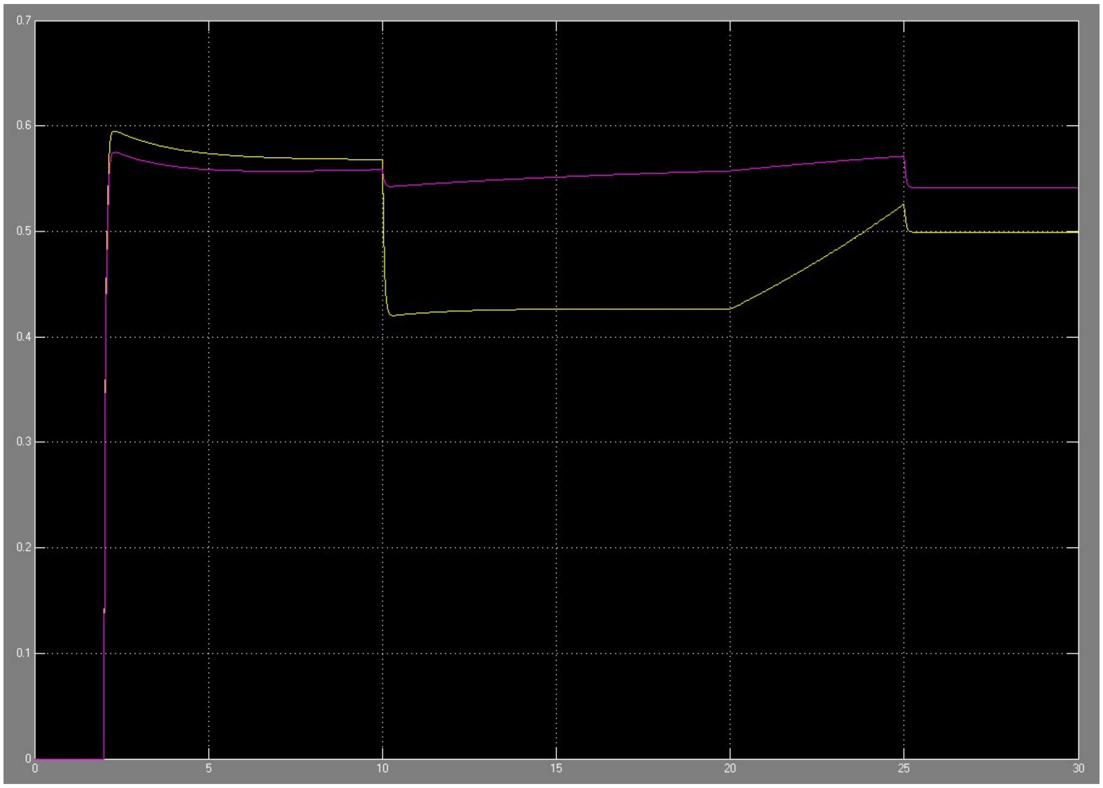

Figure 8

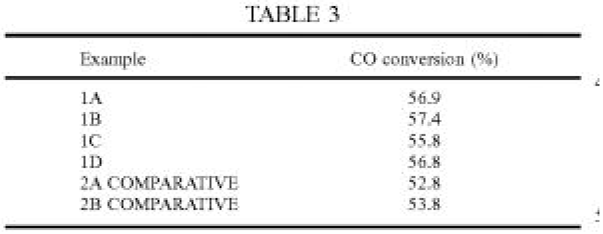

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Figure 9