

A Simplified Three-Way Catalyst Model for Use in On-Board SI Engine Control and Diagnostics

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ABSTRACT

Automotive emissions are severely regulated. Since 1980, a three-way catalyst (TWC) has been used to convert harmful emissions of hydrocarbons, carbon monoxide, and oxides of nitrogen into less harmful gases in order to meet these regulations. The efficiency of conversion of these gases is dependent on the mass ratio of air to fuel (A/F) in the mixture leaving the exhaust manifold and entering the catalyst, the velocity of the exhaust mass, and the temperature of the catalyst. The goal of this paper is to develop a dynamic, control-oriented model of a TWC. First, the importance of developing such a model will be explained. Then, a simplified dynamic catalyst model that can be determined on the basis of medium bandwidth A/F measurements and low bandwidth temperature and emission measurements will be introduced and validated.

NOMENCLATURE

A/F	air-fuel mass ratio
C	represents the effective catalyst “capacity,” or the volume of active sites for oxygen storage, expressed in terms of the mass of oxygen that can be stored in the catalyst
F	mass of fuel in the feedgas
S	stoichiometric ratio for the air-fuel mixture, normally near 14.6
T	temperature

Greek Symbols

α	relative oxygen release/absorption rate
η	catalyst conversion efficiency
λ	relative air-fuel ratio, with stoichiometry at $\lambda = 1$
ρ	a function that describes the exchange of oxygen between the exhaust gas and the catalyst

Subscripts

FG	feedgas (pre-catalyst)
L	(fuel) lean
R	(fuel) rich
TP	tailpipe (post-catalyst)

INTRODUCTION AND BACKGROUND

California and Federal emissions regulations for 2000 and beyond, in combination with customer performance demands, are engendering significant mechanical design changes to the basic internal combustion engine. Examples of innovations include variable displacement engines (VDE), variable cam timing (VCT) engines, and camless engines. To be operated effectively, these engines require sophisticated multivariable control systems, with higher bandwidths than typically used before in the automotive industry (Stefanopoulou, 1996). The design of these controllers requires good fidelity dynamic models of the engine as well as the three-way catalyst (TWC) used to post-treat the engine's exhaust, or feedgas. This paper addresses itself to

developing a phenomenological model of the TWC that is useful for control design. The same model will also be useful for developing diagnostics; cf. Cussenot et al. (1996).

The three major automotive pollutants are carbon monoxide (CO), unburned hydrocarbons (HC), and oxides of nitrogen (NO_x). Catalytic converters were first used to post-treat exhaust feedgas in production automobiles beginning in 1975 in order to meet emission control regulations. These catalysts were oxidation catalysts, also known as two-way catalysts, since they oxidized HC and CO , converting them to carbon dioxide (CO_2) and water vapor (H_2O). In 1980, the catalytic converter was enhanced with the ability to reduce NO_x as well (Environmental Protection Agency, 1994), giving rise to the so-called three-way converter. A catalytic converter does not work efficiently until it reaches a sufficiently high temperature, in the range of 650°F . When a catalyst is cold, neither the reduction of NO_x nor the oxidation of CO or HC occur within the converter. As the catalyst warms up, these reactions occur more completely. The catalyst is commonly said to *light off* when HC conversion efficiency reaches 50%.

Detailed chemical and thermodynamic-based mathematical models of TWC's have been proposed in the literature (Montreuil et al., 1992; Pattas et al., 1994). One problem with these models in an industrial setting is that by the time one is able to determine the values of the various physical parameters in the model for a given catalyst composition, technology advancements will have already driven a change in the TWC's formulation. In addition, the models are typically given by several coupled nonlinear partial differential equations, so working with them for control design is unwieldy.

In this paper, a simplified dynamic model of a three-way catalytic converter will be presented and validated against dynamic air-fuel ratio (A/F) and emissions data. The data are from a 1996 production palladium-platinum-rhodium catalyst.

SIMPLIFIED TWC MODEL

The structure of the proposed TWC model is shown in Fig. 1. The basic idea is to decompose the model into three parts: the standard steady state efficiency curves driven by tailpipe A/F , an oxygen storage mechanism to account for the modification of the A/F of the feedgas as it passes through the catalyst, and the thermodynamics of catalyst warm-up. Germann et al. (1995) discuss the fact that this structure has some deficiencies. An oxygen storage model with similarities to the one described later in this paper can be found in Shafai et al. (1996); however, that model cannot capture such phenomena as the stoichiometric plateau, where if the feedgas is held lean for several seconds and then switched rich, the tailpipe A/F will rapidly switch from lean to stoichiometry, then remain near stoichiometry for several seconds before tracking the feedgas A/F and becoming rich. This is an important consequence of the storage capability of the catalyst. In reality, a three-way catalyst stores more than just oxygen. However, for simplicity, this modeling effort combines the effect of the overall reactant storage into a single oxygen storage submodel.

Oxygen Storage Sub-Model

Oxygen storage and release, the property of oxygen attaching to metal and cerium sites in the catalyst under lean conditions, thereby decreasing the A/F (or enriching the mixture), and the release of oxygen under rich conditions, thereby leaning the mixture, is an important feature of modern catalytic converters for vehicle applications. The goal of the oxygen storage model is to capture this property in a concise and sufficiently accurate manner.

Let $0 \leq \Theta \leq 1$ be the fraction of oxygen sites occupied in the catalyst. The oxygen storage capacity is modeled as a limited integrator in the following way:

$$\dot{\Theta} = \begin{cases} \frac{1}{C} \times F \times S \times (\lambda_{FG} - 1) \times 0.21 \times \rho(\lambda_{FG}, \Theta) & 0 \leq \Theta \leq 1 \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

The function ρ is modeled as

$$\rho(\lambda_{FG}, \Theta) = \begin{cases} \alpha_L f_L(\Theta) & \lambda_{FG} > 1 \\ \alpha_R f_R(\Theta) & \lambda_{FG} < 1 \end{cases}, \quad (2)$$

with $0 \leq f_L \leq 1$ representing the ‘‘probability’’ of an oxygen atom (combined or free) from the feedgas sticking to a site in the catalyst, and $0 \leq f_R \leq 1$ representing the ‘‘probability’’ of an oxygen atom being released from the catalyst and recombining with the feedgas. In Eq. (2), f_L and f_R vary with the percentage of occupied oxygen sites and potentially with the feedgas (or ‘‘space’’) velocity as well. In the model, f_L is assumed to be monotonically decreasing, with value one at $\Theta = 0$ and zero at $\Theta = 1$, and f_R is assumed to be monotonically increasing, with value zero at $\Theta = 0$ and one at $\Theta = 1$. Typical functions f_L and f_R are shown in Figs. 2 and 3. Finally, the parameters α_L and α_R are included to represent the fact that the catalyst's storage and release rates of oxygen are different, with the release rate normally being higher than the storage rate.

For the oxygen storage submodel, the effects of feedgas and catalyst temperature are currently not included. The effects of space velocity also need further elucidation.

The quantity $F \times S \times (\lambda_{FG} - 1) \times 0.21$ represents the differential total mass of oxygen (combined or free) in the feedgas with respect to stoichiometry. When multiplied by ρ , it gives the mass of oxygen that is deposited in (or released from) the catalyst. The resulting equivalent tailpipe A/F can be directly computed by the following:

$$\lambda_{TP} = \lambda_{FG} - (\lambda_{FG} - 1) \times \rho(\lambda_{FG}, \Theta). \quad (3)$$

The block diagram representation of the oxygen storage submodel is shown in Fig. 4. In order to automate the tuning process of this submodel against data, an optimization routine was created to adjust key model parameters in a systematic fashion. The cost function is set up as a penalty on the distance between the model's predicted tailpipe A/F and measured data. This cost can be selected to depend on a single data set or any group of data for which an optimized fit is desired.

The accuracy of the model in predicting tailpipe A/F for a warmed-up catalyst is shown in Fig. 5. Note the plateau in the

data near stoichiometry as well as in the model, especially when the feedgas is switched from lean to rich. To capture this in the model, it is necessary that f_R be equal or nearly equal to one for some nontrivial range of Θ near zero, as in Fig. 3.

Heat Transfer Sub-Model

In order to characterize the conversion efficiencies of a TWC in an arbitrary drive cycle, catalyst temperature must be taken into account. Catalyst temperature plays a key role in determining the light-off time especially during cold start. Before light-off, catalyst temperature changes are due to thermal energy absorption from the feedgas. After light-off, these temperature changes are due to a combination of thermal and chemical processes.

It is assumed that the flow through the catalyst is one-dimensional and incompressible. Any physical variable or parameter of the catalytic converter used in the model is "lumped," and its average value is assumed. The catalyst temperature is primarily a function of feedgas temperature, exhaust mass flow rate, reaction rate of each species, and other geometric considerations. To maintain a simple model structure for control design and yet retain sufficient accuracy, a first order dynamic equation with a nonlinear algebraic function is used. The model consists of first order dynamics on the feedgas temperature cascaded with an algebraic function that depends on the feedgas temperature and feedgas HC and CO concentrations, as well as HC and CO conversion efficiencies. The brick temperature model is as follows:

$$\dot{T}_b = \begin{cases} \frac{1}{\tau_1} [-T_b + f_{cold}(T_{fg\downarrow})] & T_b < \text{threshold} \\ \frac{1}{\tau_2} [-T_b + f_{hot}(HC, CO, \eta_{hc}, \eta_{co}, T_{fg\downarrow})] & T_b > \text{threshold} \end{cases} \quad (4)$$

where T_b represents the brick temperature; \dot{T}_b is its time derivative; τ_1 and τ_2 are the time constants; HC and CO represent feedgas emission levels of hydrocarbons and carbon monoxide, respectively; and η_{hc} and η_{co} represent the efficiencies of the TWC in oxidizing the feedgas HC and CO emissions. The left bank feedgas temperature ($T_{fg\downarrow}$) was chosen for illustrative purposes. If the brick temperature on the right bank were to be modeled, then the right bank feedgas temperature would be used. The nonlinear functions $f_{cold}(T_{fg\downarrow})$ and $f_{hot}(HC, CO, \eta_{hc}, \eta_{co}, T_{fg\downarrow})$ and the two time constants are determined by regressing the measured data.

There are two reasons for not using NO_x information in the brick temperature model. The first reason is that the heat generated by NO_x reduction is less than that generated by HC and CO oxidation. The second reason is that the data for NO_x conversion efficiency and concentration are not very repeatable. Although NO_x conversion also contributes to the temperature increase, it is difficult to identify and validate the corresponding model structure and parameters based on available data.

Static Conversion Curves

The static behavior of a TWC is characterized by the conversion efficiencies of HC , CO , and NO_x as functions of the tailpipe

air-fuel ratio. These functions for the specific TWC package are plotted in Fig. 6 for a constant brick temperature. There is a narrow window of air-fuel ratio around the stoichiometric point within which the high conversion efficiencies of all three pollutants can be achieved for a typical three-way catalyst. However, the inlet temperature, which is measured at about half an inch from the face of the first brick of TWC, also affects the conversion efficiency, and the effects are significant enough to make a difference in the subsequent control design and optimization analysis.

Tests were conducted to map the catalyst conversion efficiency for different air-fuel ratio and brick temperature setpoints. The data used in this part of the modeling work were collected under steady state, warmed up engine conditions. For each engine speed/load point, the spark timing was adjusted to meet the desired temperature before a ± 1.0 air-fuel ratio sweep was applied. The dynamometer test data show that the HC , CO , and NO_x conversion efficiencies are sensitive to the variations in temperature.

The nonlinear functions representing the static efficiency curves are derived by regressing the dynamometer test data with respect to normalized air-fuel ratio and brick temperature. The HC conversion efficiency is then corrected by a linear function of the mass air flow rate, which accounts for the effect of space velocity on the catalyst performance.

In order to achieve better numerical results, the temperature and air-fuel ratio variables are first normalized as follows:

$$\hat{T}_b = \frac{T_b - 496}{1188} \quad (5)$$

$$r_H = \frac{r_{pc} - r_{st} + 3.885}{7.43} - 0.0339\hat{T}_b + 0.0058$$

$$r_C = \frac{r_{pc} - r_{st} + 3.68}{7.43} - 0.0086 \quad (6)$$

$$r_N = \frac{r_{pc} - r_{st} + 3.6}{7.43}$$

where \hat{T}_b, r_H, r_C, r_N are normalized variables for the brick temperature, HC specific, CO specific, and NO_x specific air-fuel ratio respectively. Then the static catalyst performance is described by the following conversion efficiency equations for the three pollutants:

$$\eta_H = 1.0021 \left(\gamma_H + \frac{(0.998 - \gamma_H)r_H^{14}(-0.1r_H + 1.061)}{p_H(r_H)} + (-0.073\dot{m}_a - 0.0075) \right) \quad (7)$$

$$\eta_C = 1.0229 \left(\gamma_{C1} + \frac{0.9886r_C^{16}\gamma_{C2}}{p_C(r_C)} \right) \quad (8)$$

$$\eta_N = \frac{1}{1 + e^{-\frac{r_N - 0.49304}{0.00576}}} \left(-1.5425 + \frac{7.32456}{1 + e^{-\frac{\hat{T}_b + 2.95654}{1.47271}}} \right) - \frac{0.05074}{1 + e^{-\frac{\hat{T}_b + 2.95654}{1.47271}}} + 1.00475 \quad (9)$$

where $\gamma_H, \gamma_{C1}, \gamma_{C2}$ reflect the temperature effects on HC and

CO conversion efficiency, empirically defined as:

$$\begin{aligned}\gamma_H &= 0.9136\hat{T}_b - 0.0956 \\ \gamma_{C1} &= 0.4752\hat{T}_b - 0.0616 \\ \gamma_{C2} &= 0.0706\hat{T}_b^2 - 0.6981\hat{T}_b + 1.2058 \\ &\quad - r_C(0.1411\hat{T}_b^2 - 0.4459\hat{T}_b + 0.2924),\end{aligned}\quad (10)$$

where p_H and p_C are Chebyshev polynomials of 14th and 16th order, respectively, whose coefficients are defined in Table 1.

OVERALL MODEL EVALUATION

Figure 7 shows a comparison between test data and simulation data from the dynamic catalyst model of the previous section. At this warm condition, the feedgas A/F is the only input to the model, and the comparison is shown to be quite favorable for tailpipe A/F as well as NO_x and CO conversion efficiencies. However, the model seems to underestimate the HC conversion efficiencies during the rich portions of the test.

Table 2 provides a further comparison between simulation and test data, showing results from the standard FTP cycle. The table shows accumulated tailpipe mass emissions from each bag of the cycle along with the model estimate of these values. The differences in the results from Bags 1 and 3 highlight the need for further work on the model's performance under startup conditions. However, the Bag 2 results, especially for HC and CO , are encouraging, despite the need for improvement in tailpipe NO_x estimation. Further encouragement can be drawn from the favorable comparison between modeled brick temperature and data during Bag 1, as shown in Fig. 8.

CONCLUSIONS AND REMAINING ISSUES

In this paper, a simplified dynamic model of a three-way catalytic converter was presented and validated against dynamic A/F and emissions data. This model is based on a 1996 production palladium-platinum-rhodium catalyst.

The preliminary validation of the model against data seems quite favorable. There are, of course, many issues that remain to be investigated. For example, certain types of input signals yield significant errors in the tailpipe A/F predictions and, consequently, in the conversion efficiencies and tailpipe emissions. For example, for certain rich/lean triangular wave patterns that lead to breakthrough (demonstrated by significant departure from stoichiometry in tailpipe A/F) only on the lean side, the model tends to predict breakthrough also on the rich side, even though this is not present in the data.

Further work needs to be done to determine the source of this error. Some possible sources are as follows: There could be a space velocity dependency that is not being included properly in the storage model. Perhaps the TWC's properties as a fuel storage or reductant storage device, both of which are currently neglected, may be more important than estimated. The investigation of these and other issues is a topic for future research.

In addition, more startup data (cold and hot start) needs to be collected in order to expand the capability of the thermal model. Additional data will provide the means for further iden-

tification and validation of that submodel. This will then allow for improvement in the accuracy of the model in its prediction of tailpipe emissions for Bags 1 and 3 of the FTP cycle.

Finally, the TWC converter is clearly a distributed device. A single lumped element model has been presented in this paper. The oxygen storage model in particular can be cascaded with itself in order to better approximate the distributed nature of the catalyst. A cascaded model may also be useful for representing TWC's that are composed of multiple bricks of different catalytic material. Each brick could then be represented by an individual oxygen storage block.

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Function Term	HC Efficiency par.	CO Efficiency par.
const.	0.0058232	0.0020713
x^2	-0.081526	-0.034509
x^4	0.44839	0.23355
x^6	-1.2228	-0.82298
x^8	1.712	1.6064
x^{10}	-1.1416	-1.7026
x^{12}	0.28549	0.88634
x^{14}	1	-0.1759
x^{16}	0	1

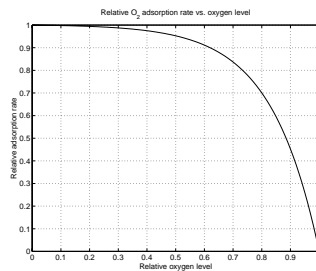


Figure 2: Typical function f_L .

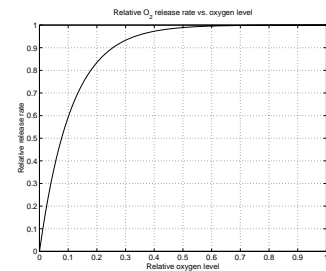


Figure 3: Typical function f_R .

TABLE 1: Catalyst Static Efficiency Function Parameters for HC and CO

		Simulation	Bag Data
Bag 1	HC	2.7413	2.3835
	CO	16.1527	19.1365
	NO _x	0.76195	1.0259
Bag 2	HC	0.02333	0.02485
	CO	0.2343	0.2323
	NO _x	0.2184	0.2794
Bag 3	HC	0.2690	0.1977
	CO	0.3654	0.2827
	NO _x	0.5796	0.6794

TABLE 2: Comparison of mass emissions (in grams) between simulation and bag data.

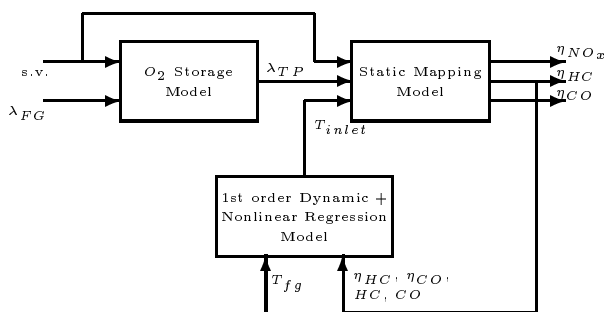


Figure 1: Structure of the TWC model developed in this paper.

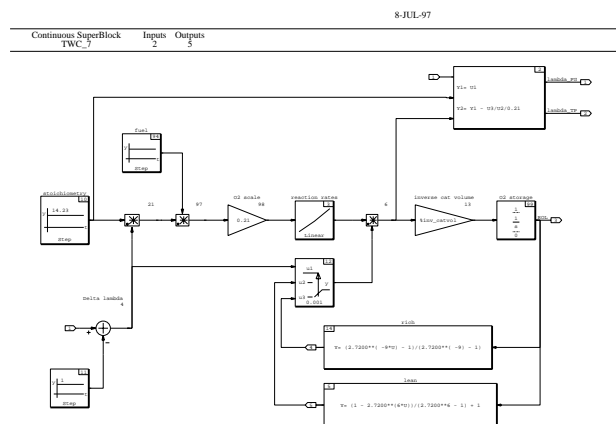


Figure 4: Structure of the oxygen storage submodel.

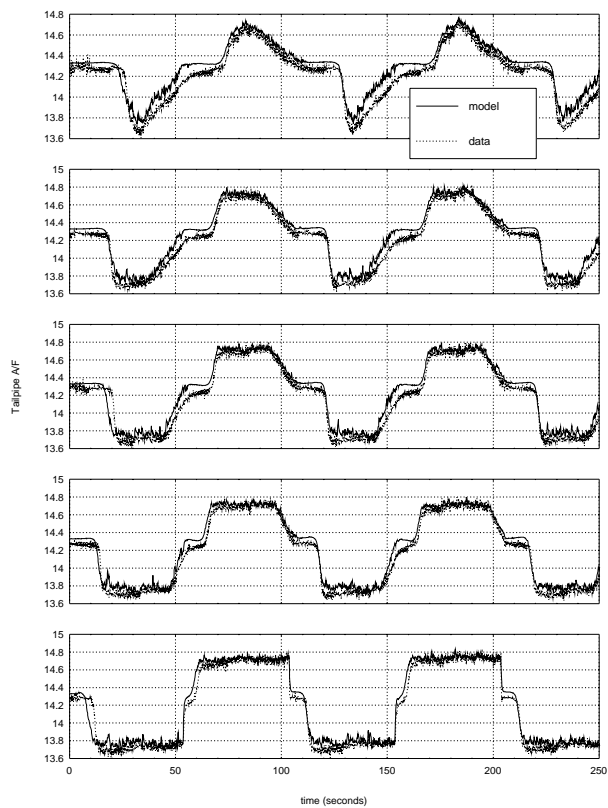


Figure 5: Model validation data for warmed-up catalyst.

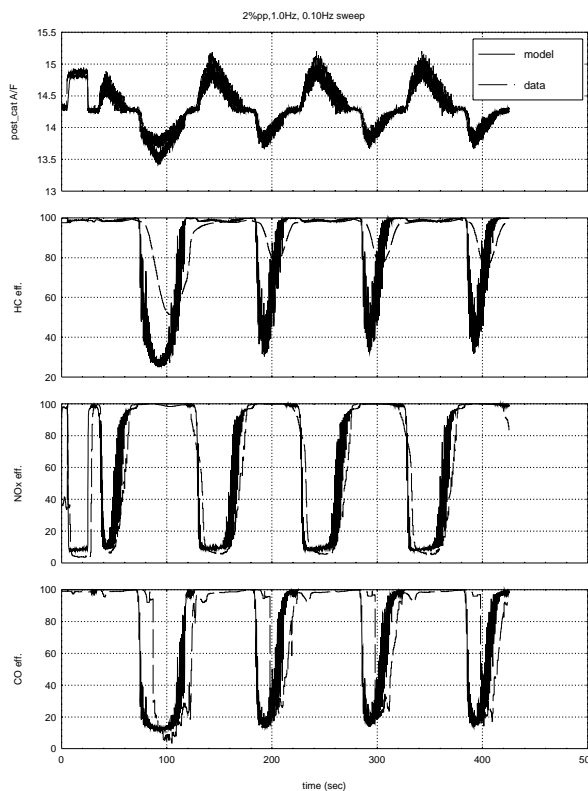


Figure 7: Validation data for warm TWC model.

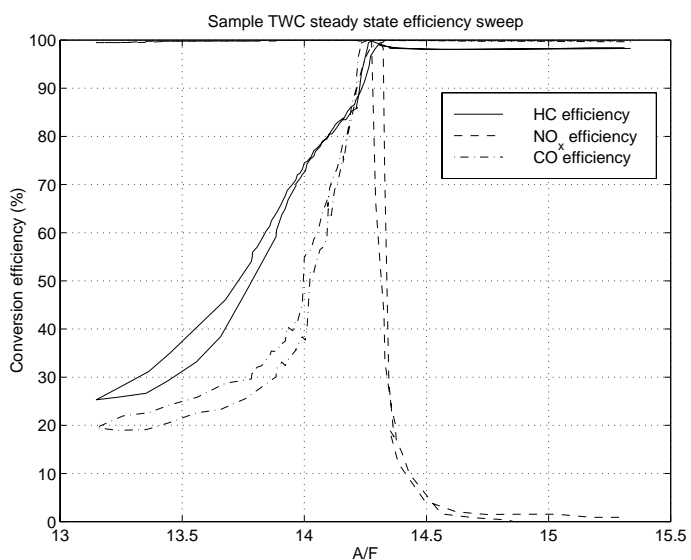


Figure 6: Sample steady state TWC efficiency data (forward and backward sweeps).

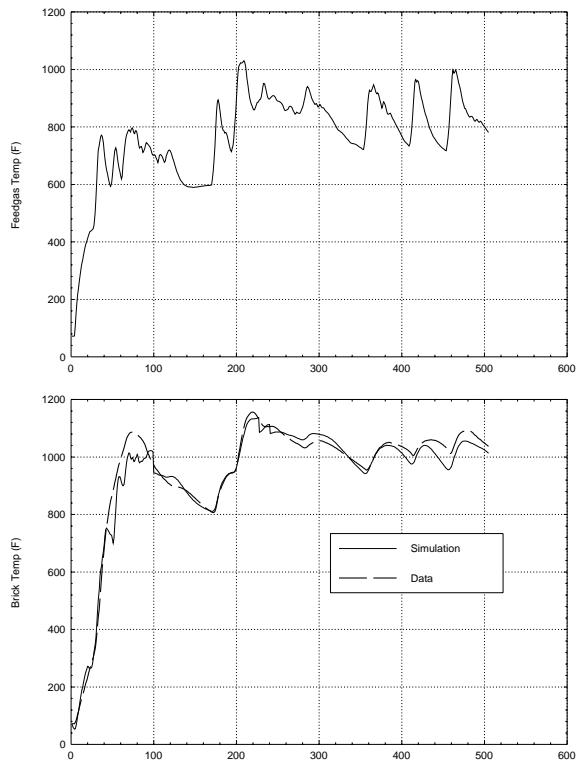


Figure 8: Feedgas and brick temperatures vs. time in Bag 1.