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A NUMERICAL MODEL TO PREDICT THE EFFECTS OF EXHAUST GAS RECIRCULATION ON NO EMISSIONS

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Abstract. *The claim for reducing* NO_x *emissions from internal combustion engines sources has led to the application of Exhaust Gas Recirculation (EGR) technology. By such means, the temperature of the products mixture is lowered reducing NO formation from the Zeldovich mechanism (thermal NO). The injection of hot products back to the combustion chamber may alter significantly the performance of the system This paper presents a numerical model to predict the influence of EGR for a wide range of air/fuel dilution by the inert gas. A routine, which calculates complex states of chemical equilibrium, is employed thus allowing a great number of species to be treated by the model. The models allow the predictions of EGR for wide range of hydrocarbon fuels, including alcohol, in IC engines, boilers, and turbines. Experimental results from an internal combustion engine test facility are then used to validate the model as well as to establish the practical limits for recirculation.*

Key-words: *EGR-Exhaust gas recirculation,IC engines, Gas turbines.*

1. INTRODUCTION

The exhaust gas recirculation (EGR) technology was introduced back to 1972 as a mean to reduce vehicular emissions. The exhaust gas mixed with the fresh mixture reduces the combustion temperature as it is burned again. This in turn diminishes the quantity of oxides of nitrogen, a harmful emission, produced. The application of EGR technology to other types of combustors has the potential for significantly improving and controlling environmental contaminating pollutants. Moreover, when used in a regenerative semiclosed cycle turbine engine, an improvement in performance, economy, and weight to power ratio can be achieved. However, recirculating regenerative engines require an innovative burner concept to operate with large quantities of diluent, which reduces the oxygen concentration as well as the availability of secondary combustion air that represents a departure from conventional burner designs. The application of EGR to a combustion process alters the final product composition and temperature, and, in some cases, final pressure. In most of the applications, the process is either at constant pressure, like in gas turbine, or at constant volume, characteristic of IC engines. Computational tools that, under some assumptions, may simulate the final thermodynamic state of chemically reacting systems are of great interest. In this work we present a numerical code that permits the investigation of EGR technology applied to IC engines as well as gas turbines for a variety of hydrocarbons fuels, including alcohol. The computational code was developed by a group of students to be used in the Applied Thermodynamic Laboratory (ATL) of the Mechanical Engineering Department (University of Brasília). The ATL has an internal combustion engine test facility with an EGR valve that can recycle combustion products to be mixed with the fresh air/fuel charge in a variety of proportions.

Exhaust gas recirculation has been under investigation both therorically as well as experimentally, though with more attention for the latter (Musser *et al.* 1971, Benson and Stebar, 1971). Morgan and Kirling (1977) observed that compression rate has no effects in NO_x emissions and maximum levels of formation occur at the air to fuel ratio of 16:1. A simulation model that includes exhaust gar recirculation was presented by Benson and Baruah (1977). The model was later improved as to simulate the EGR system in combination with a multi-cylinder sapark ignition engine (Baruah *et al.* 1978). Predictions were carried out only under steady state condition and full carburettoor throttle. Application of recylcled gases have shown that emissions of nitric oxide can be reduced up to 50% at peak NO condition.

Recently, experimental work was conducted by de Souza (1997) on application of EGR in a 1000 cm^3 motor. The measurents provide emissions curves for a wide range of recirculation if different engine refimes.

As regarded to the formation of nitrogen oxides, three main routes have been identified (Turns, 1996). The chemical mechanisms that involve nitrogen from the air are the thermal and prompt, s well as the N_2O-intermediate. In rich conditions,the Fenimore mechanism plays an important role. NO formation from the N_2O-intermediate mechanism is important in very lean, low temperature combution processes. In spark ignition engines, the mixture is set to vary near the stoichiometric ratio, thus dicharging mechanisms other than the thermal. The thermal mechanism dominates in procees that experiment very high combustion temperatures, over a wide range oc equivalence ratios.

Nitrogen oxides may be also formed from the nitrogen in the fuel. The nitrogen content in hydrocarbon fuels, however, is too low compared to the potential of the atmospheric nitrogen to form NO.

The intermediate species that play a major role in the Zeldovich mechanism (thermal) can be assumed in their equilibrium state, if time scales involved are sufficiently long the NO formation can be calculated separately from the fuel combustion chemistry. This simplification is adopted in specifying global rate expressions for NO formation.

Figure 1 shows the schematic representation applied in exhaust-gas recirculation system for a spark-ignition engine (Turns, 1996).

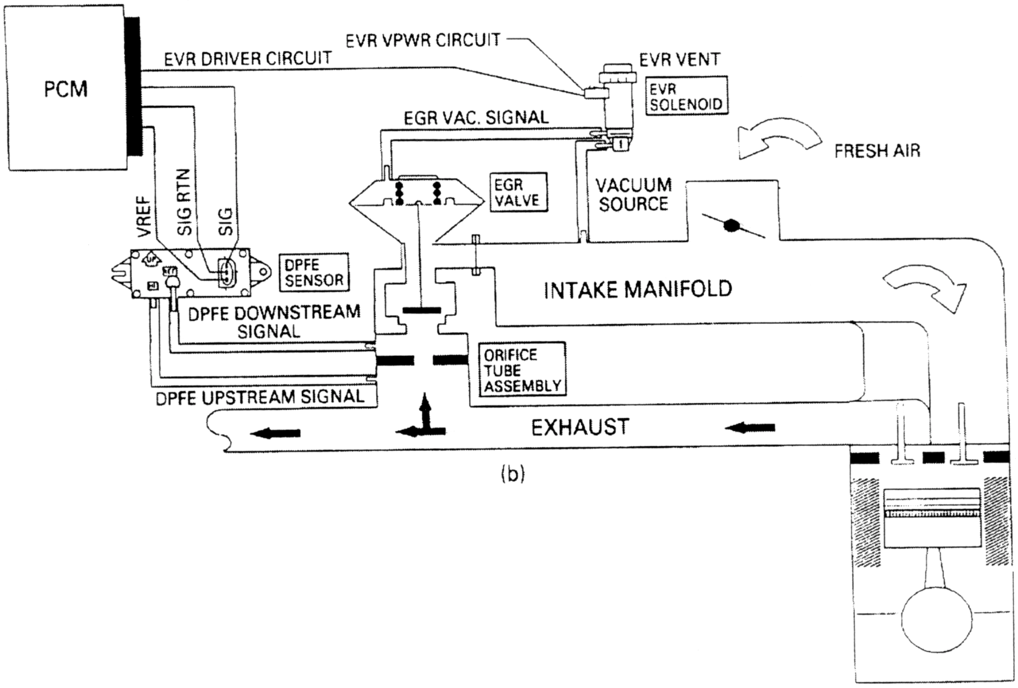

Figure 1- Schematic exhaust-gas recirculation system for IC engine (Turns, 1996).

2. MATHEMATICAL FORMULATION

In order to simplified the formulation, the composition of the recycled gas is assumed to consist of undissociated products of the hydrocarbon fuel reaction with air. That is, all the carbon in fuel is converted to CO_2, the hydrogen is converted to H_2O and the nitrogen in air is an inert gas. The final gas composition, after combustion, is assumed to be in equilibrium. As pointed by Heywood (1988), the characteristic time for the NO formation process (τ_{NO}) is usually comparable or longer than times characteristic of changes in the engine conditions. The NO formation, thus, is kinetically controlled. Hence, the process should be dynamically modeled. However, close to the stoichiometric condition and at very high pressures and temperatures, τ_{NO} is of the same order as typical combustion times (≈1ms) resulting that equilibrium NO concentrations may be attained. In general, the departure from stoichiometry in IC engines is undesirable thereby allowing this simplification. For gas turbines and other combustors, as regarded to the equivalence ratio, the range of operation is wider, however residence times are longer. Hence, the applicability of an equilibrium code is deemed adequate. To calculate the complex state of equilibrium, we made use of the Olikara and Borman (1975) computer code. This program calculates the properties of combustion products of adiabatic constant-volume and adiabatic constant-pressure processes, typical of IC engines and gas turbines, respectively. The routine HPFLAME calculates the adiabatic flame temperature, equilibrium composition and properties of the products for the adiabatic constant-pressure case while UVFLAME is used in the adiabatic constant-volume case. In both routines, the user is asked to specify fuel composition, reactant enthalpy, equivalence ratio, and initial temperature and pressure. For EGR, the problem has the additional difficulty of, given the amount of recycled gas to be used the above mentioned variables need calculation. Once all the input data is obtained, the appropriate routine HPFLAME or UVFLAME can be automatically executed by the user main program.

Initial gas temperature and pressure are either given by the user or calculated by the program. These parameters are calculated when a constant-volume problem is of interest. In both cases, the program calculates the remaining variables (H_{reac}, N_{reac}/N_{fuel} *and* W_{reac}) when recycled gas is employed, in any proportion. In addition, the user is asked to supply the equivalence ratio of the fresh air/fuel mixture.

The enthalpy of reactants (H_{reac} *)* before the combustion process can be calculated by

$$H_{reac} = N_F \bar{h}_F + N_A \bar{h}_A + N_{EGR} \bar{h}_{EGR} . \tag{1}$$

By definition,

$$N_{EGR} \equiv (N_A + N_F)\%EGR . \tag{2}$$

In Equation 1, *N* is the number of moles of a species and *F*, *A*, and *EGR* stands for, fuel, air and recycled gas, respectively. In Equation 2, *%EGR* is the amount of recirculation that is being applied (porcentage of exhaust gas recirculation).

The molecular weight of the mixture has also to be provided. The preogram them calculates this variable as a function of the *%EGR*. The molecular weight of a mixture is given by

$$W_{mix} = \sum x_i W_i . \tag{3}$$

For the reactants,

$$W_{reac} = \frac{N_F W_F + N_A W_A + N_{EGR} W_{EGGR}}{N_F + N_A + N_{EGR}} . \tag{4}$$

The molecular weight of the recycled gas appearing in Eq. 4 has to be determined. The composition of combustion products is a mixture of many species. At the temperature level reached in IC engines as well as in gas turbines is hih enough to cause dissociation. This woul imply the usage of about 1o to 15 species. However, CO_2, H_2O and N_2 together, accounts for more than 95% of the whole mixture. For simplicity, it is assumed that the composition of any hydrocarbon conversion, at the stoichiometry, consists of undissociated products as shown by the reaction

$$\mathrm{C_xH_yO_mN_n} + a(\mathrm{O_2} + 3.76\mathrm{N_2}) \rightarrow b\mathrm{CO_2} + c\mathrm{H_2O} + d\mathrm{N_2} . \tag{5}$$

Therefore, the product composition is given by the stoichiometric coefficients *b*, *c*, and *d*.

In IC engine calculations, the initial pressure and temperature after compression are input data to the UVFLAME routine. The program then calculates the initial state of the mixture as a function of the characteristics of the motor, namely, compression ratio. The equations are as follows

$$T_2 = T_1 (V_1 / V_2)^{\gamma - 1} . \tag{6}$$

and

$$p_2 = T_1 (V_1 / V_2)^{\gamma - 1} . \tag{7}$$

where γ is the polytropic exponent, T_1 and P_1, is the state of the fresh mixture before compression and T_2 and P_2 the same variables before constant-volume combustion. The user has then to supply the polytropic exponent and the compression ratio, the program calculates the state of the mixture prior to combustion as required by the UVFLAME routine.

The user program was written in Fortran 90 and the executable file can be run in personal computers. The program automatically calls the appropriate equilibrium routine, HPFLAME or UVFLAME, as determined by the problem type. Final composition is calculated for a mixture containing H, O, N, H_2, OH, CO, NO, O_2, H_2O, CO_2 and N_2.

The diagram in Fig. 2 shows the schematic representation of the computer program. The user needs to supply the requested parameters as to set up a problem. Using these inputs, the main routine calculates the necessary variables and runs the appropriated equilibrium routine. The HPFLAME or UVFLAME routine prints the output file containing the combustion products mixture assuming dissociation, as well as equilibrium temperature and pressure.

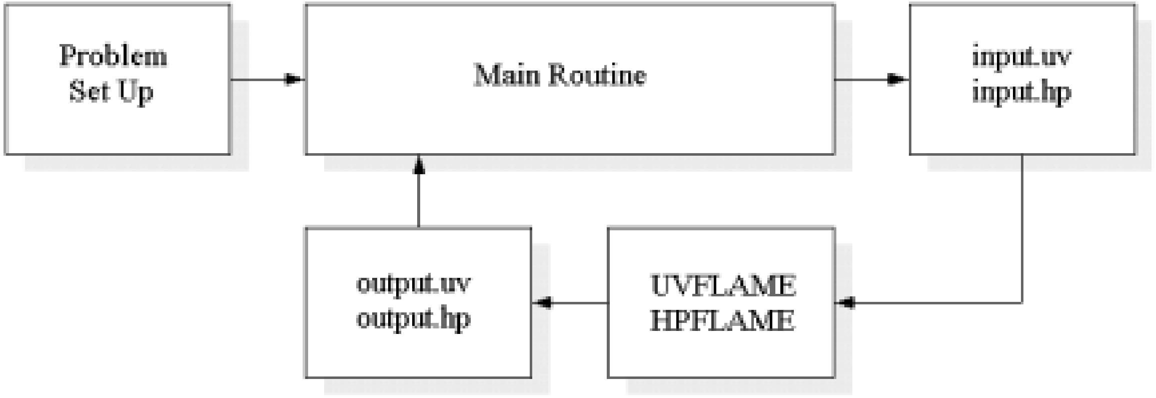

Figure 2- Schematic representation of the computer program.

The experimental apparatus consists of IC engine, 994.4 cm^3, 4 cylinders, fitted with EGR system. All the tests were performed with gasoline, thus having the compression ratio fixed at 8:1. The EGR valve has a screw finely threaded that allows to set the desired proportions of recycled gas, better used in the range of 0 to 20% of recirculation. The data acquisition system incorporates pressure, temperature, shaft speed (rev/min), and crank angle measurements. The exhaust gas sampling system measures the concentration of CO, CO_2, HC, O_2 and NO_x. Details about the test facility can be seen elsewhere (de Souza, 1997).

3. RESULTS AND DISCUSSION

We considered a spark-ignition engine whose fuel/air mixture prior to compression is at 0.5 atm and 300 K, the %EGR was then varied from 0 to 20%. Figure 3 shows the calculated temperature and pressure versus the amount of recycled gas. As it can be seen, by diluting the fresh fuel/air mixture a great reduce in the adiabatic temperature is attained and consequently, NO formation due to the thermal mechanism is expected to reduce as well. In fact, the combustion process is not at constant-volume as approximated by the model. Hence, a deviation from experimental results is expected.

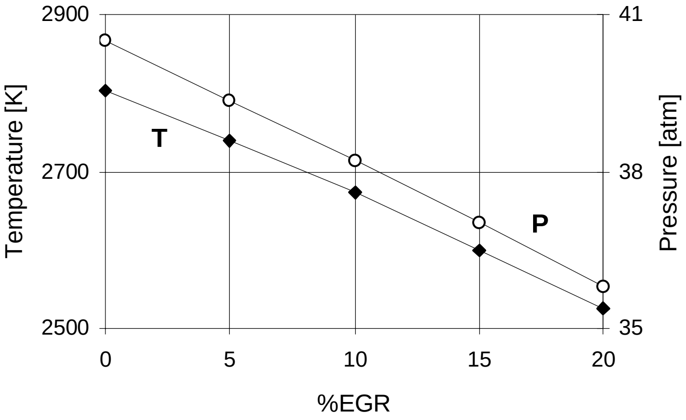

Figure 3- Final temperature and pressure versus the amount of recycled gas.

Based on experimental investigation, a parametric study may provide means to correct the predicted values. The peak pressure as obtained experimentally is in close agreement to the equilibrium values calculated by the program. The final temperature as calculated by the model may be over predicted since the combustion products loose heat to the cylinder walls. Therefore, the calculated NO may be in excess when compared to the measured values. Since the mixture inside the cylinder is approximately uniform, the dynamic of NO formation is coupled to the kinetic mechanism with the pressure/temperature history during combustion and the early part of the expansion process.

If the mass fraction burned can be estimated as a function of the pressure (crank angle) then the NO concentration at equilibrium for different burned mass fractions can be determined. Integration of the NO curve from unburned to totally burned mixture will give the average exhaust mass fraction (NO_{exh}).The program, however, in its actual configuration is not able of performing such calculations. This is the second step of the project. Nonetheless, qualitatively speaking, the model shows the trends as EGR is applied to an IC engine. In gas turbine, this problem does not arise since pressure is kept constant throughout combustion and residence times are comparable longer thereby approaching equilibrium composition.

Figure 4 shows the amount of NO reduction (%) versus %EGR applied.

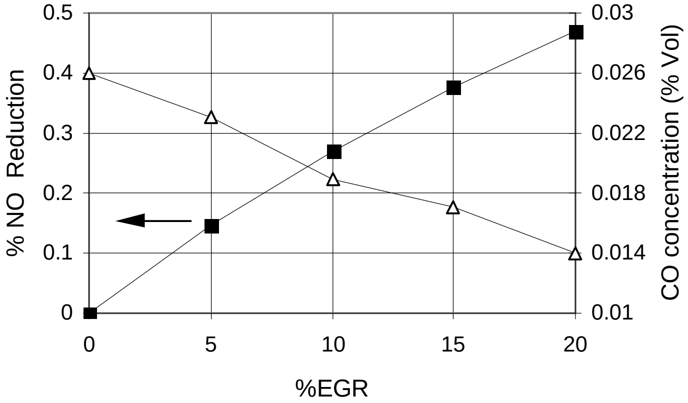

Figure 4- NO and CO amounts versus the amount of recycled gas applied.

As it can be seen, a 47% reduction is achieved when 20% of recycled gas employed as a diluent of the fresh fuel/air mixture. The experimental results indicated the same level of reduction when EGR= 11%, when the shaft speed was set to 2000 rev/min. The absolute levels of NO observed experimentally are much lower than those predicted by the model. With no recirculation, the concentration of NO measured was near 2000 ppm while the equilibrium model predicted about 8000 ppm. However, increasing the speed of the motor sharply increases the NO levels measured, up to 3000 ppm at 4000 rev/min. As previously observed, the model calculates the NO concentration at the peak of the cylinder pressure.

Baruah *et al.* (1978) have measured NO formation at four levels of recirculation in a 2000 cm^3 engine. With no recycled gas added to the fresh fuel/air charge NO concentrations as high 4200 ppm were observed. With the EGR valve fully open, the NO concentrations reduced to about 25%.

The model has to be further increased to take into account the transient effect of pressure in the NO chemistry. In its actual version, however, the application of the model to flue-gas recirculation in constant-pressure combustors such as boilers and turbines is straightforward.

In practice, the amount of recycled gas that can be reintroduced to the combustion chamber is limited by flame speed concerns. Dilution decreases the flame speed, which may have a substantial effect on the performance of the engine when %EGR increases. Turns (1996) calculated a decrease in flame speed from 73.8 to 50.6 cm/s of gasoline-air mixtures with 15% (mass basis) of exhaust gas recirculation.

4. CONCLUSIONS

A model for the predictions of NO emissions on exhaust gas recirculation was developed. Predictions have shown that a 47% decrease in emissions of NO is possible with up to 20% of EGR is applied. This same level of reduction was accomplished with 11% of EGR in the tested engine. Experimental results indicated that at higher levels of EGR has significant effect on the engine performance.

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