Warsaw Univeristy of Technology

Faculty of Power and Aeronautical Engineering

Computer methods in combustion - Project

Gas turbine combustion chamber model using Cantera constant volume reactor net - nitrogen oxides emission analysis

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1 Introduction

Emission prediction is a complex problem involving the coupling between the flow field and chemistry. Most of the time CFD is the preferred modeling approach, yielding predictions with varying degrees of accuracy. But because of a high computational cost, CFD investigations are often limited to the use of reduced chemical mechanisms. In this work the specific features of chemical reactor networks are exploited to build a faster emission estimator. Simple chemical reactor networks, based on the well - stirred reactor plus plug flow reactor scheme, are analyzed using the Cantera package and the GRI - 3.0 chemical kinetics mechanism. The focus is put on the final NO_x concentration.

2 Literature : scientific background

2.1 Gas turbine combustion chamber

A combustion chamber is a component or area of a gas turbine where combustion takes place. It is also known as a burner, combustor or flame holder. In a gas turbine engine, the combustor is fed high pressure air by the compression system. The combustor then heats this air at constant pressure. After heating, air passes from the combustor through the nozzle guide vanes to the turbine.

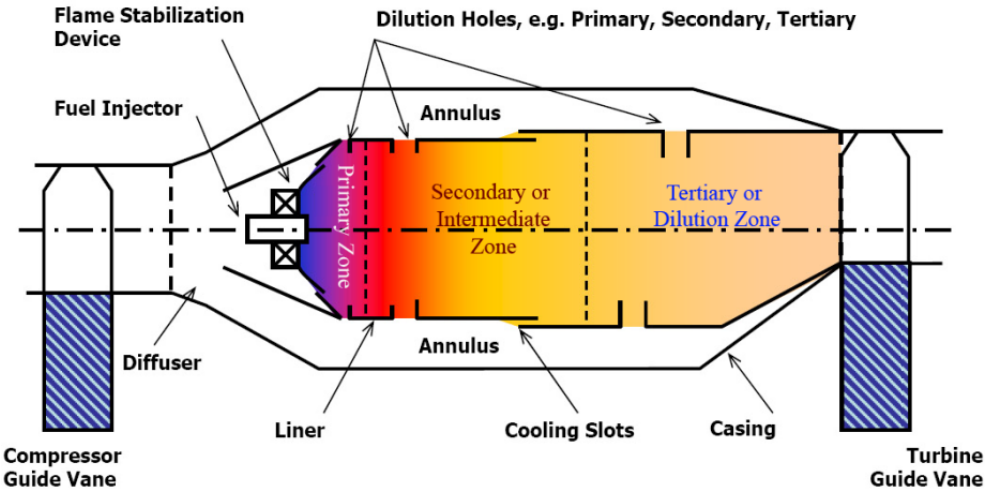


Figure 1: Combustor chamber scheme

A combustor must contain and maintain stable combustion despite very high air flow rates. To do so combustors are carefully designed to first mix and ignite the air and fuel, and then mix in more air to complete the combustion process.

Combustors play a crucial role in determining many of an engine's operating characteristics, such as fuel efficiency, levels of emissions and transient response (the response to changing conditions such as fuel flow and air speed).

2.2 Nitrogen oxides (NO_x)

Combustion systems can produce nitrogen oxides through the reaction of molecular nitrogen contained either in the fuel or in the air. The nitrogen oxides family regroups a variety of compounds among which the most relevant to combustion systems are: nitric oxide NO, nitric dioxide NO_2 and nitrous oxide N_2O. These are also the main nitrogen oxides found in the atmosphere. The first two compounds are commonly grouped together and referred to as NO_x while NO_2 is not included in the definition since it is in majority being produced naturally. Additionally, fractions higher than 90 % of the NO_x in the exhaust of a combustion system is NO. The oxidation of NO to NO_2 occurs later in low temperature regions.

Because of its role in combustion and the subsequent impacts, the chemical kinetics of NO_x formation have received detailed attention. Different pathways have been identified and their relative importance varies depending on the combustion conditions.

Thermal NO or Zeldovich mechanism: This pathway consists in the oxidation of atmospheric nitrogen via the following mechanism known as the extended Zeldovich mechanism

$$N_2 + O \rightarrow NO + N$$

$$N + O_2 \rightarrow NO + O$$

$$N + OH \rightarrow NO + H$$

This route has then a high temperature dependence, hence the name.It is considered that this pathway becomes active and significant at temperatures above 1800 K.

Prompt NO or Fenimore mechanism: This route is intimately linked to the combustion chemistry of hydrocarbons and depends on local combustion conditions rather than on temperature. Fenimore discovered that some NO was rapidly produced in the flame zone of laminar premixed flames long before the characteristic time of the thermal NO. This rapid formation of NO was termed promp.Because prompt NO is formed in the presence of CH radicals (among others), its formation is favored in fuel rich zones and its importance is significant at low temperatures and small residence times (before the thermal pathway activates). The Fenimore mechanism can simplistically be written as follows:

$$CH + N_2 \rightarrow HCN + N \rightarrow ... \rightarrow NO$$

Fuel NO: Some fuels contain nitrogen in their molecular structure (e.g. coal can contain bound nitrogen up to 2 % in mass). The thermal decomposition of the nitrogen-bound compounds of the fuel in the reaction zone leads to the creation of radicals, mainly hydrogen cyanide HCN and ammonia NH_3. These radicals are subject to a following reaction path : they are oxidized into NO in the presence of oxygen, but they can also contribute to reduce NO into N_2.

3 Emission modeling of a gas turbine combustor

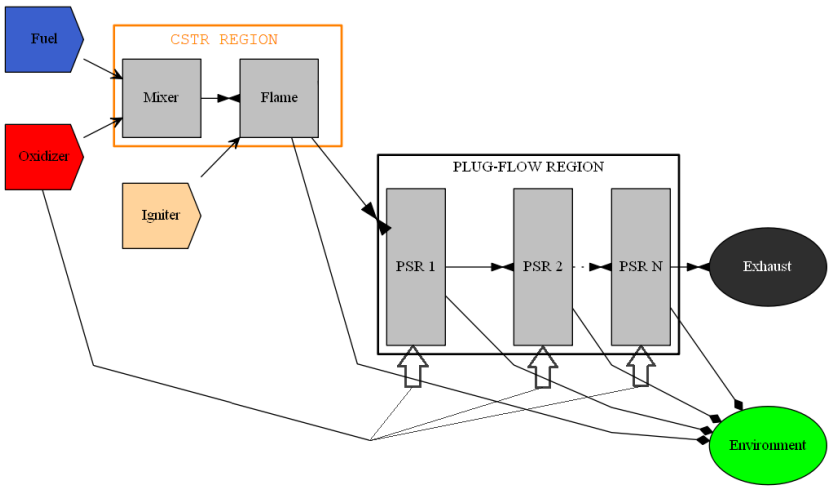


Figure 2: Reactor net scheme

The general architecture used consists of a hybrid CSTR - PFR network: a CSTR cluster of 2 reactors is used to model a mixing region and a flame/ignition region while a PFR is used for the post - flame region. The plug flow reactor is represented by a linear chain of zero -dimensional CSTR reactors. The gas at the inlet to the first one has the specified inlet composition, and for all others the inlet composition is fixed at the composition of the reactor immediately upstream. Since in a PFR model there is no diffusion, the upstream reactors are not affected by any downstream reactors, and therefore the problem may be solved by simply marching from the first to last reactor, integrating each one to steady state. An igniter inlet is added to make sure the flame reactor ignites and the reaction is sustained while not impacting the steady - state solution.

This model has inlet parameters as a typical power production cycle (combustion pressure 25 bar, combustor inlet air temperature 700 K). The fuel is a pure methane.

To define simulation components' attributes such as thermodynamic and transport properties or the reaction rates GRI - 3.0 mechanism is used. The GRI - 3.0 is a chemical mechanism developed by the Gas Research Institute to model natural gas combustion, including full NO_x chemistry. It is a compilation of 325 reactions involving 53 species. A particular feature of GRI - 3.0 is that it has been optimized as a whole towards targets related to methane and natural gas combustion. The GRI - 3.0 mechanism is considered one of the best when it comes to CH_4/NO_x chemistry for natural gas combustion and it is widely used.

4 Results

Simulation has been run considering change of 2 parameters. It's cause was to find temperature distribution and nitrogen oxides concentration over the combustor length. First was equivalence ratio given as:

$$\Phi = \frac{fuel\,to\,oxidizer\,ratio}{(fuel\,to\,oxidizer\,ratio)_{stoichiometric}}$$

Second was parameter X, which I defined as:

$$X = 1 - \frac{dilution\,air\,mass\,flow}{total\,air\,mass\,flow}$$

Only example data will be shown to preserve the brevity of the article. As a result of varying X parameter the following results have been obtained:

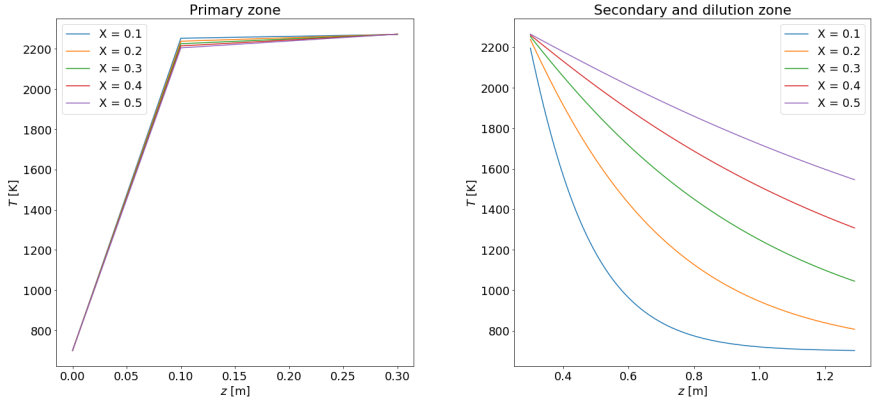


Figure 3: Temperature distribution over combustor length, $\Phi = 0.8, X = var$

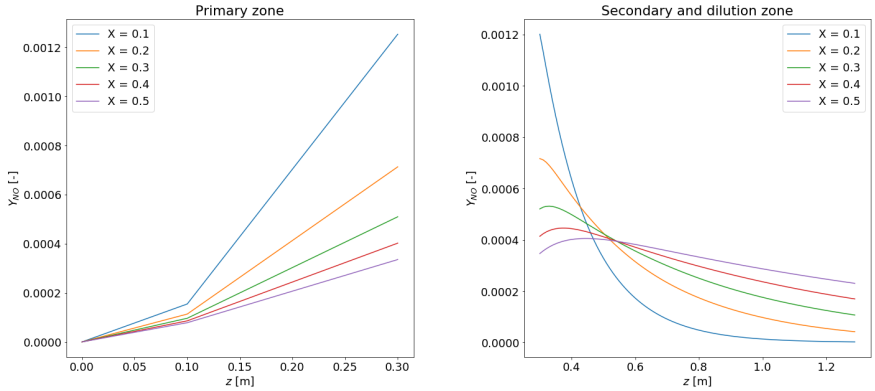


Figure 4: NO mass fraction over combustor length, $\Phi = 0.8, X = var$

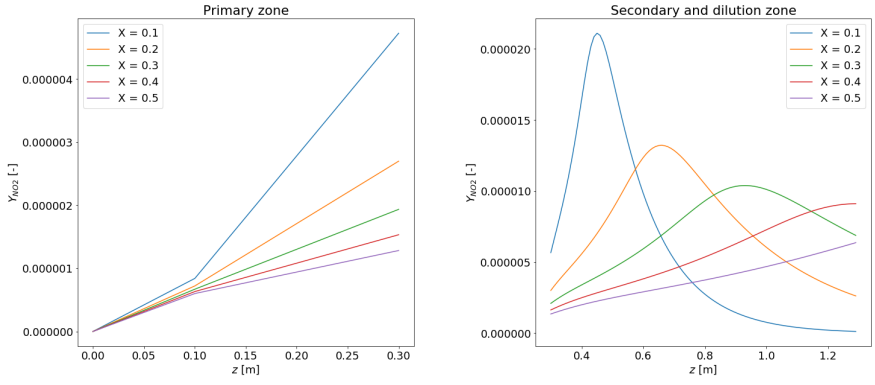


Figure 5: NO2 mass fraction over combustor length, $\Phi = 0.8, X = var$

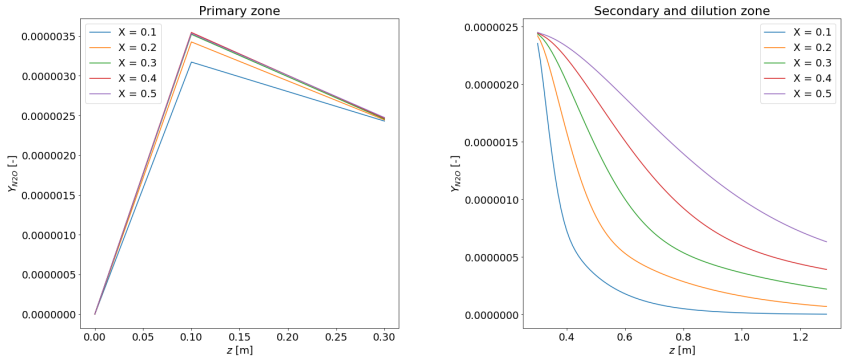


Figure 6: N2O mass fraction over combustor length, $\Phi = 0.8, X = var$

As a result of varying Φ parameter the following results have been obtained:

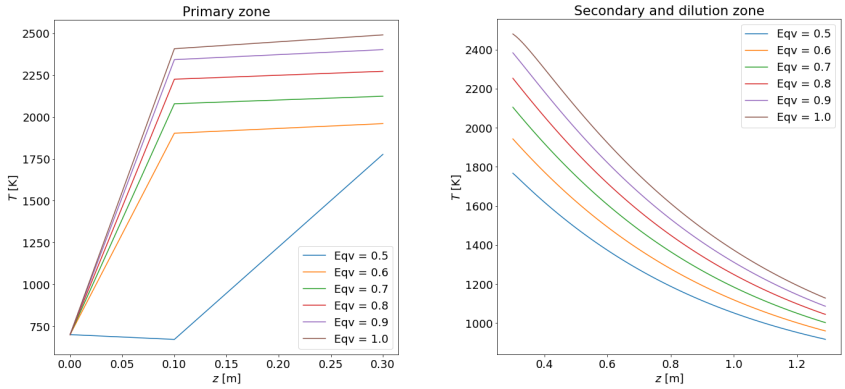


Figure 7: Temperature distribution over combustor length, $X = 0.3, \Phi = var$

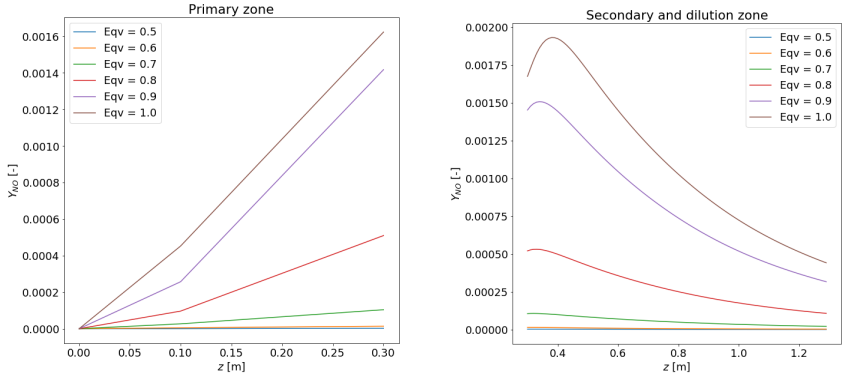


Figure 8: NO mass fraction over combustor length, $X = 0.3, \Phi = var$

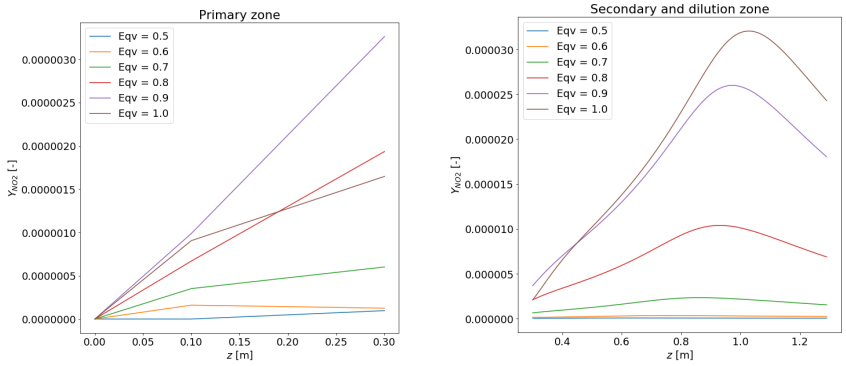


Figure 9: NO2 mass fraction over combustor length, $X = 0.3, \Phi = var$

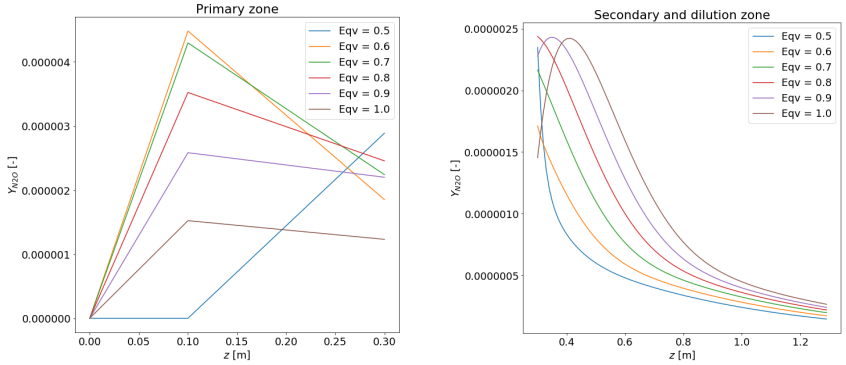


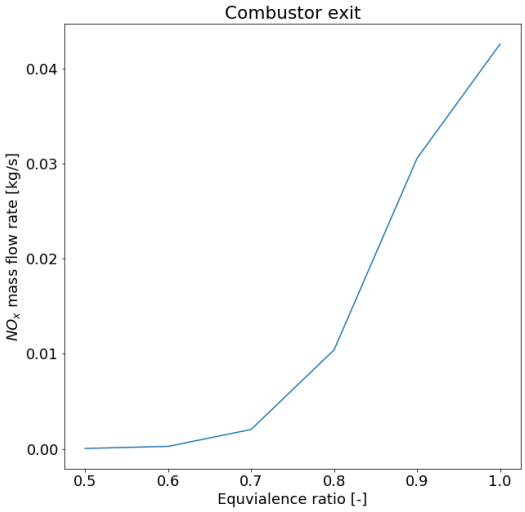
Figure 10: N2O mass fraction over combustor length, $X = 0.3, \Phi = var$

It is important to note that lines in the primary zone charts are not data but trend lines created using 3 data points acquired at the beginning of mixer, between mixer and primary zone and at the end of primary zone. It has been done this way because it is impossible to track parameters through CSTR reactor length, it is possible only at the beginning and the end of the reactor.

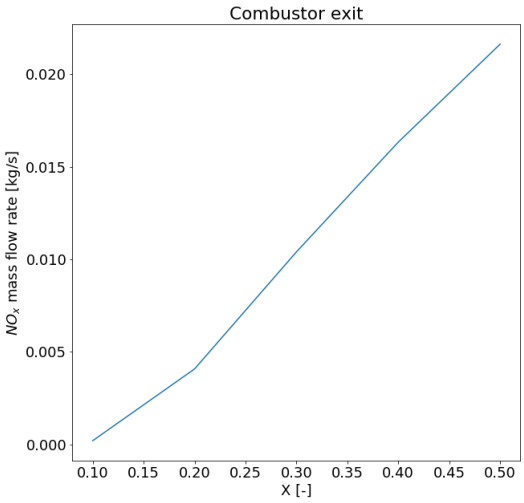
5 Conclusion

From the all nitrogen oxides (NO_x) a nitric oxide (NO) is the element created the most during the combustion reaction in the chamber, and we should mainly concentrate on limiting its emission.

In case of the following graphs all the previous elements emissions were summed to created one general NO_x emission.



(a) NOx mass flow at exit over Φ



(b) NOx mass flow at exit over X

As can be seen from graph (a), the emission of nitrogen oxides increases with the equivalence ratio. Therefore, we can reduce the amount of nitrogen oxides emitted to the atmosphere by carrying out the combustion process with a smaller Φ coefficient, i.e. with a larger excess of air. It leads to a decreased peak temperature, therefore preventing thermal NO_x formation.

This technique is called lean combustion and is employed in nearly all combustion technology sectors, including gas turbines, boilers, furnaces, and internal combustion engines. This wide range of applications attempts to take advantage of the fact that combustion processes operating under fuel lean conditions can have very low emissions and very high efficiency. Unfortunately, achieving these improvements and meeting the demands of practical combustion systems is complicated by numerous problems such as low reaction rates, instabilities and sensitivity to mixing.

As can be seen from graph (b), the emission of nitrogen oxides increases with the X coefficient, which means with the larger part of total air injected directly into burning zone. Therefore, we can reduce the amount of nitrogen oxides emitted to the atmosphere by splitting the combustion air in a number of streams, which are delivered to the combustor at convenient locations. It leads to reducing the formation of NO_x by limiting the availability of NO promoters such as O_2, O, and OH.

This technique is called air staging and it was first used in pulverized coal and oil fired boilers, but with time the technique was adjusted for a variety of other applications such as fluidized bed combustors and gas turbines. Air staging works best under highly fuel-rich conditions and in a range of temperatures that depends on additional variables such as pressure, hydrocarbons availability.

An interesting prospect of Cantera is the ability to generate reaction path diagrams. The reaction path diagram tool aids in the generation of chemical path diagrams for reacting flow systems. For reacting flow systems, the nodes of this graph represent chemical species, and the arrows connecting the nodes represent the flow of a conserved quantity between species. Analyzing these graphs can easily provide information about what NO_x creation mechanism is dominant during considered process and thus what type of solution should we choose to limit their emissions. An example diagram generated during the results analysis is presented below.

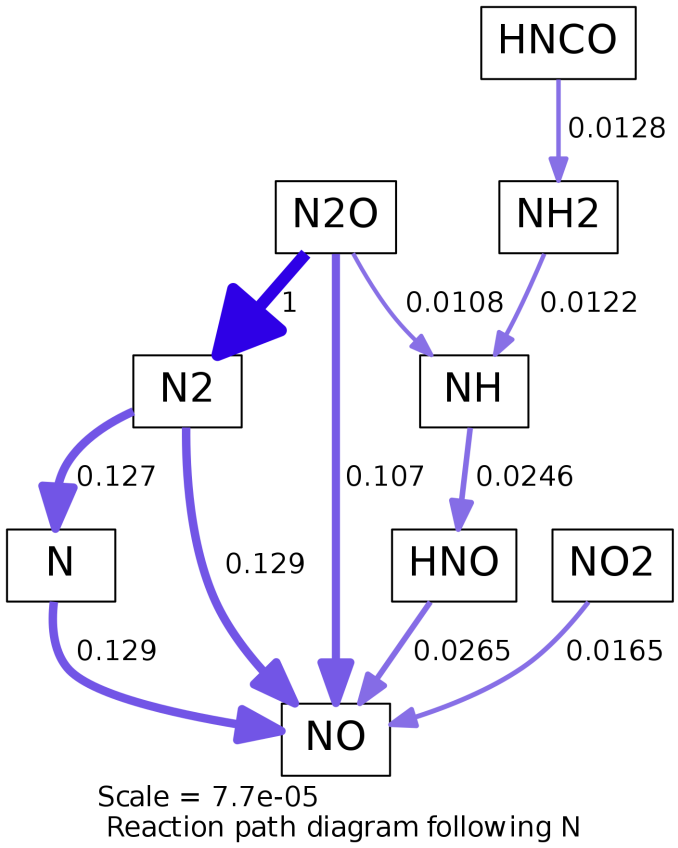


Figure 11: NO_x pathway analysis for $\Phi = 0.5$, X = 0.1, T = 1784 K

6 Sources

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