Tutor/s

Dr. Jordi Bonet Ruiz
Departament Enginyeria Química

Dr. Joan Llorens Llacuna
Departament Enginyeria Química

Màster en Enginyeria Química

Treball Final de Màster

Study of Combustion Using a Computational Fluid Dynamics Software (ANSYS)

Estudio de la Combustión Usando Software de Dinámica de Fluidos Computacional (ANSYS)

Jose Manuel Iglesias Fernández

February, 2015

UNIVERSITAT DE BARCELONA

Dos campus d'excel·lència internacional
B:KC Barcelona Knowledge Campus
HUB Health Universitat de Barcelona Campus

No se equivoca el hombre que prueba distintos caminos para alcanzar sus metas,
se equivoca aquél que por temor a equivocarse no actúa.
Anónimo

En primer lugar, agradecer toda la dedicación y trabajo de mis tutores, y profesorado que han estado implicados en la realización de este trabajo. También agradecer a todas aquellas personas, familia, amigos, compañeros, maestros, etc. Que de alguna manera u otra han estado presentes, animándome para seguir siempre adelante y crecer tanto como persona como como profesional.

Contents

1. SUMMARY

This work is a study of the effect of water addition to a combustion chamber. Starting from a review of the art and literature to understand the NOx formation phenomena and then, using the commercial computational fluid dynamics software ANSYS FLUENT to perform a sensitivity analysis of this water addition.

More specifically, first is a description of what can be found when searching for computational fluid dynamics and water injection engines. Secondly, there is shown the structure and the main characteristics of a simulation performed in ANSYS FLUENT. Finally, there's posed a sensitivity analysis in order to see the effect of the water addition to a combustor, and the influence of the contact mode used to implement this addition.

2. INTRODUCTION

Combustion is present in many different aspects of our lives, from lighters or water heating in home-scale heaters to airplane reactors. Since the phenomena of combustion is a very important part of our daily lives and it's the main source of heat used in the industry it results in a very attractive field of study for many reasons. The next paragraphs can illustrate some of this reasons.

Firstly, as a main source of energy, there's the necessity to maximize the efficiency of the combustion systems and obtain the maximum profit from the resources. Secondly, it is not just the concern about the efficiency what boost the studies about combustion. These processes must be environment-friendly and one of the most limiting aspect for the optimization of the combustion systems is the pollution associated with it. All the pollution associated with these systems (NOx, SOx, VOC's,CO,CO_2) and it's direct relation with global warming is a strong reason to spend resources in technology to improve the combustion systems. For instance, in these days the newsletters has been filled of news about the production of oxidized compounds of nitrogen (NOx) in diesel engines and possible measures to solve the problem [8].

On the other hand, computational resources are increasing in an astonishing rate, which allows us to perform simulations in such detail and velocity that was unbelievable a few years ago. Also, this allows to reduce the time spent in an investigation as the use of computation can be useful for a first approach and save time and money in expensive experiments.

This final project is intended to use the advantages resulting from the availability of these computational resources and apply it to the study of NOx emissions in combustion systems. More exactly, the effect of water addition to combustion systems.

3. OBJECTIVES

The objective of this work is the study of NOx formation in systems where vapour-water is present in the reaction system by using a commercial Computational Fluid Dynamics software (ANSYS: Fluent). In order to carry out this study, the work has been divided in some specific, measurable, achievable, realistic and time-based objectives.

Those objectives are:

- See what has been done in the field of the study of combustion by using CFD and systems where vapour-water is used to reduce the pollution due to NOx (a review of the state of the art).
- Learn how to use the selected commercial simulator and its capabilities.
- Select an appropriated case study.
- Provide a virtual laboratory to study the combustion.
- Perform a sensitivity analysis to see the effect of water addition into the combustion system in the NOx emissions.

4. REVIEW OF THE STATE OF THE ART

4.1. NUMERICAL SIMULATION OF COMBUSTION

The study of NOx production by using CFD is not widely used. When searching for papers related to it, just a few but interesting results can be found. Specifically, *Byeonghun et al (2015) provides* a recent clear example about the concern about this subject. In this paper, the authors carry out a study of the NOx emission characteristics when burning a methane-air mixture in a combustor. The study includes both experimental and computational data referring the NOx emissions. The experimental device scheme used in their study is shown in figure 1.

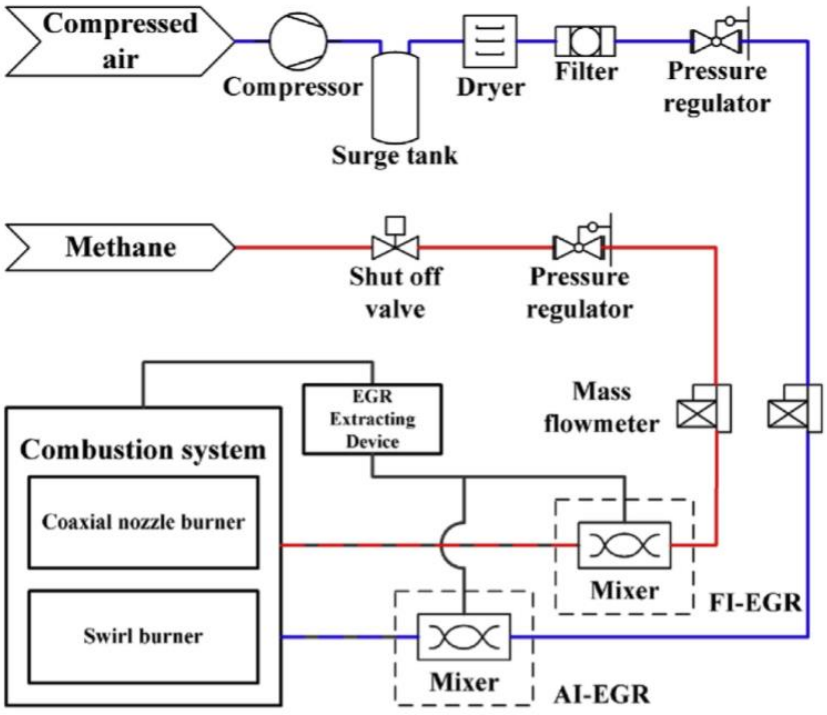

Figure 1: Schematic diagram of the experimental apparatus (Byeonghun et al, 2015).

The combustion system consists of a combustion chamber that can operate as a coaxial combustor (Non-premixed combustion) or as a swirl combustor (pre-mixed combustion), a fuel inlet (Methane), a compressed-air inlet and an exhausted gas recirculation (EGR) device (Figure 1). A scheme of the combustion chamber used in the experiments is presented in Figure 2.For their study, the researchers set the system to work as a non-premixed combustor and studied the NOx emissions for different ratios of EGR in the fuel stream (FI-EGR) and in the air stream (AI-EGR).For the computational part of the research, they use the commercial software ANSYS-Fluent to study the effect of the EGR ratio in the NOx production and the GRI-3.0 reaction mechanism.

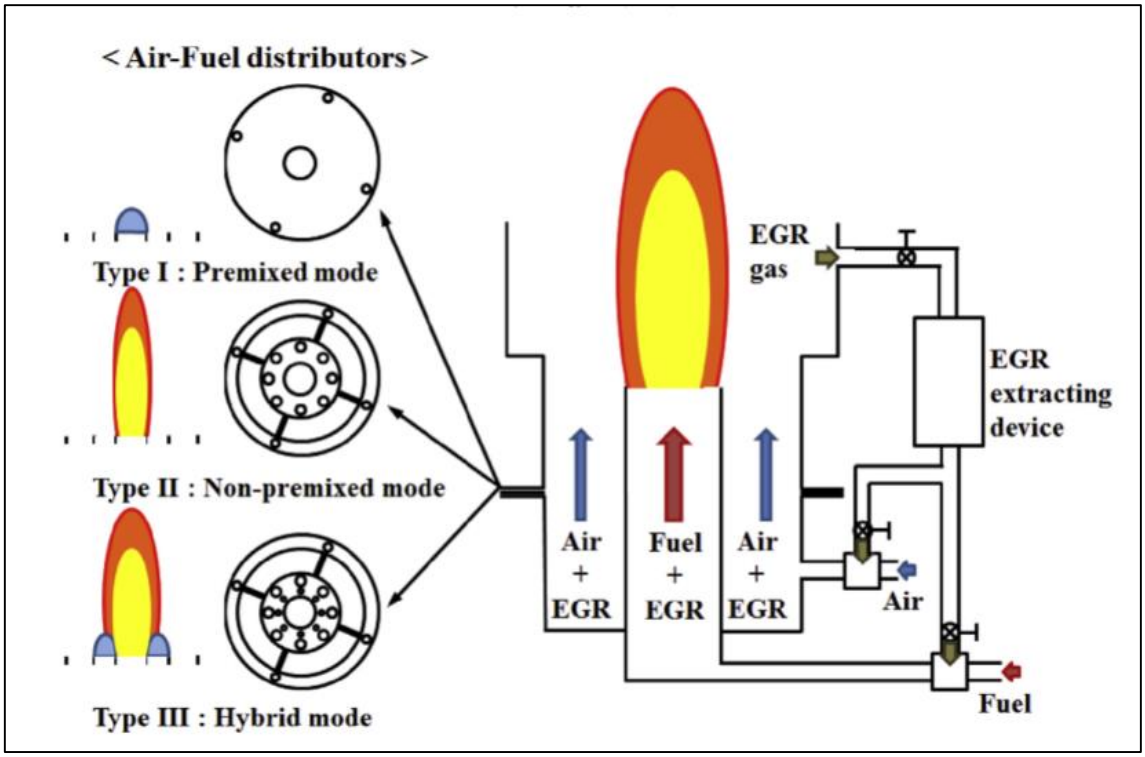

Figure 2: Shematic picture of the combustion apparatus (Byeonghun et al, 2015).

4.2. WATER ADDITION IN COMBUSTION SYSTEMS

Several experiments has been carried out in the last years, showing the positive effects in terms of pollutants reductions when water-injection engines are employed (e.g. (2)). However, it is not only a laboratory field of study. The water-injection engines has been commercially used in aircraft engines, marine engines and automation engines. Those systems can help to overcome the challenge arisen from the increasingly restrictive legislation about the NOx emissions [10].

The addition of water have some effects when talking about the thermodynamic and the chemistry of the combustion system. An example of the effects in the thermodynamics is that the initial injection of water, cools the fuel-air mixture significantly, resulting in an increase of the compression ratio that can be acquired in the system. Also, the addition of water minimizes the temperature peaks during the combustion process, hence a reduction of NOx formation will happen, as it tend to appear at high temperatures.

Besides the NOx reduction associated with a combustion temperature decrease, the presence of water influences directly to the reaction mechanism. Chybowski et al [2] describe the following reaction mechanism for the NOx reduction by water addition *(Figure 3,* Figure 4*)*. Notice that the water supplied into the combustion chamber reduce the concentration of atomic oxygen and promote the formation of hydrogenated species as HCN or HNCO, which cannot convert directly to NO.

$$H_2O \rightarrow OH + H$$
$$H_2O + O \rightarrow OH + OH$$
$$H_2 + O \rightarrow H + OH$$
$$H + O_2 \rightarrow OH + O$$

which influences the reaction speed:

$$O + N_2 \leftrightarrow NO + N$$
$$O + N_2 + OH \leftrightarrow N_2O + OH.$$

Figure 3 : Atomic oxygen reduction due to water (Byeonghun et al, 2015).

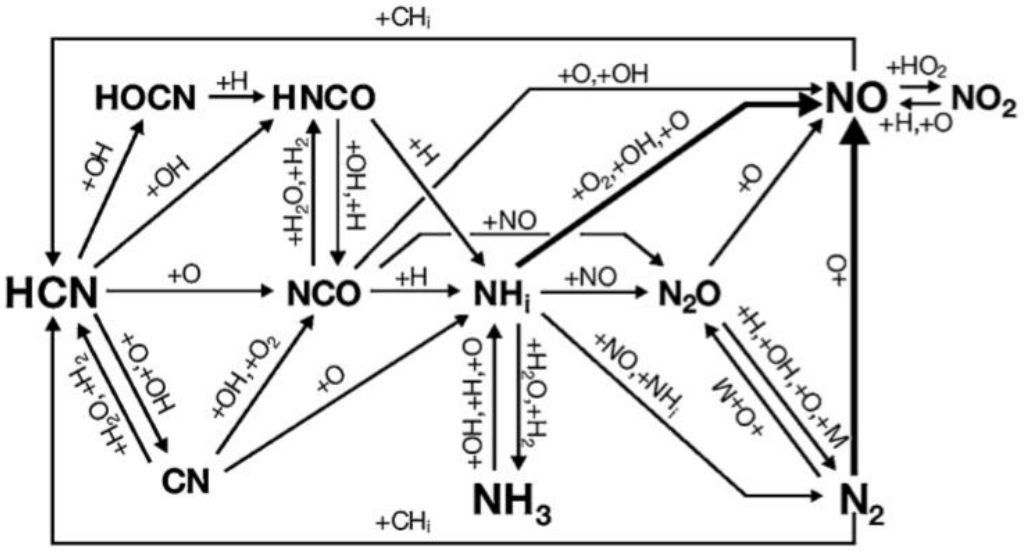

Figure 4 A simplified diagram of nitrogen oxides integration and disintegration during the combustion process (Byeonghun et al, 2015).

5. COMPUTATIONAL FLUID DYNAMICS: ANSYS-FLUENT

Computational Fluid Dynamics (CFD) simulation provides a virtual laboratory to perform experiments in the early stages of design without building the physical apparatus. Virtual environments decreases the unit design costs as the number of unsatisfactory experimental devices that ends to scrap decrease drastically. Otherwise, the cost of experimental device and its operation until obtain satisfactory results can become very huge. Simulations can be done by CFD modelling using commercial or own software with the same base: *"CFD simulations use mathematical models which represents the different phenomena occurring in the system."*

The accuracy of a CFD simulation to the real solution depends on the appropriated selection of the models. Hence, the use of a commercial and widely use commercial software, which its models are widely accepted and validated against experimental data, is recommended. In this work, the CFD software used was ANSYS.

5.1. PERFORMING A SIMULATION IN ANSYS: FLUENT

ANSYS is a software suit that spans the entire range of physics, providing access to lots of fields of engineering simulation that a design process require. In particular, the module FLUENT is appropriate for this work. FLUENT's models are focused on fluids flow and chemical reactions, including a very good model to run a first-approach simulations of combustion systems.

In the next sections, it's explained the main characteristics of how to perform a simulation using ANSYS: Fluent. Starting, but not focusing, on the geometry and mesh creation, and continuing on how to set up the models and run the calculations. the ANSYS FLUENT Tutorial Guide (ANSYS, **2015**), to perform this kind of simulations it is required to attain the *"Chapter 16: Modelling Species Transport and Gaseous Combustion", example problem number 16.* In this problem, it's studied the combustion of methane in air, in turbulent flow, and using a simple reaction mechanism. Once achieved the basic skills from the tutorial, we are ready to simulate the effect of water addition to the NOx formation.

To perform a simulation in ANSYS FLUENT, the next steps are followed:

- Design the geometry of the system.
- Discretise the geometry by generating an appropriated mesh.
- Set up the models to represent the reality adequately.
- Configure the calculation's parameters to run the simulation and obtain results.
- Results retrieval and visualization.

5.1.1. Geometry design

Figure 5 provides the configuration and dimensions of the combustion chamber used in the simulations as well as the fuel and air rates passing through the system.

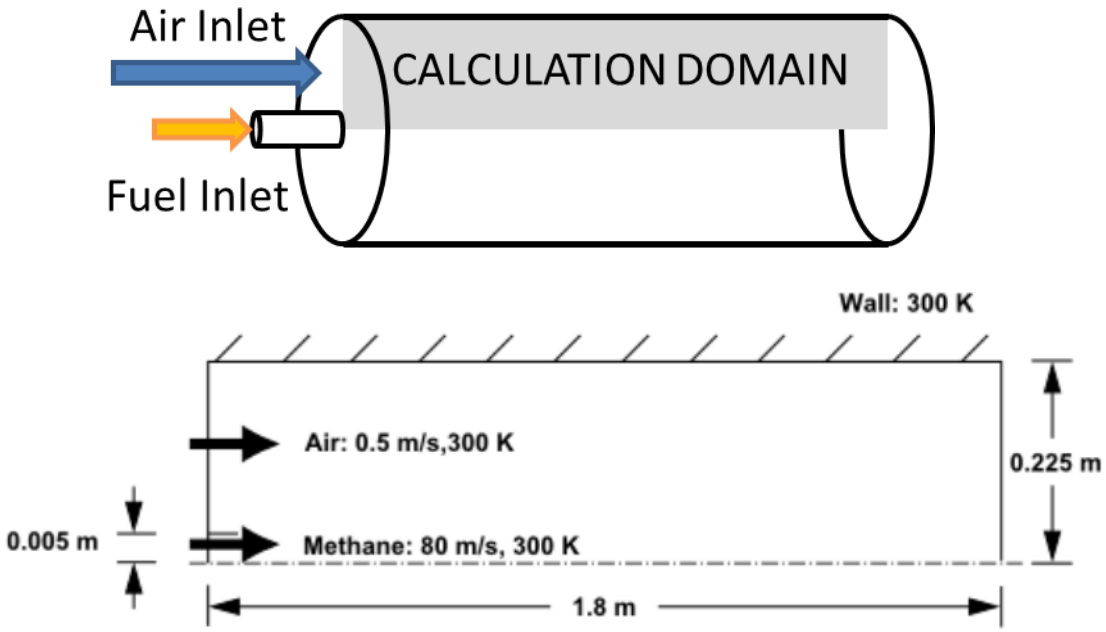

Figure 5 : Calculation domain (ANSYS, 2015)

This is a representation of a non-premixed combustion chamber but, due to the high level of symmetry present in the system, the calculation domain can be reduced to a 2D problem assuming no variations in the radial coordinate. If done, the computational time required for the calculations decrease drastically.

5.1.2. Mesh generation

Concerning the microscopic balances, notice that all the governing equations are differential equations with a continuous solution along the space. The system discretisation is the way to assign the mathematical model to a finite element of the system, transform those differential equations in algebraic equations, and then, solve the system. That is called finite element method.

The approximation of differential equations to finite increments introduce an error that is bigger as bigger is the size of the finite element but, the error associated to a determined point is also dependant of the derivatives intensity. Hence, if there is a zone

where an intense phenomena is occurring (i.e. intense chemical reactions or high energy turbulences), the size of the elements must be reduced to improve solution accuracy. Undiscrimate use of an uniform tiny mesh size everywhere leads to unachievable computing power requirements.

In the combustion chamber, the mesh must be refined all long near the center (symmetry axis) and close the fuel inlet, because there is where the combustion reaction occurs. For this purpose, the combustion chamber has been discretised using ANSYS's own meshing program, introducing a sphere of influence and an inflation ratio to refine the mesh in the important zones of the system. In the figure below, is presented a view of the sphere of influence, and the final mesh used for the calculations with the sphere and inflation applied.

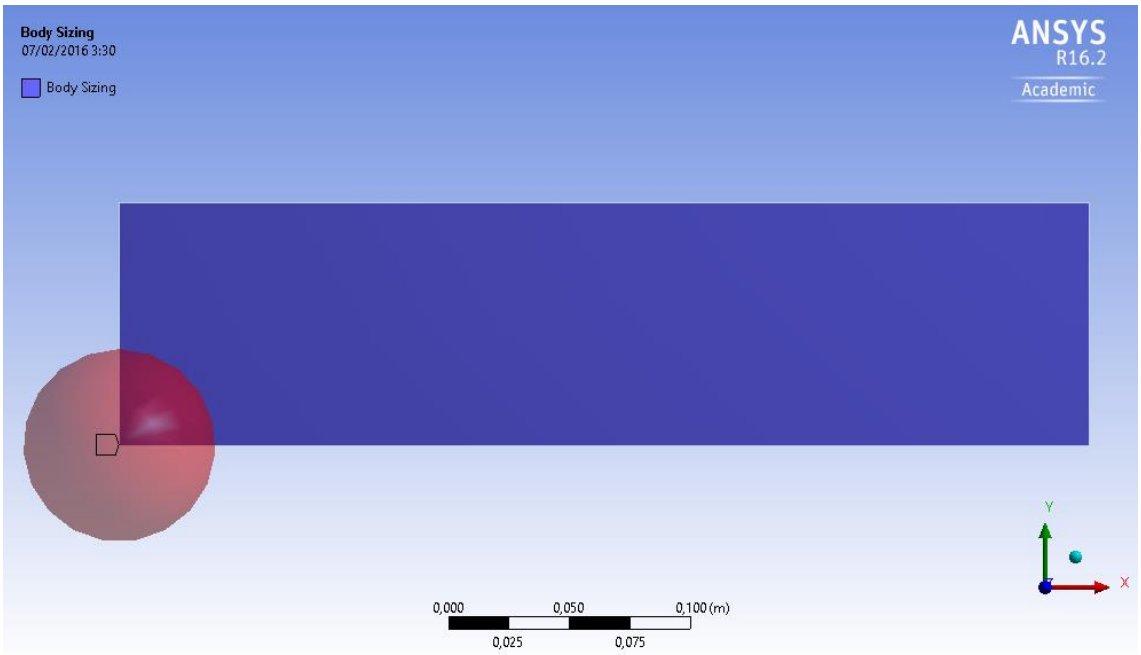

Figure 6: Refining the mesh using a sphere of influence near the inlets.

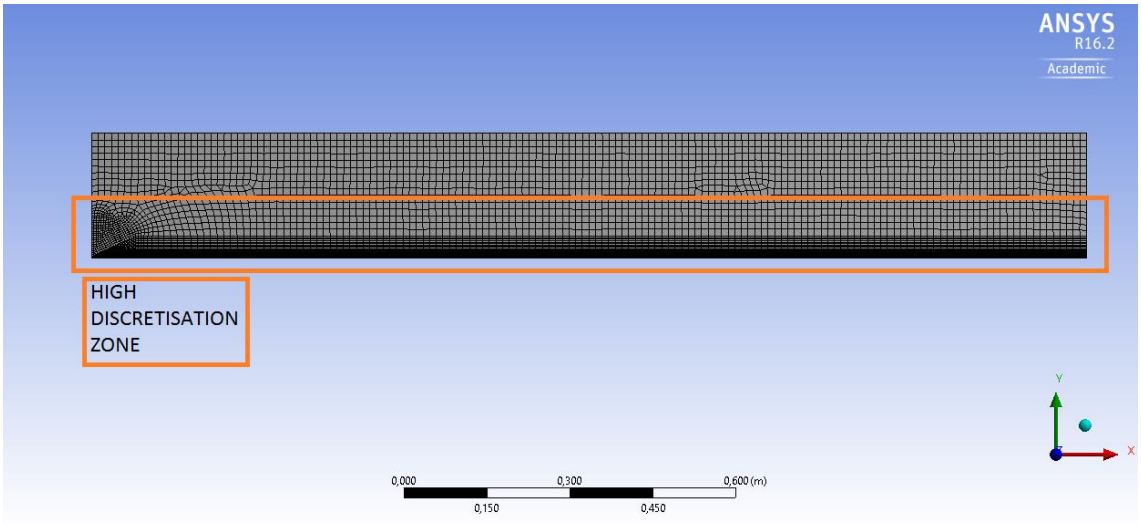

Figure 7: Final mesh with the sphere of influence in the fuel inlet and the inflation factor in the symmetry axis.

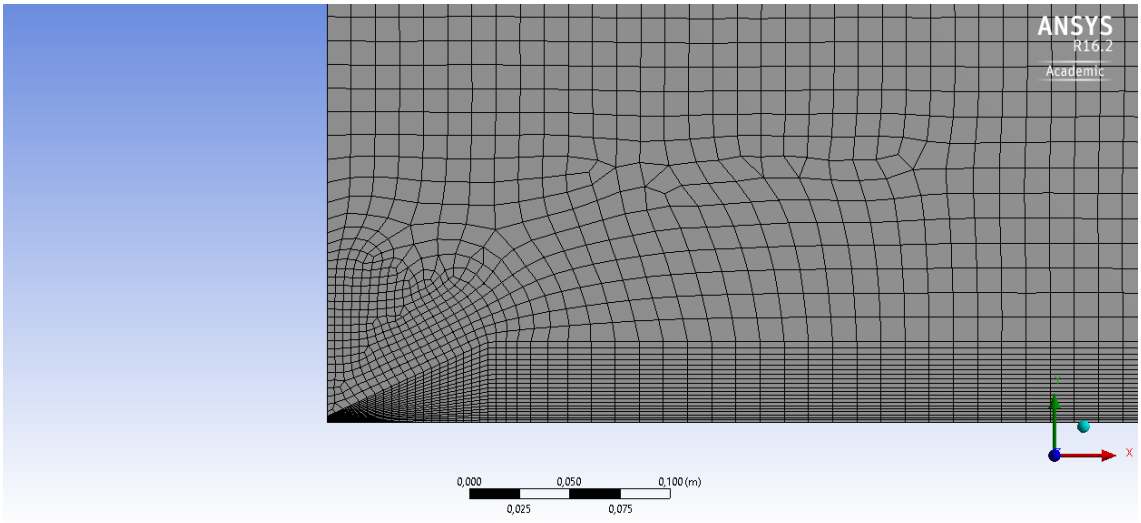

Figure 8: Zoom-in at the zone of high discretisation.

5.1.3. Simulation Setup

As commented before, this is the step where all the models are assigned to the design modelled in the previous parts. ANSYS has some valid applications available that could solve the problem posed in this work. The software ANSYS FLUENT has been selected because it incorporates a good package for simulate the combustion phenomena. Inside FLUENT the setup consists in the following parts, necessary to perform the calculations.

- Models definition: it is the part where is defined which models are selected to as describe the different phenomena present in the system.
- Boundary Conditions: Set the different inlets, outlets and limits of the system.
- Calculation Parameters: Set the solution methods and controls.

Models definition

CFD calculation and mathematical processes are governed by fluid flow governing equations. The equations are series of balances and fluid properties, which are the overall mass balance (continuity equation) (equation 1), momentum balance (equation 2), energy balance (equation 3 or 4) and partial mass balances (equation 5).

Those governing equations are:

Continuity

$$\frac{\delta \rho U}{\delta t} + \nabla . \rho U = 0 \qquad \textit{Equation 1}$$

Momentum

$$\frac{\delta \rho U}{\delta t} + (\nabla . \rho U U) = -\nabla p + \nabla . \tau + \rho g \qquad \textit{Equation 2}$$

Enthalpy

$$\frac{\delta \rho h}{\delta t} + \nabla . \rho U = \nabla . \lambda_e \nabla T - \nabla . q_r + \nabla . \sum_l \rho h_l(T) D_e \nabla m_l \qquad \textit{Equation 3}$$

Temperature

$$\rho C_p \frac{DT}{Dt} = \nabla . \lambda_e \nabla T - \nabla . \sum_l \rho h_l(T) D_e \nabla m_l - \rho \sum_l \frac{D m_l}{Dt} h_l(T) \qquad \textit{Equation 4}$$

Species mass fraction

$$\frac{\delta \rho m_l}{\delta t} + \nabla . \rho U m_l = \nabla . D_e \rho \nabla m_l - R_l \qquad \textit{Equation 5}$$

FLUENT discretise those governing equations for every point of the system. To obtain de different properties that are needed to solve those discretised equations (i.e. viscous behaviour, radiation energy transfer, or chemical reactions) FLUENT resorts to different models in order to estimate these parameters. The use and selection of these models depends on the nature of the problem to be solved. For this work all this equations need to be solve and the following models must be activated to estimate the turbulences (viscous model), the radiation term, and the species distribution and kinetics.

Viscous model

The viscous model must be activated because there is a fluid flowing through the system. One of the most accepted and used models to estimate the turbulent-flow behaviour of the combustion systems is the k-epsilon model (6).This model is practical for many flows and its convergence is usually easy. The model is composed by two equations including the turbulent kinetic energy (k) (equation 6) and the turbulent dissipation rate (ϵ) (equation7).

$$\frac{\delta(\rho k)}{\delta t}+\frac{\delta(\rho k u_i)}{\delta x_i}=\frac{\delta}{\delta x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\delta k}{\delta x_j}\right]+P_k+P_b+\rho\epsilon-Y_M+S_k \quad \textit{Equation 6}$$

$$\frac{\delta(\rho\in)}{\delta t}+\frac{\delta(\rho\in u_i)}{\delta x_i}=\frac{\delta}{\delta x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\in}\right)\frac{\delta\in}{\delta x_j}\right]+C_{1\in}\frac{\in}{k}(P_k+C_{3\in}P_b)-\rho C_{2\in}\frac{\epsilon^2}{k}+S_\in \quad \textit{Equation 7}$$

Radiation model

The radiation model must be activated because of the high temperature achieved in the system. The P-1 radiation model is the simplest case of the more general P-N model, which is based on the expansion of the radiation intensity I into an orthogonal series of spherical harmonics. The radiation flux term ($-\nabla\cdot q_r.$) in the energy balance equation (equation 3) is provided by the equation 8. For more information see *section 5.3.3: P-1 Radiation Model Theory* (7).

$$-\nabla\cdot q_r=aG-4an^2\sigma T^4 \quad \textit{Equation 8}$$

Where a is the absorption coefficient, n is the refractive index of the medium, σ is the Stefan-Boltzmann constant and G is the incident radiation.

Species transport: non-premixed model

As commented before, the non-premixed combustion occurs when the fuel and the oxidizer enter the reaction zone in distinct streams.Under certain assumptions, the thermochemistry can be reduced to a single parameter: the mixture fraction. The mixture fraction, denoted by f, is the mass fraction that originated from the fuel stream. In other words, it is the local mass fraction of burnt and unburnt fuel stream elements (C, H, etc.) in all the species (CO_2, H_2O, O_2, etc.). Hence, the mixture fraction is a conserved scalar quantity, and therefore its governing transport equation does not have a source term. Combustion is simplified to a mixing problem. Hence, all the species' parameters required for the transport equations are defined in terms of the mixture fraction and the difficulties associated with closing non-linear mean reaction rates are avoided for *non-premixed combustion* (7).

The basis of the non-premixed modelling approach is that under a certain set of simplifying assumptions, the instantaneous thermochemical state of the fluid is related to a conserved scalar quantity known as the mixture fraction, f. The mixture fraction can be written in terms of the atomic mass fraction (equation 9).

$$f = \frac{Z_i - Z_{i,OX}}{Z_{i,fuel} - Z_{i,OX}} \qquad \textit{Equation 9}$$

Where Z_i is the elemental mass fraction for element, i. The subscript *OX* denotes the value at the oxidizer stream inlet and the subscript *fuel* denotes the value at the fuel $Zi - Zi,OXZi,fuel - Zi,OX$Equation 9 is identical for all elements, and the mixture fraction definition is unique. The mixture fraction is thus the elemental mass fraction that originated from the fuel stream.

NOx formation:

The formation of NOx can be attributed to four distinct chemical kinetic processes: thermal NOx formation, prompt NOx formation, fuel NOx formation, and intermediate N_2O (7). Thermal NOx is formed by the oxidation of atmospheric nitrogen present in the combustion air. Prompt NOx is produced by high-speed reactions at the flame front, and fuel NOx is produced by oxidation of nitrogen contained in the fuel. At elevated pressures and oxygen-rich conditions, NOx may also be formed from molecular nitrogen (N_2) via N_2O.

The formation of thermal NOx is determined by a set of highly temperature-dependent chemical reactions known as the extended Zeldovich mechanism. The principal reactions governing the formation of thermal NOx from molecular nitrogen are as follows:

$$O + N_2 \rightleftharpoons N + NO$$

$$N + O_2 \rightleftharpoons O + NO$$

A third reaction has been shown to contribute to the formation of thermal NOx, particularly at near-stoichiometric conditions and in fuel-rich mixtures:

$$N + OH \rightleftharpoons H + NO$$

The rate of formation of NOx is significant only at high temperatures (greater than 1800 K) because fixation of nitrogen requires the breaking of the strong N_2 triple bond. Also, will increase with increasing oxygen concentration. It also appears that thermal NO formation should be highly dependent on temperature but independent of fuel type. In fact, the thermal NOx production rate doubles for every 90 K temperature increase beyond 2200 K.

To evaluate the NOx formation, the concentration of O atoms and the free radical OH will be required, in addition to the concentration of stable species (i.e., O_2, N_2). Following the suggestion by Zeldovich, the thermal NOx formation mechanism can be decoupled from the main combustion process, by assuming equilibrium values of temperature, stable species, O atoms, and OH radicals.

Reffering to Prompt NOx, there is good evidence that can be formed in a significant quantity in some combustion environments, such as in low-temperature, fuel-rich conditions and where residence times are short.

At present the prompt NOx contribution to total NOx from stationary combustors is small. However, as NOx emissions are reduced to very low levels by employing new strategies (burner design or furnace geometry modification), the relative importance of the prompt NOx can be expected to increase.

Prompt NOx is most prevalent in rich flames. The actual formation involves a complex series of reactions and many possible intermediate species. The route is as follows:

$$\begin{aligned} CH + N_2 &\rightleftharpoons HCN + N \\ N + O_2 &\rightleftharpoons NO + O \\ HCN + OH &\rightleftharpoons CN + H_2O \\ CN + O_2 &\rightleftharpoons NO + CO \end{aligned}$$

A number of species resulting from fuel fragmentation have been suggested as the source of prompt NOx in hydrocarbon flames (e.g., CH, CH_2, C, C_2H), but the major contribution is from CH_2 via:

$$CH_2 + N_2 \rightleftharpoons HCN + NH$$

The other two mechanisms won't have an effect on the NOx formation of this study because, the fuel NOx are associated to Nitrogenized hydrocarbons (not presents as the fuel is pure methane) and the NO_2 intermediate mechanism is associated to high pressure systems.

For this case, as the non-premixed combustion model has been used, and the model estimates the concentration of O and OH radicals, the instantaneous O and OH radicals' model for the NOx calculations has been used.

6. SENSITIVITY ANALYSIS

Once some practice with ANSYS FLUENT has been acquired, one can use it to perform parametric analysis of a system, where almost all the variables stay static but a few change. That allows to see and the effect of this change. The first step is to set a base case. The next table show the flow rates of this case and the excess percentage referring to the stoichiometric flow rate. The results obtained from this simulation will be named as "0% water", (it is the dry case run).

Table 1 0% simulation flow rates.

Fuel Rate [kg/s]	Air Rate [kg/s]	Excess Air Percentage [%]
$4.095 \cdot 10^{-3}$	$9.020 \cdot 10^{-2}$	25

In order to observe the effect of water addition, a serie of simulations will be run varying the amount of water added to the system and maintaining the fuel and air flow rates constant. The amount of water added is referred as fuel mass percentage, and it will vary from 0% to 25% in 5% increments.

Also, it's thought that not only the amount but the contact mode influences the NOx formation. Hence, the previous values of added water will be simulated for the case when it's added mixed with the air (cases named WA) and for the case when it's mixed with the fuel (cases named WF). The next tables resume the values used to configure the simulations.

Table 2: Water with fuel(WF) cases. Rates and percentages used in ANSYS FLUENT.

	Water mass %	Methane-H2O Rate [kg/s]	Air Rate [kg/s]	Methane mass %	Water mass %	N_2 mass fraction	O_2 mass fraction
WF	0	$4.09 \cdot 10^{-3}$	$9.02 \cdot 10^{-2}$	1	0	$7.67 \cdot 10^{-1}$	$2.33 \cdot 10^{-1}$
	5	$4.30 \cdot 10^{-3}$	$9.02 \cdot 10^{-2}$	9.52·10-1	$4.76 \cdot 10^{-2}$	$7.67 \cdot 10^{-1}$	$2.33 \cdot 10^{-1}$
	10	$4.50 \cdot 10^{-3}$	$9.02 \cdot 10^{-2}$	9.09·10-1	$9.09 \cdot 10^{-2}$	$7.67 \cdot 10^{-1}$	$2.33 \cdot 10^{-1}$
	15	$4.71 \cdot 10^{-3}$	$9.02 \cdot 10^{-2}$	8.70·10-1	$1.30 \cdot 10^{-1}$	$7.67 \cdot 10^{-1}$	$2.33 \cdot 10^{-1}$
	20	$4.91 \cdot 10^{-3}$	$9.02 \cdot 10^{-2}$	8.33·10-1	$1.67 \cdot 10^{-1}$	$7.67 \cdot 10^{-1}$	$2.33 \cdot 10^{-1}$
	25	$5.12 \cdot 10^{-3}$	$9.02 \cdot 10^{-2}$	8.00·10-1	$2.00 \cdot 10^{-1}$	$7.67 \cdot 10^{-1}$	$2.33 \cdot 10^{-1}$

Table 3: Water with Air (WA) cases. Rates and percentages used in ANSYS FLUENT.

	water mass %	H_2O-AIR Rate [kg/s]	Methane Rate [kg/s]	N_2 mas fraction	O_2 mass fraction	H_2O mass fraction
WA	0	$9.02 \cdot 10^{-2}$	$9.02 \cdot 10^{-2}$	$7.67 \cdot 10^{-1}$	$2.33 \cdot 10^{-1}$	0
	5	$9.04 \cdot 10^{-2}$	$9.02 \cdot 10^{-2}$	$7.65 \cdot 10^{-1}$	$2.32 \cdot 10^{-1}$	$2.26 \cdot 10^{-3}$
	10	$9.06 \cdot 10^{-2}$	$9.02 \cdot 10^{-2}$	$7.64 \cdot 10^{-1}$	$2.32 \cdot 10^{-1}$	$4.52 \cdot 10^{-3}$
	15	$9.08 \cdot 10^{-2}$	$9.02 \cdot 10^{-2}$	$7.62 \cdot 10^{-1}$	$2.31 \cdot 10^{-1}$	$6.76 \cdot 10^{-3}$
	20	$9.10 \cdot 10^{-2}$	$9.02 \cdot 10^{-2}$	$7.60 \cdot 10^{-1}$	$2.31 \cdot 10^{-1}$	$9.00 \cdot 10^{-3}$
	25	$9.12 \cdot 10^{-2}$	$9.02 \cdot 10^{-2}$	$7.58 \cdot 10^{-1}$	$2.30 \cdot 10^{-1}$	$1.12 \cdot 10^{-2}$

7. RESULTS

The most important parameters involved in the NOx formation as describe in the previous section are the temperature, and the O, H and OH radicals' concentration. For a visual analysis of the system, in the next pages the profiles of these parameters for each of the simulations of the sensitivity analysis are presented. In addition, it is presented the rate of thermal and Prompt NOx.

For a quantitave measure of the NOx formation, the amount of NOx produced in dry base (ppmNOx without water) for each kilogram of methane burnt, $[\frac{ppmdryNOx}{kgburntCH4/s}]$ is represented as a function of the water percentage injected on the system for the WA and WF cases. Furthermore, following the ***¡Error! No se encuentra el origen de la referencia.***, there is presented a table that shows the average temperature at the outlet, and the peak temperature of each case.

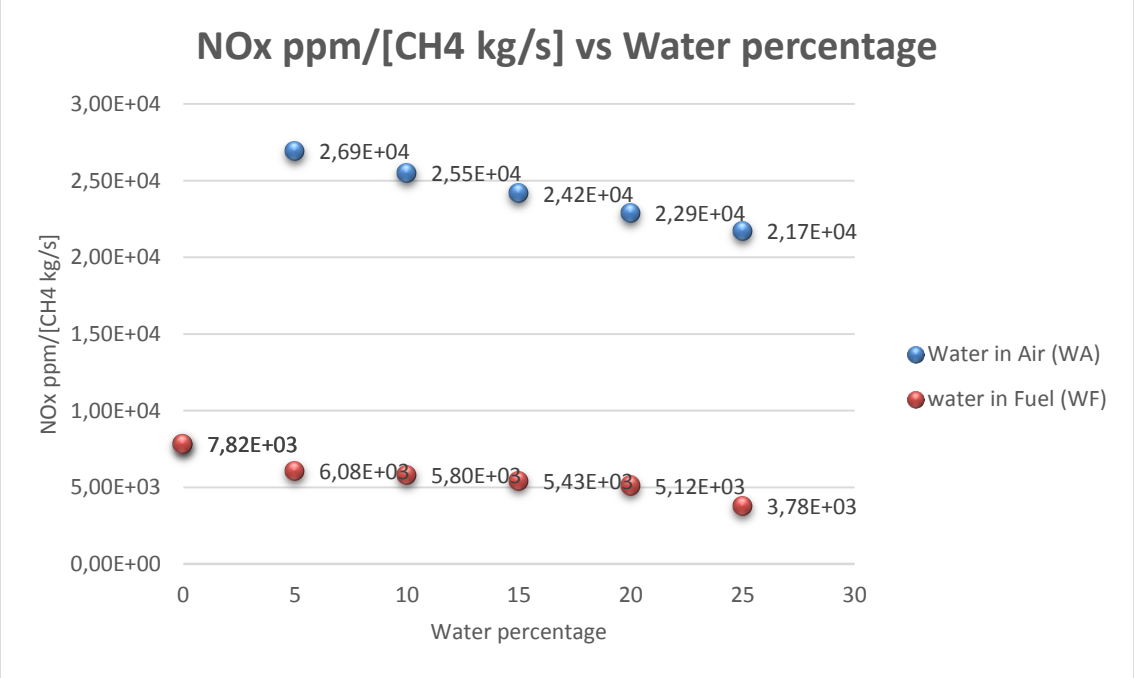

Figure 9: average outlet ppm of NOx produced for every kilogram of CH4 burnt

Case Name	Water mass percentage [%]	Average Outlet [NOx ppm]	Temperature peak [K]	Average outlet Temperature [K]
0%-W	0	32,	2050	1793
WA	5	110	2136	1737
	10	104	2133	1723
	15	99	2129	1730
	20	94	2126	1727
	25	89	2123	1724
WF	5	25	1982	1726
	10	24	2033	1715
	15	22	2029	1711
	20	21	2026	1710
	25	15	2013	1658

Table 4: Results summary

Looking at the graphic, one can notice how, as much water is added to the system, the amount of NOx formed reduce, but the mixing of the water in the air have a detrimental effect because it increase the NOx formed. Also, when comparing the NOx produced for each case with other parameters and profiles (shown below) one can notice how there's the tendency to reduce the temperature average, the temperature peak, the radicals [O] and [OH] concentration and the thermal and Prompt NOx rates, as much water is added to the system.

All the profiles presented below should be evaluated as half symmetry plane of the combustor, with the fuel inlet at the left-bottom corner. The next figure is an example of how would it look like if represented as a symmetry plane in the cylinder.

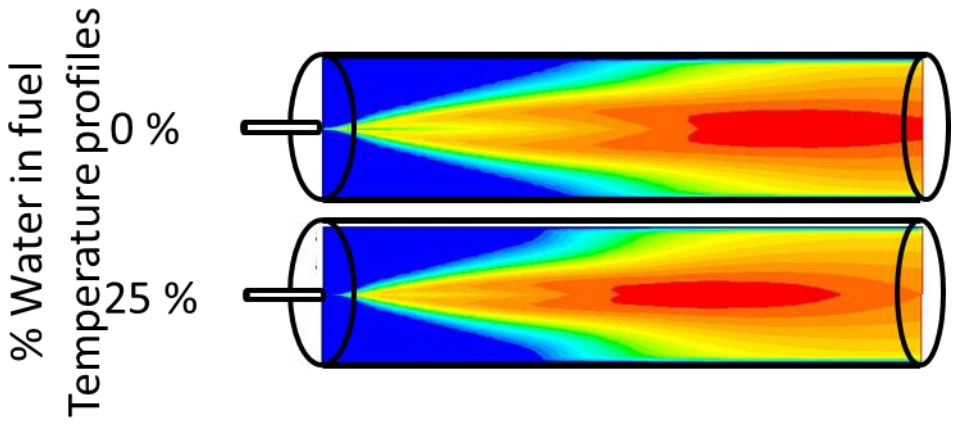

Figure 10: Symmetry plane results representation example

7.1. TEMPERATURE PROFILES

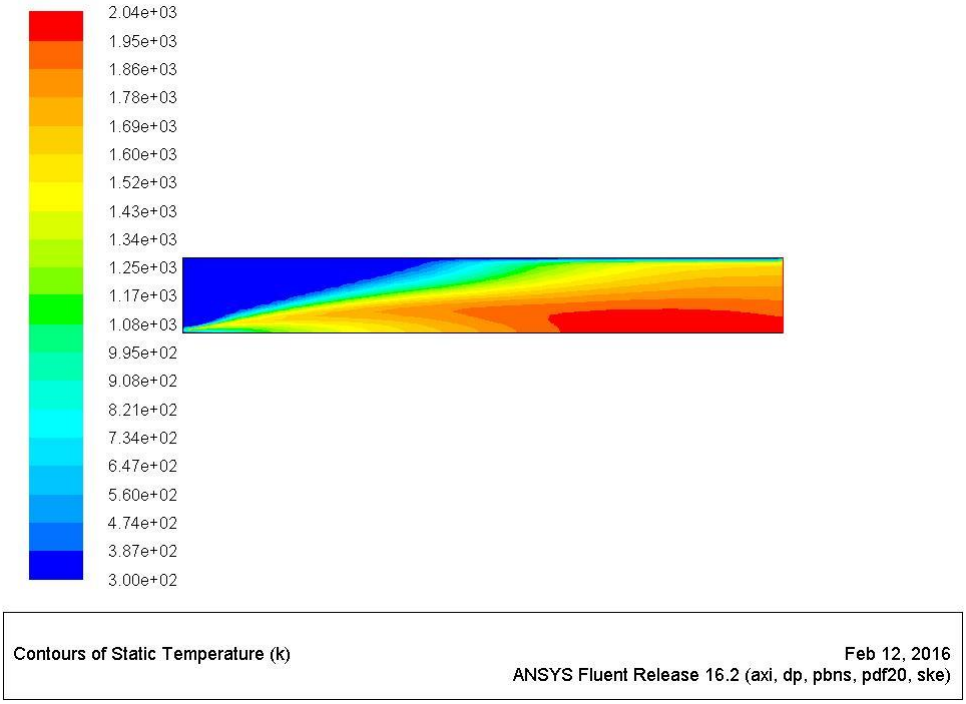

Figure 11 :0% water temperature profile

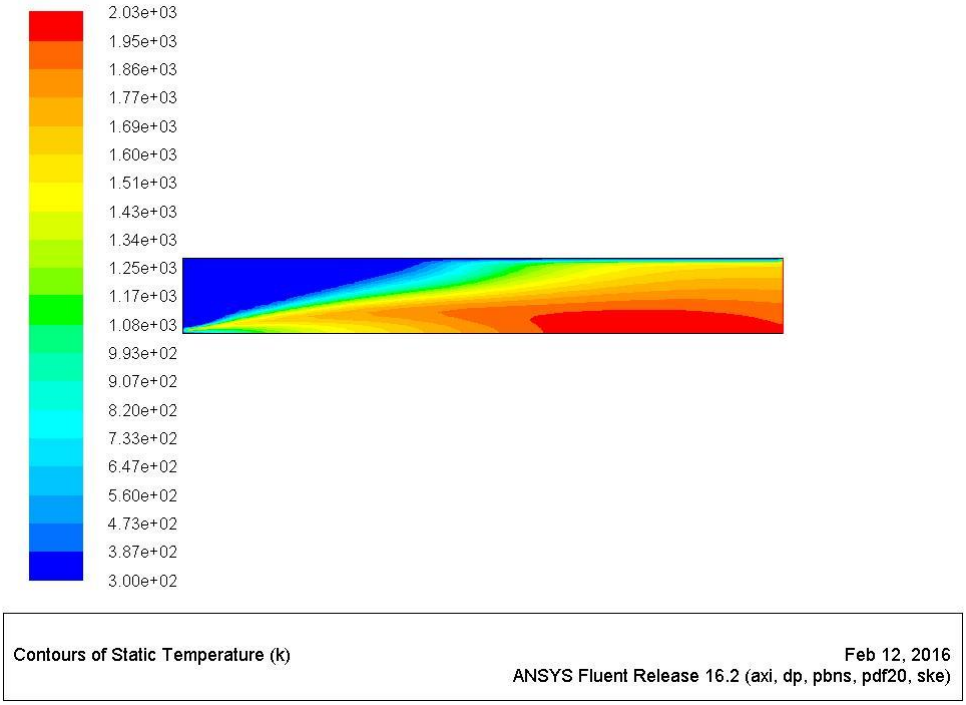

Figure 12: 5% WF temperature profile

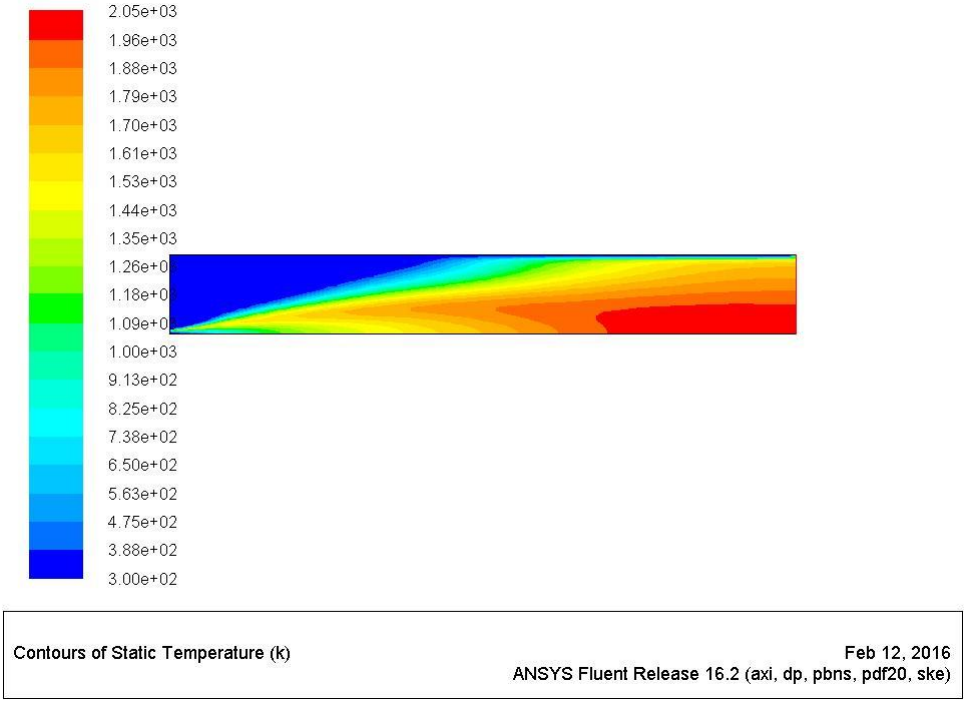

Figure 13: 10% WF temperature profile

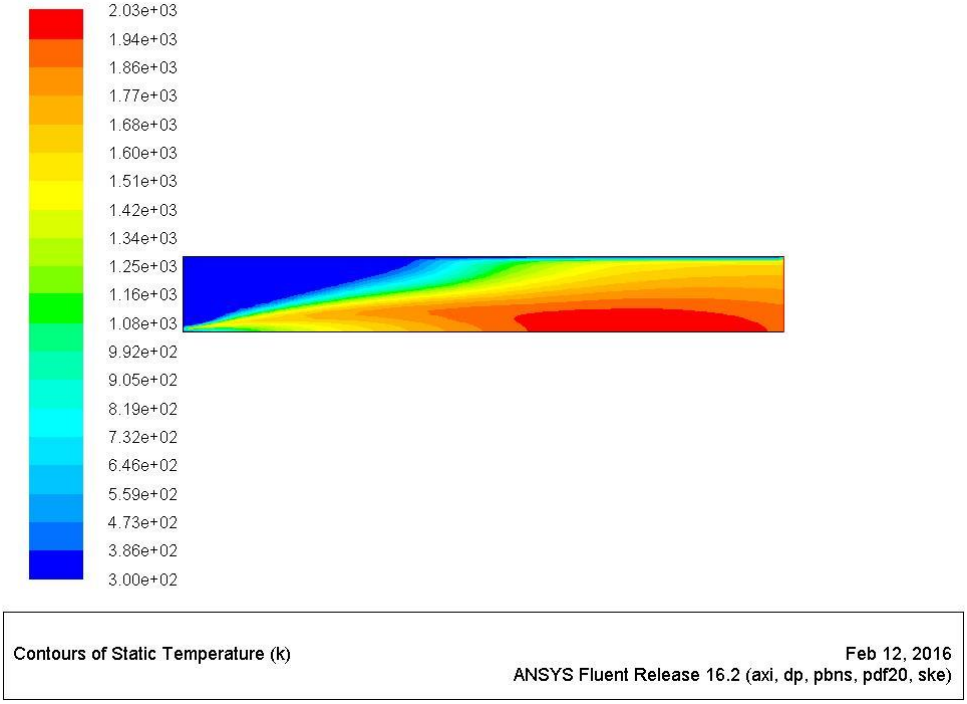

Figure 14: 15% WF temperature profile

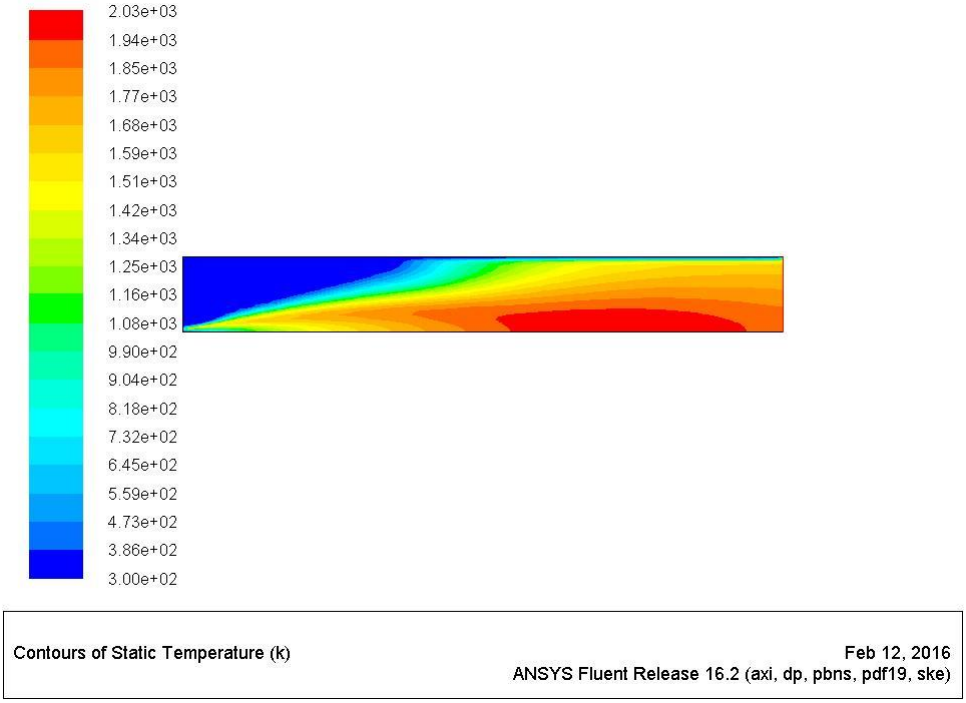

Figure 15: 20 % WF temperature profile

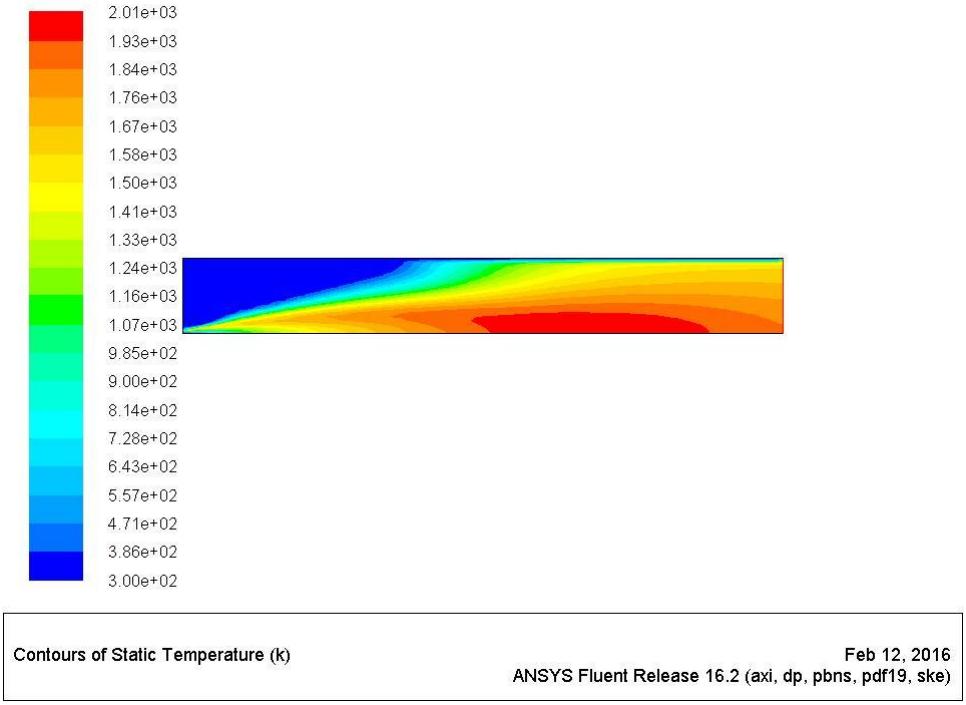

Figure 16: 25 % WF temperature profile

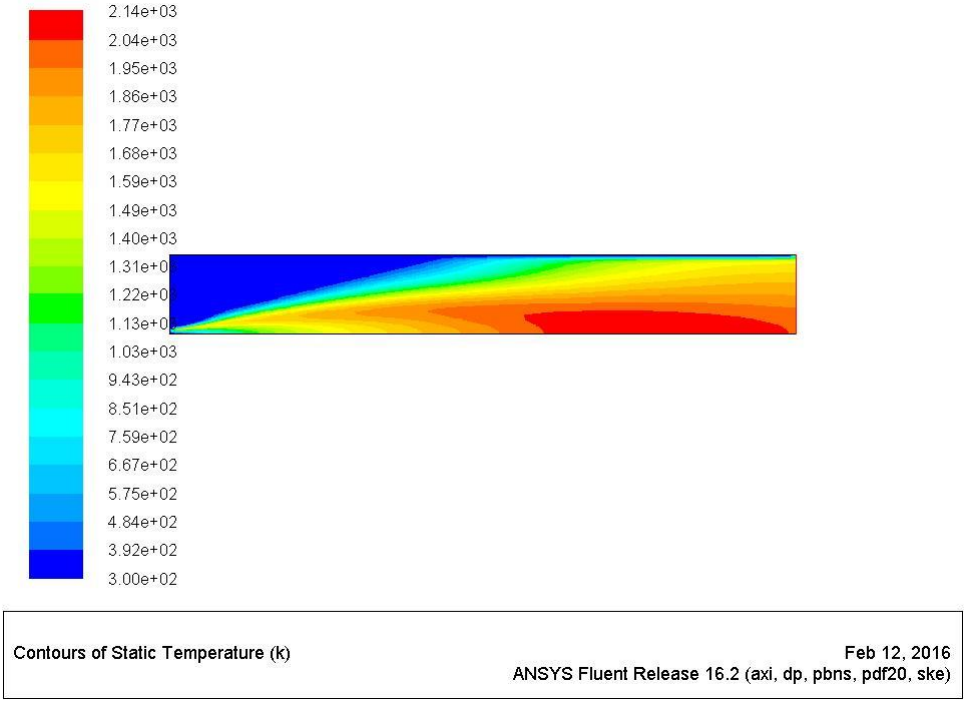

Figure 17: 5% WA temperature profile

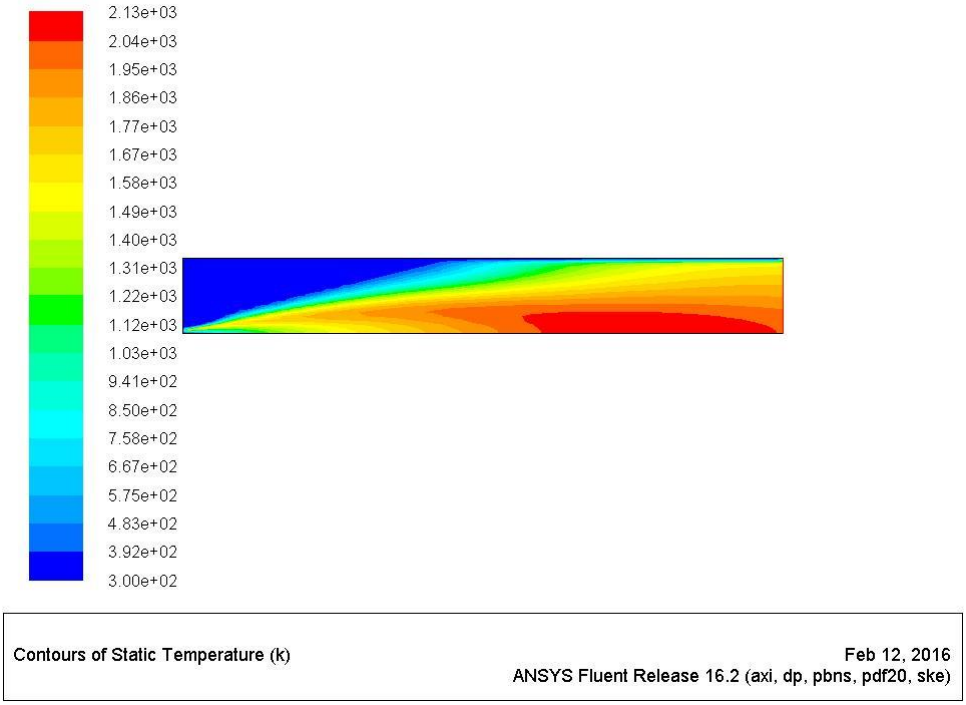

Figure 18: 10% WA temperature profile

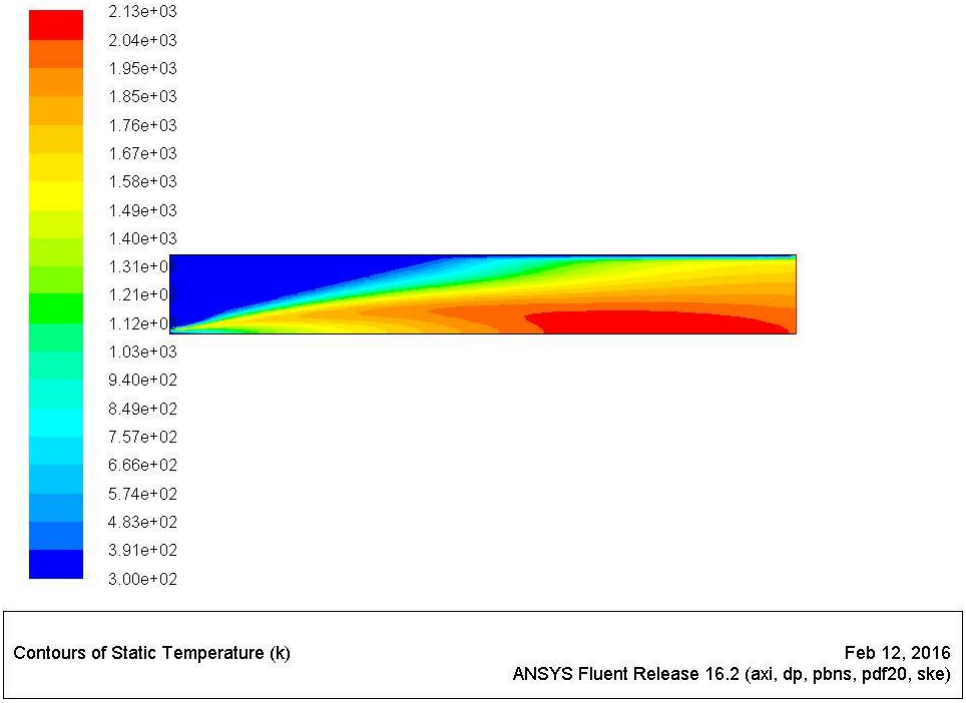

Figure 19: 15% WA temperature profile

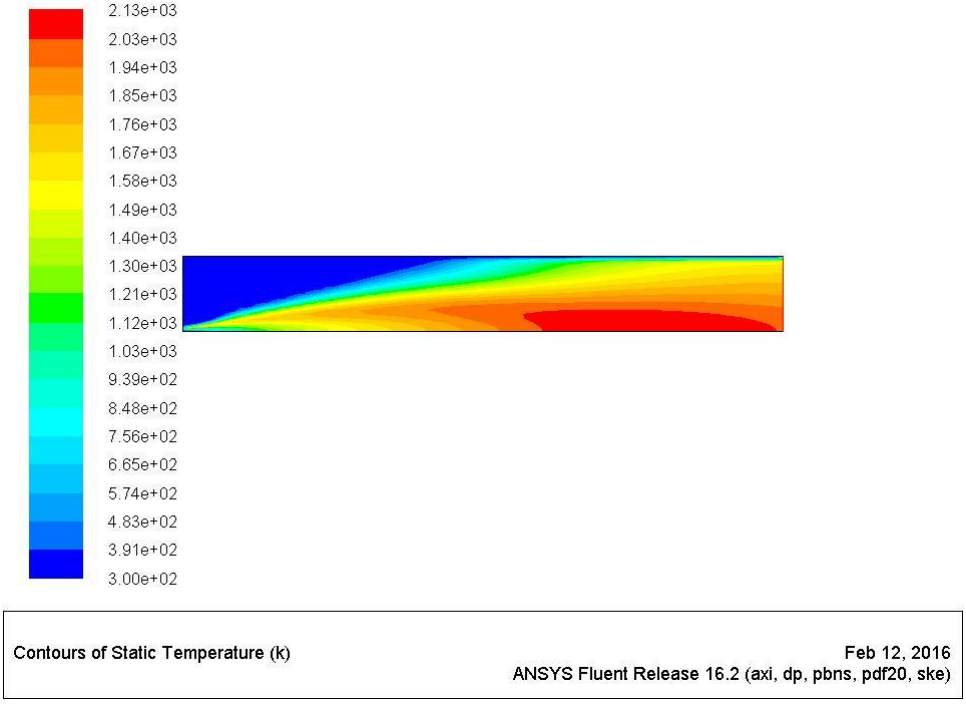

Figure 20: 20% WA temperature profile

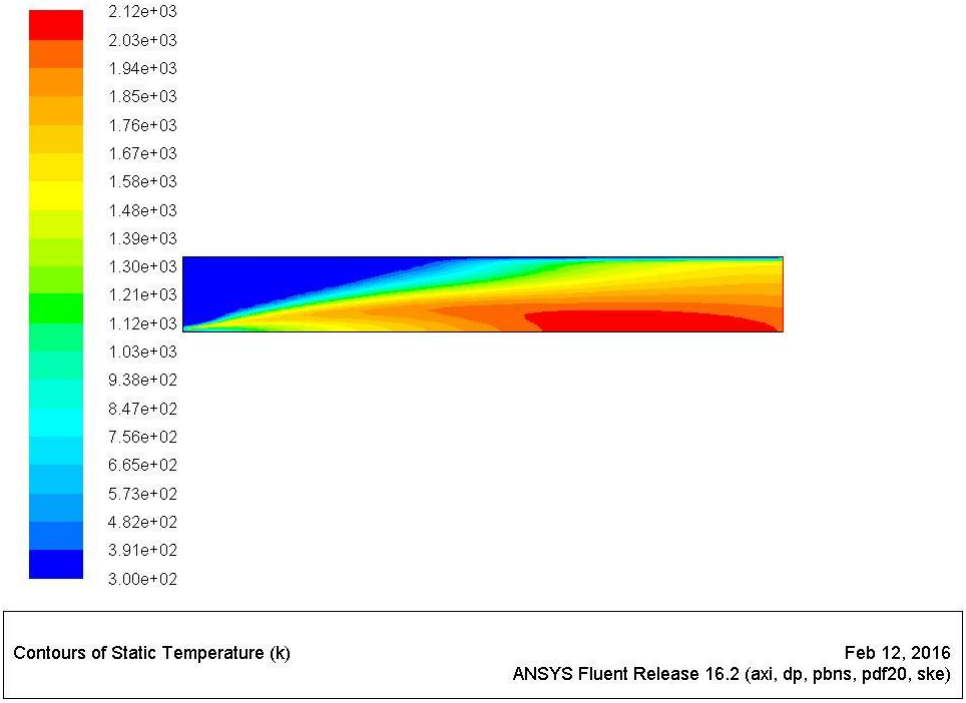

Figure 21: 25% WA temperature profile

7.2. NOX PPM PROFILES

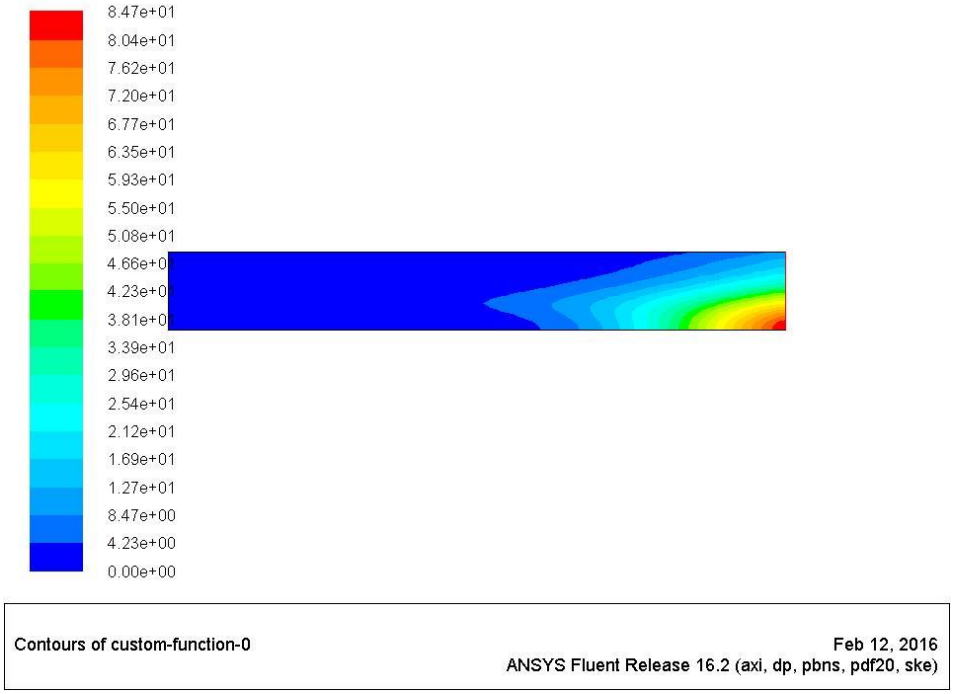

Figure 22: 0% water ppmNOx

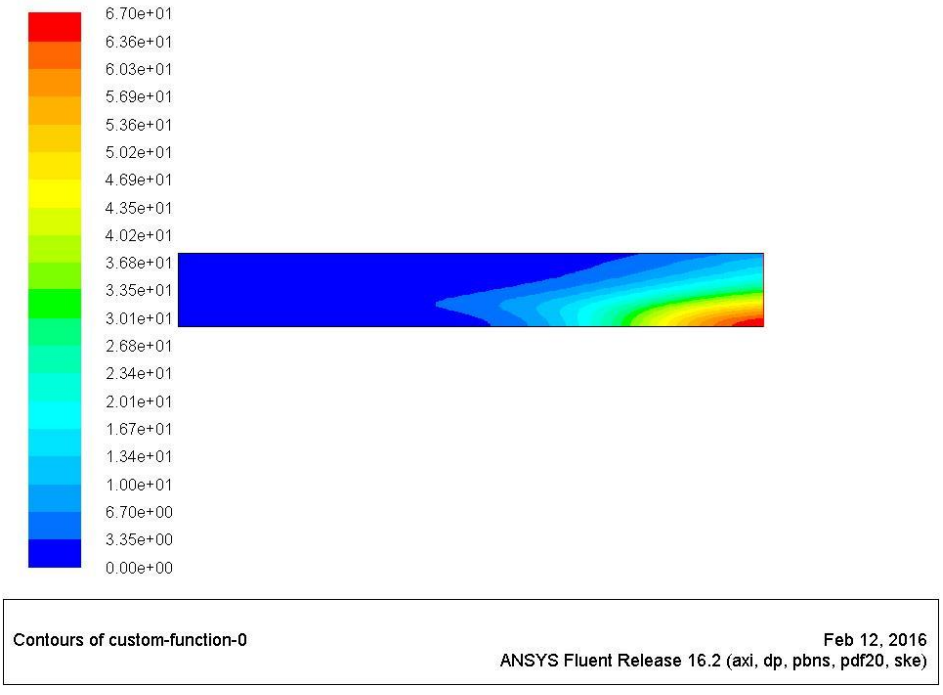

Figure 23: 5% WF ppmNOx

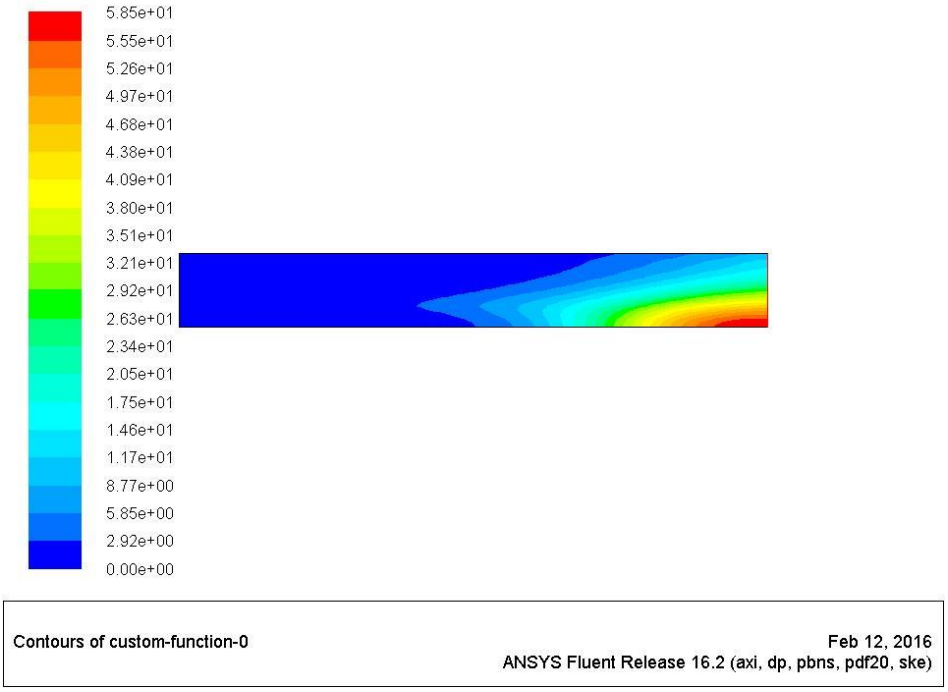

Figure 24: 10% WF ppmNOx

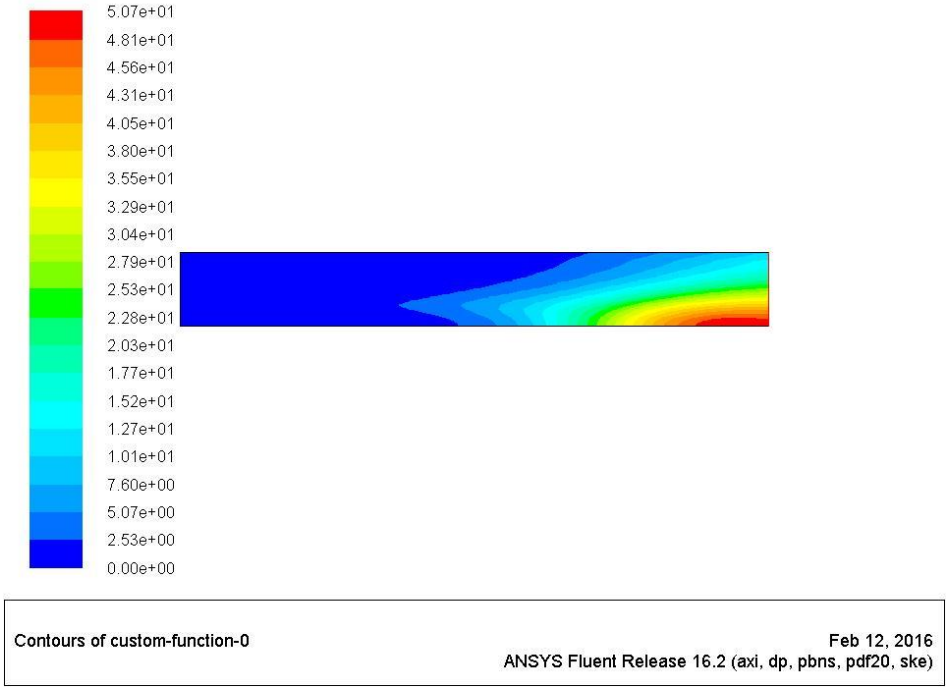

Figure 25: 15% WF ppmNOx

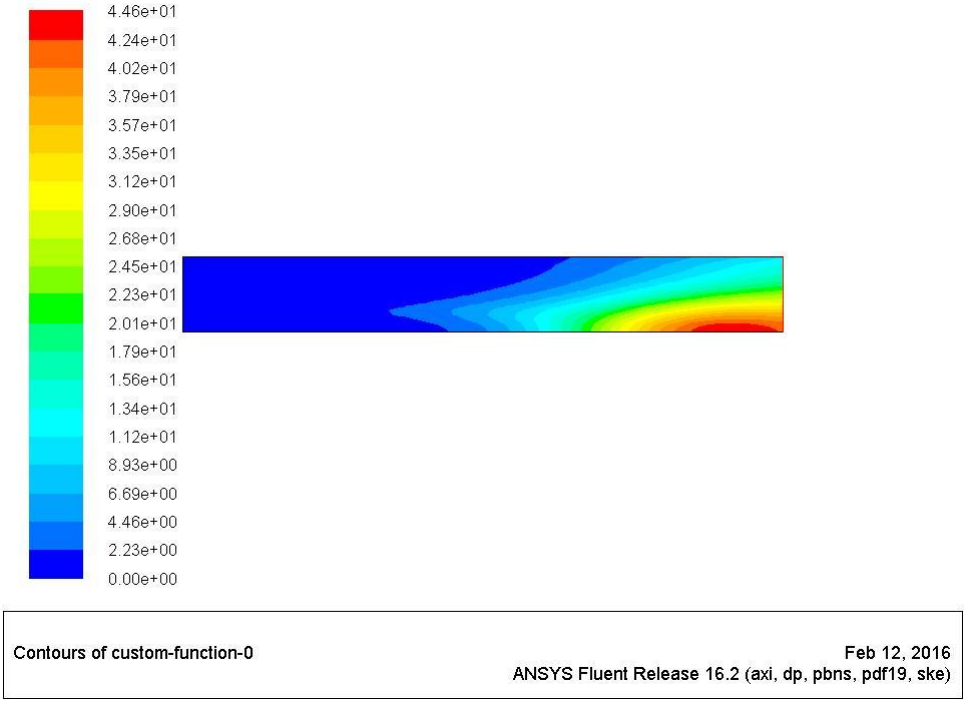

Figure 26: 20% WF ppmNOx

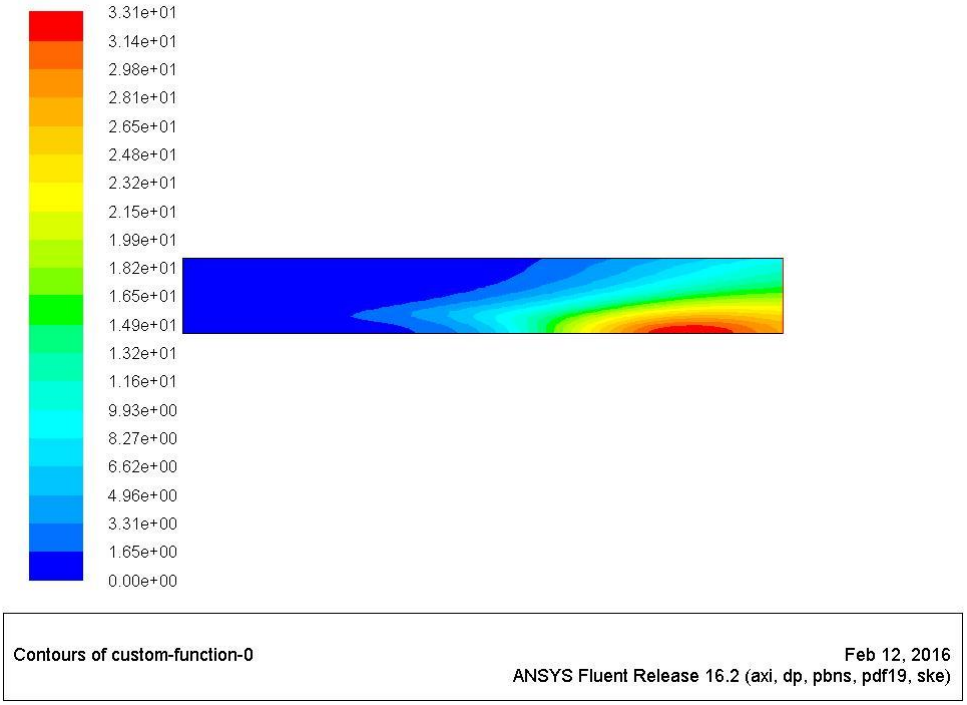

Figure 27: 25% WF ppmNOx

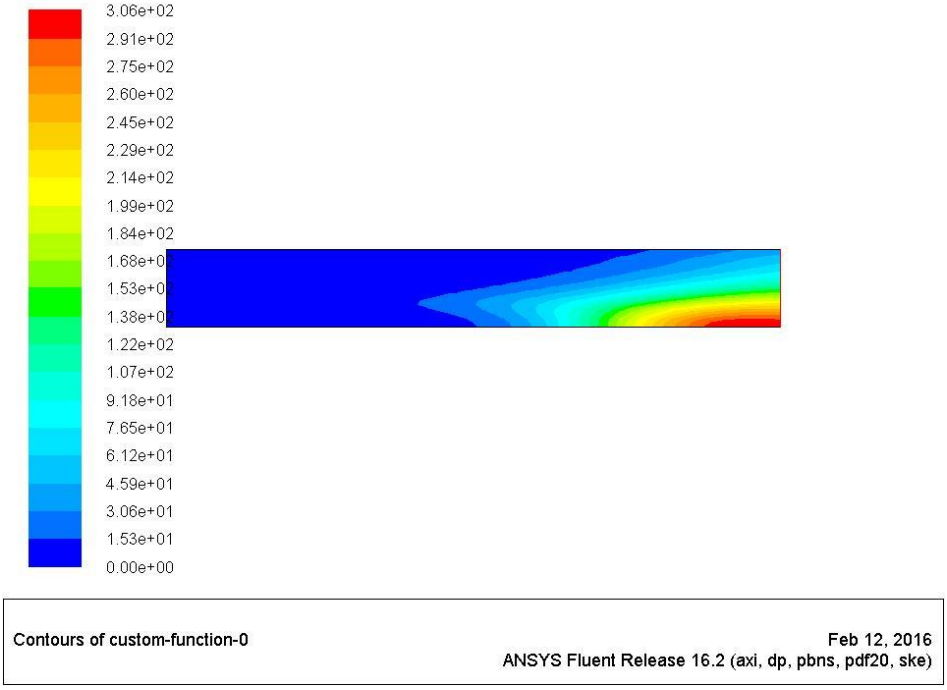

Figure 28: 5% WA ppmNOx

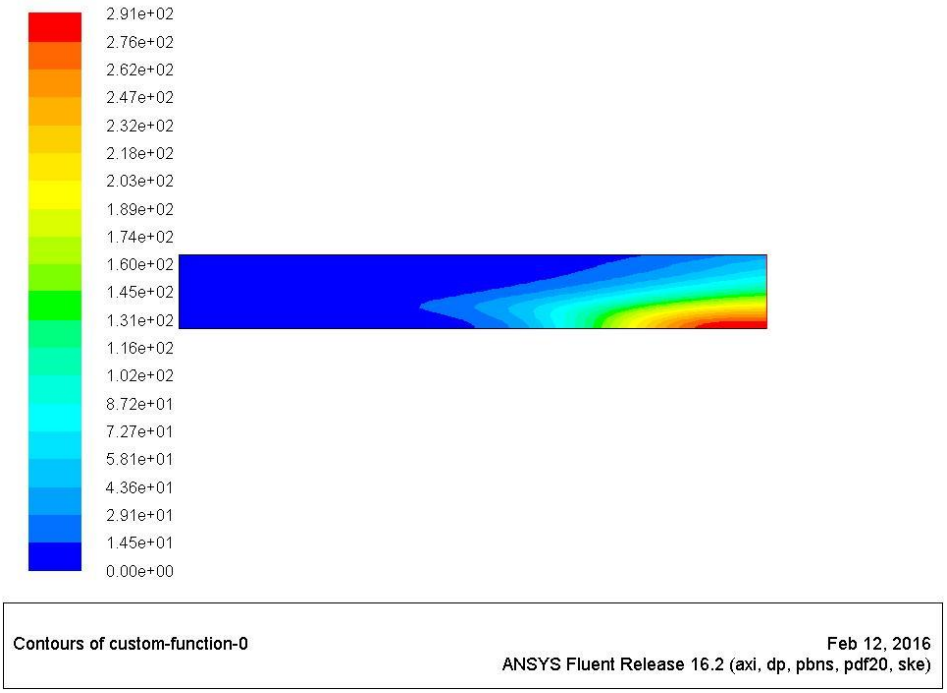

Figure 29: 10% WA ppmNOx

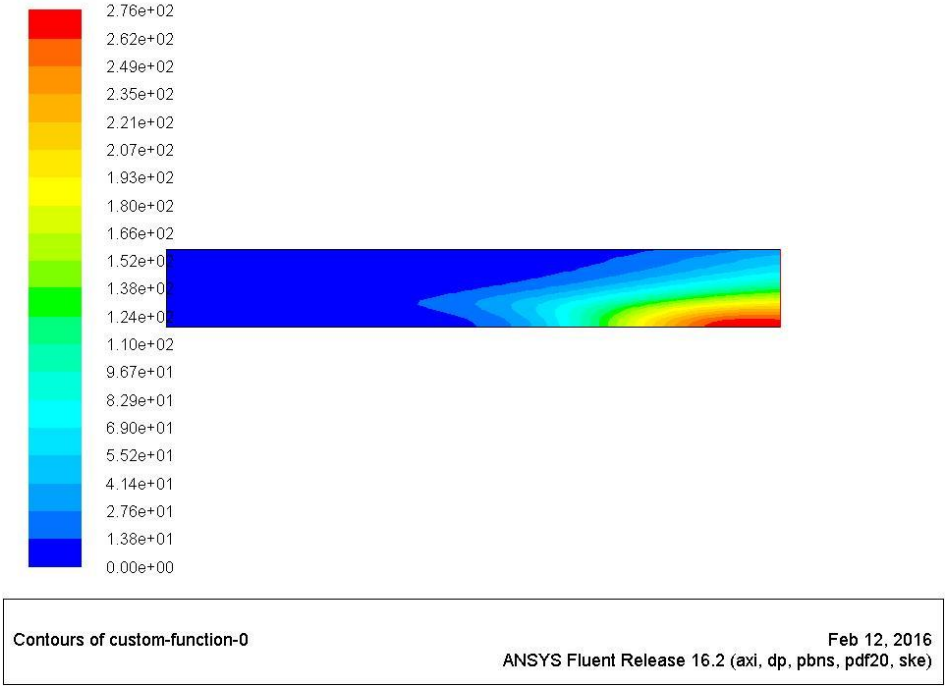

Figure 30: 15% WA ppmNOx

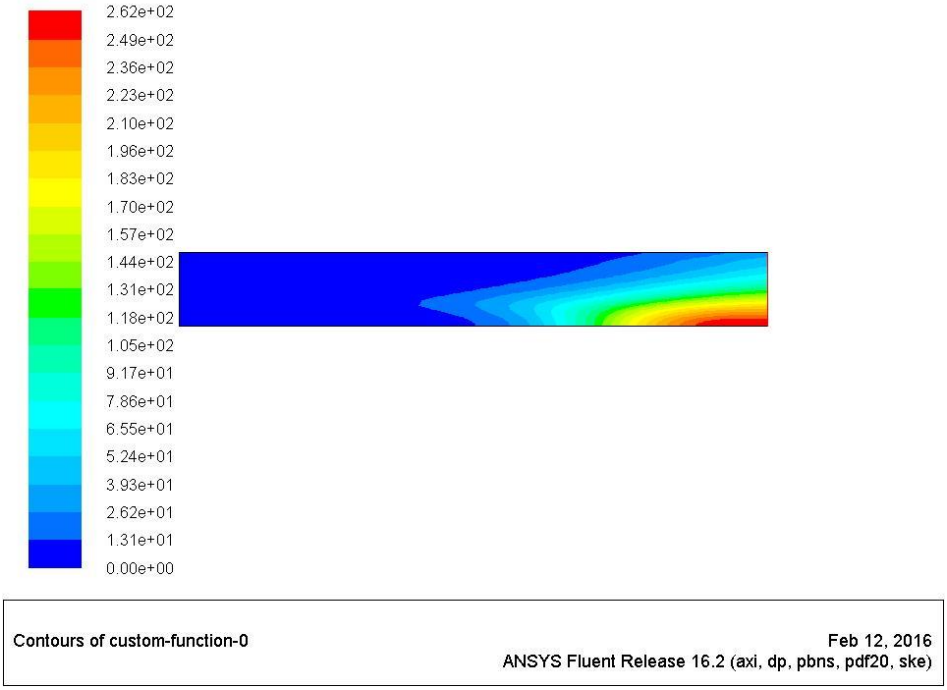

Figure 31: 20% WA ppmNOx

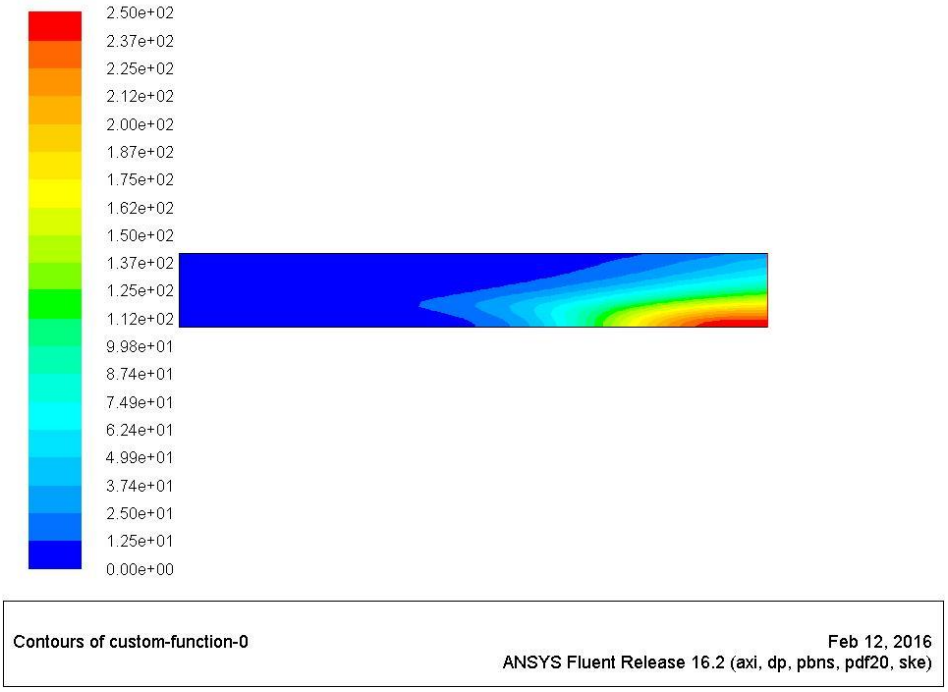

Figure 32: 25% WA ppmNOx

7.3. THERMAL NOX RATE PROFILES

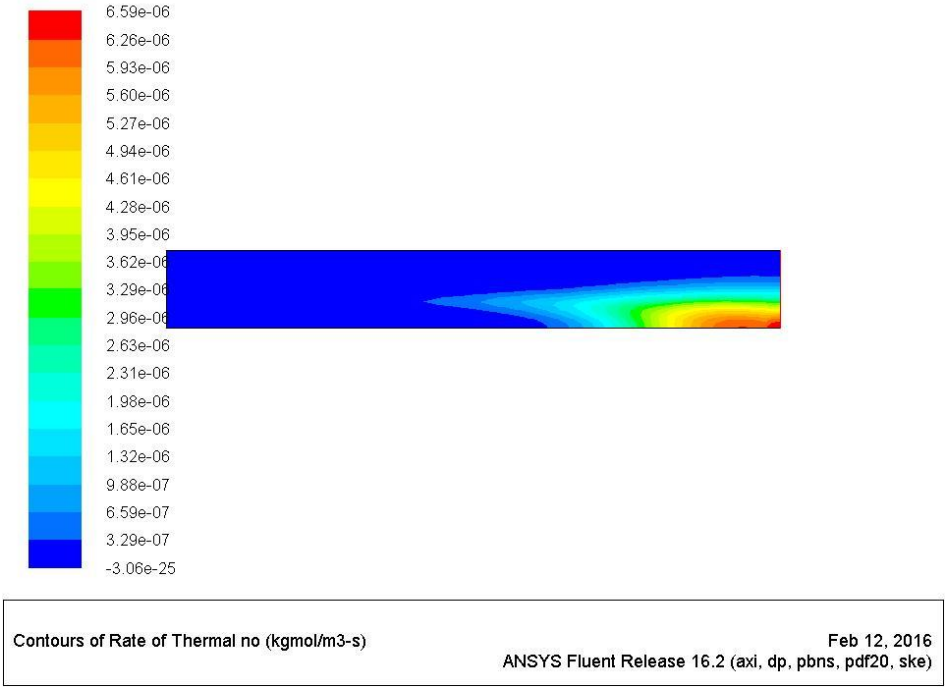

Figure 33: 0% water thermal NOx

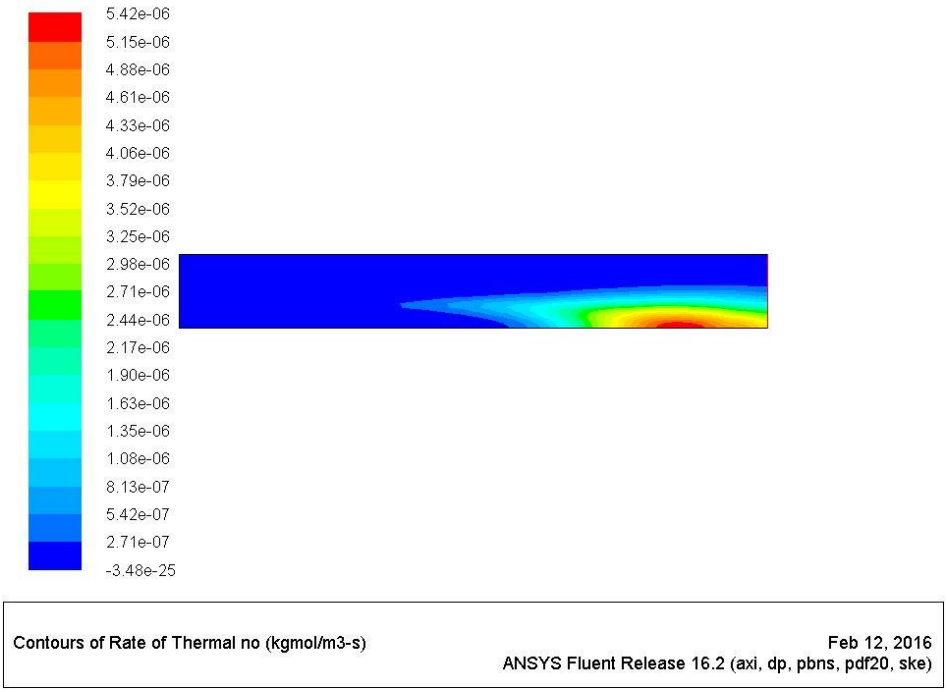

Figure 34: 5% WF thermal NOx

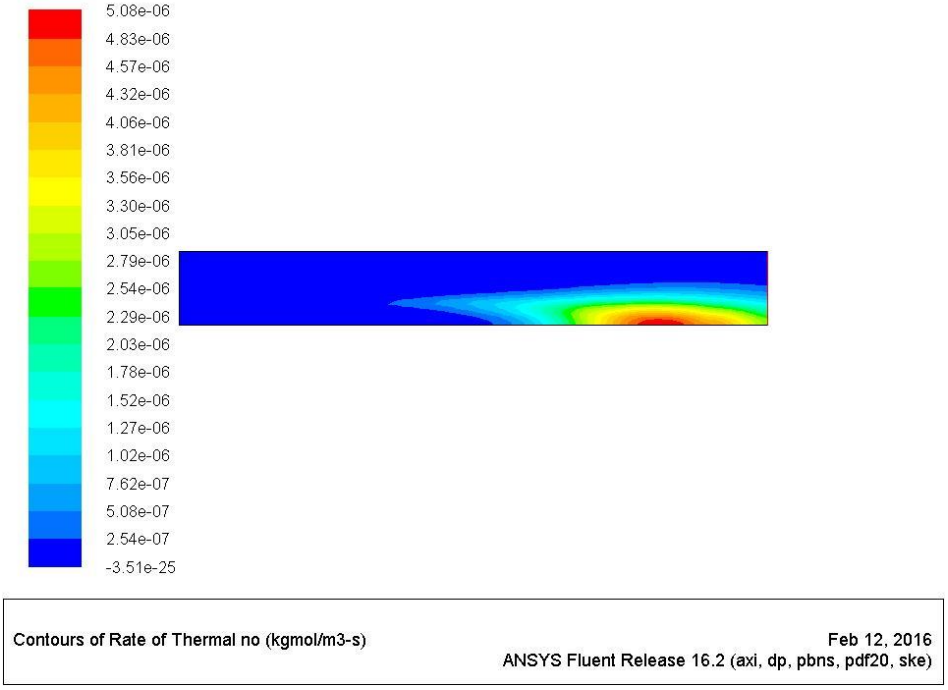

Figure 35: 10% WF thermal NOx

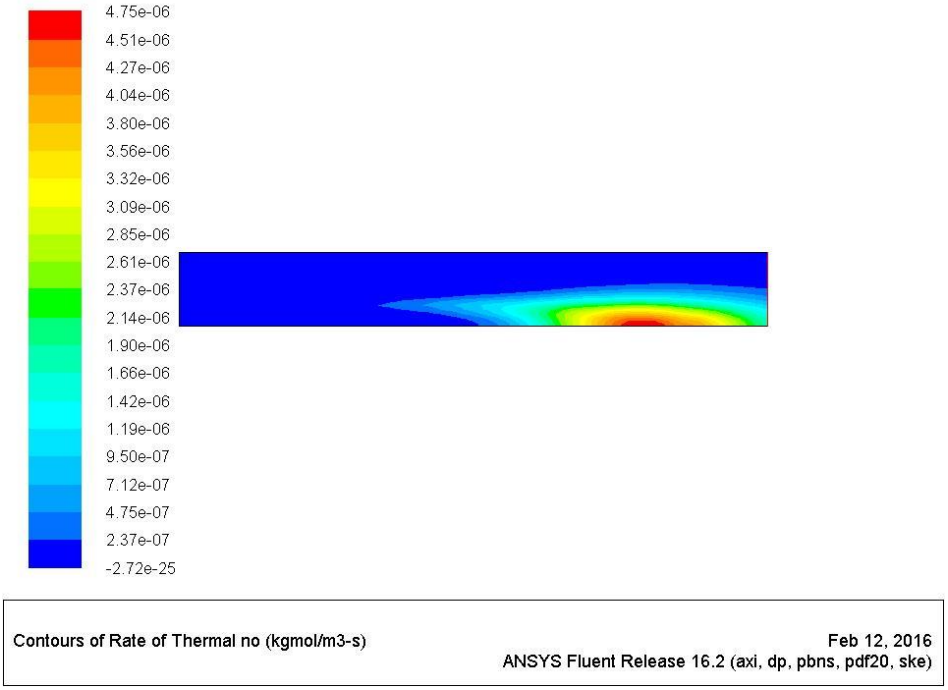

Figure 36: 15% WF thermal NOx

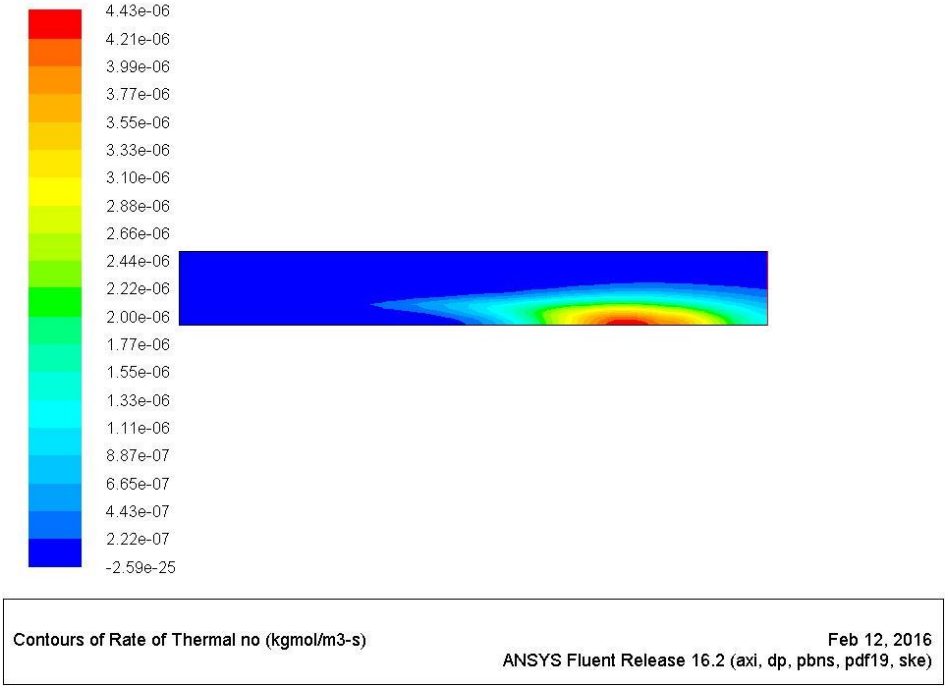

Figure 37: 20% WF thermal NOx

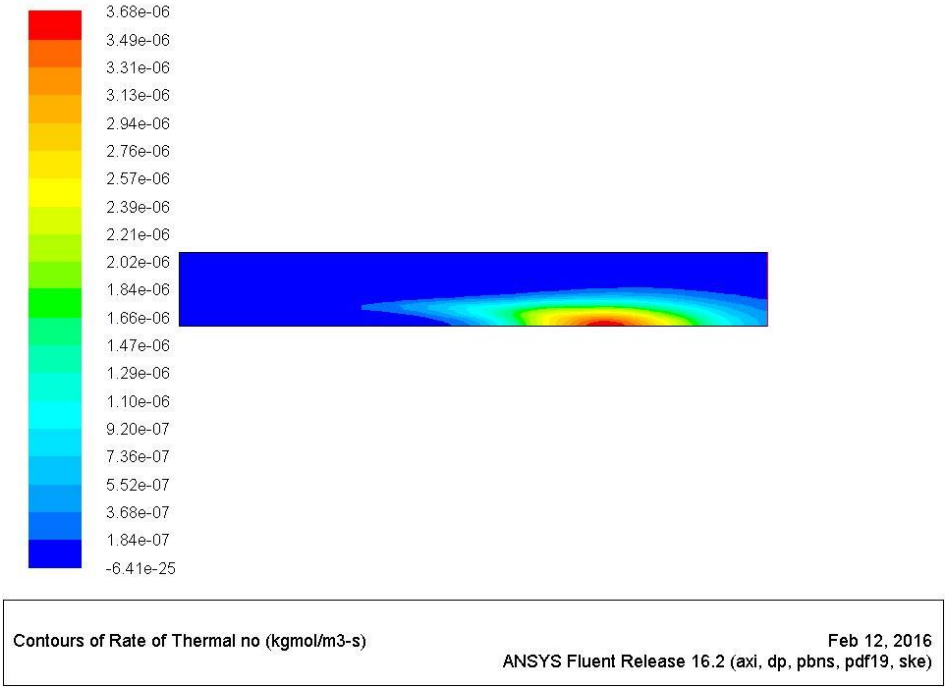

Figure 38: 25% WF thermal NOx

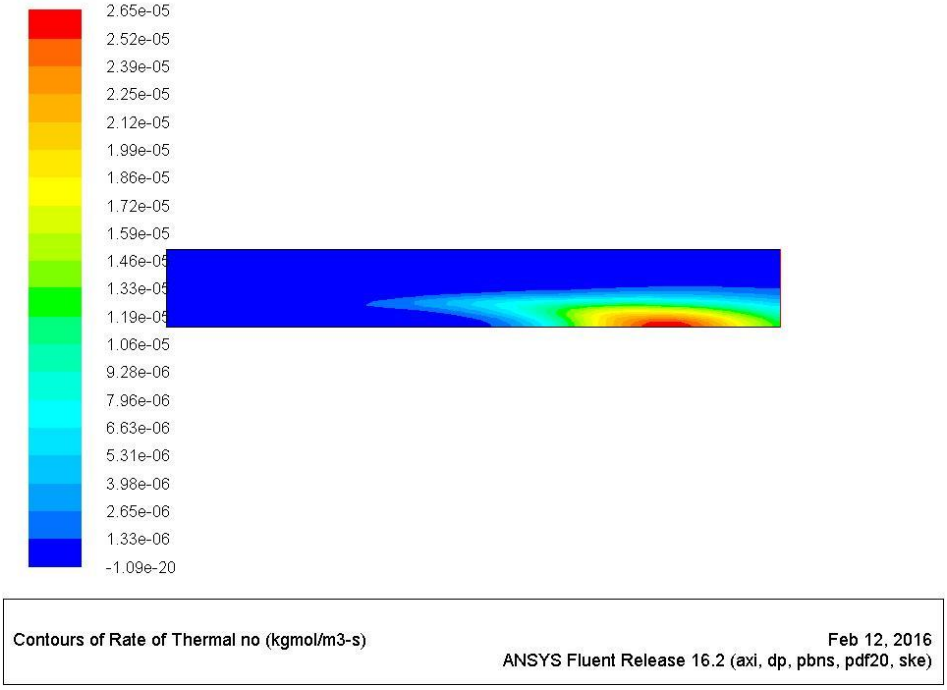

Figure 39: 5% WA thermal NOx

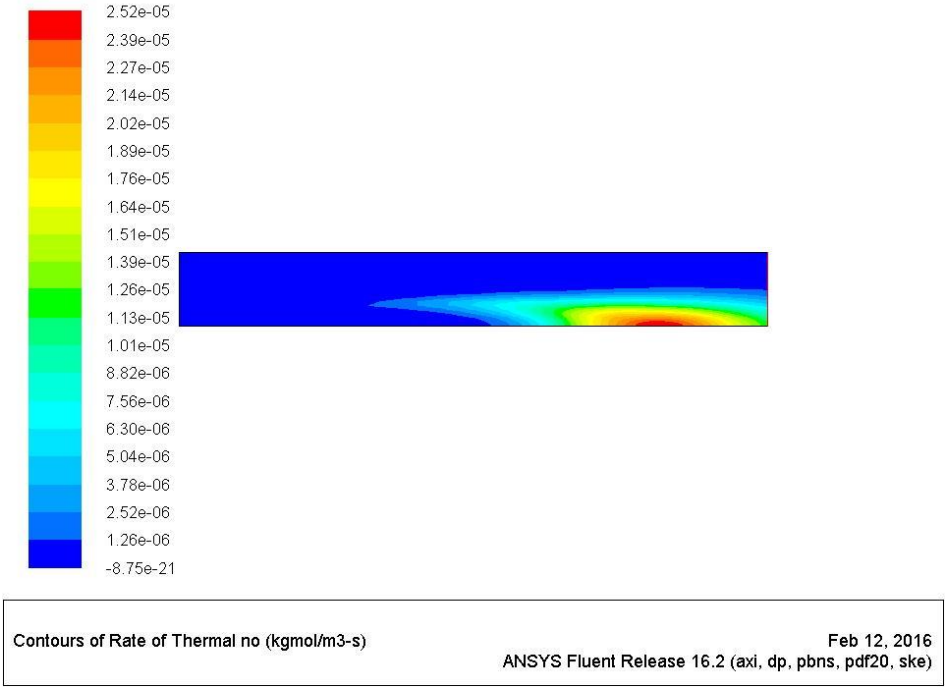

Figure 40: 10% WA thermal NOx

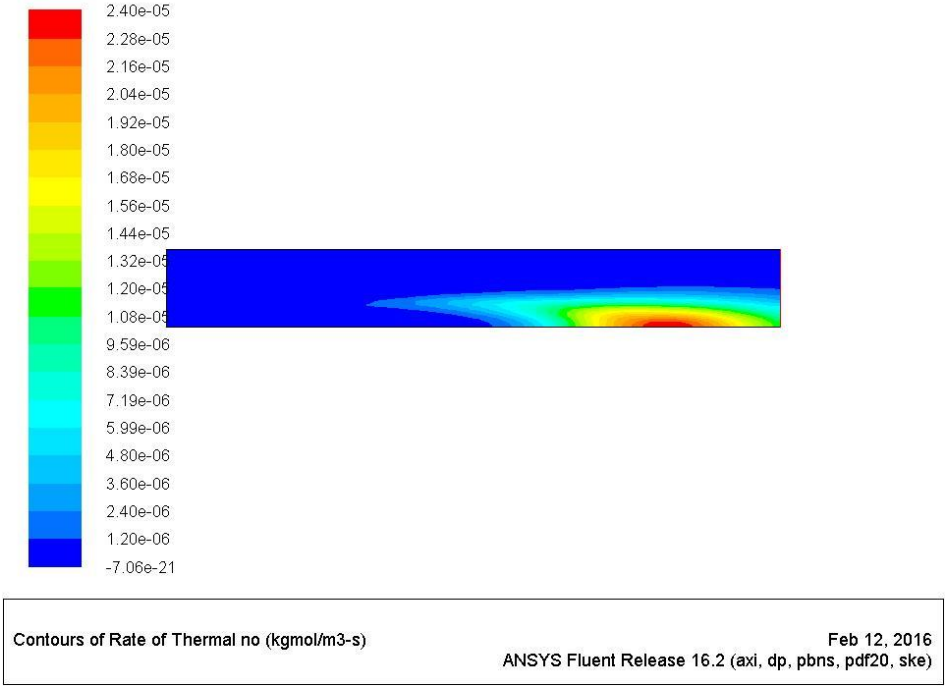

Figure 41: 15% WA thermal NOx

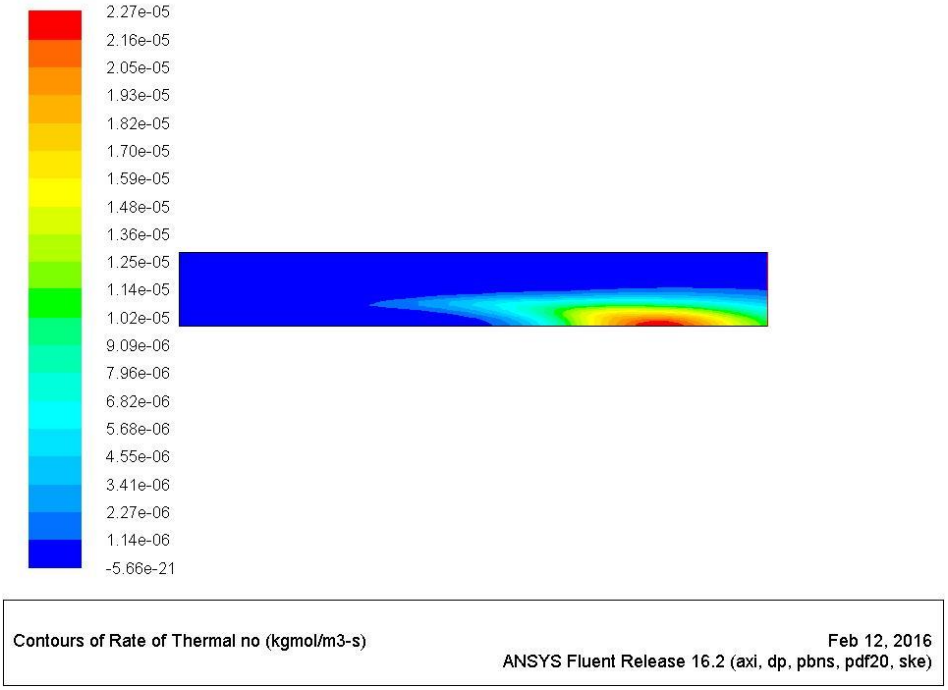

Figure 42: 20% WA thermal NOx

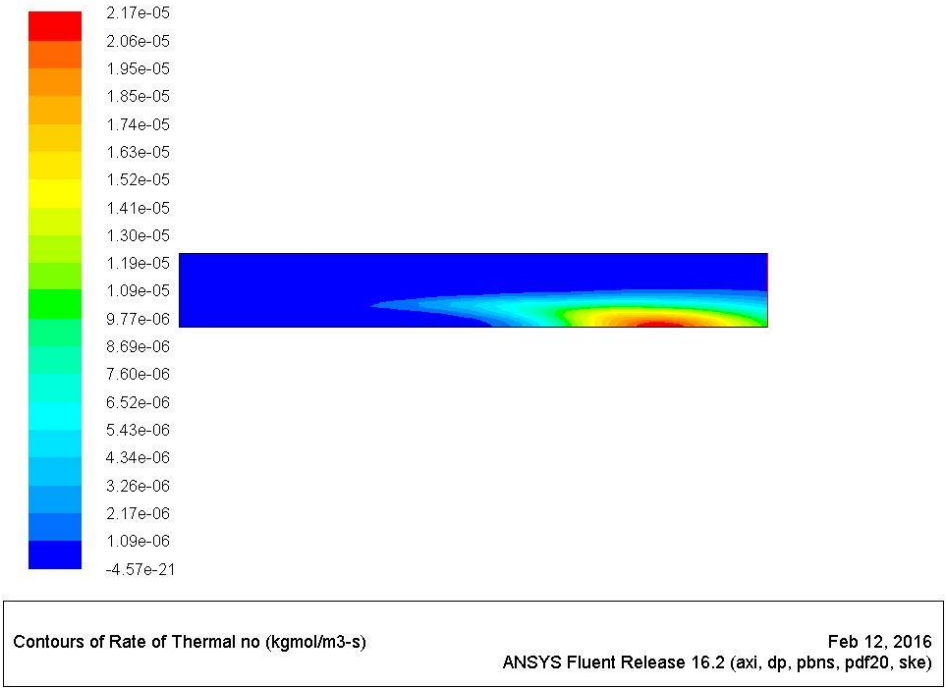

Figure 43: 25% WA thermal NOx

7.4. PROMP NOX RATE PROFILES

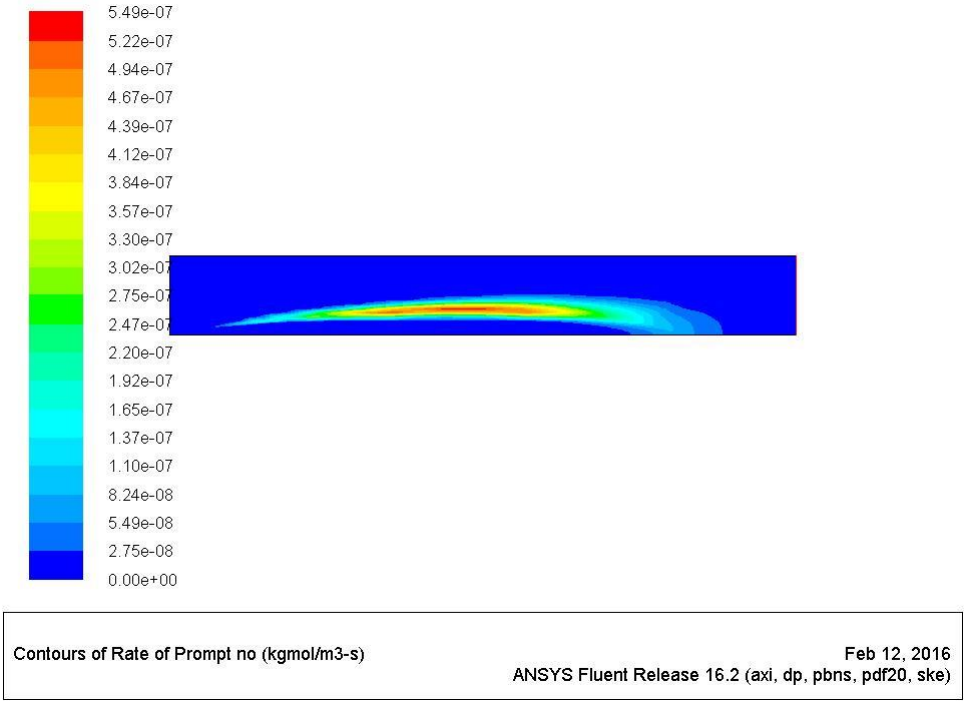

Figure 44: 0% water prompt NOx

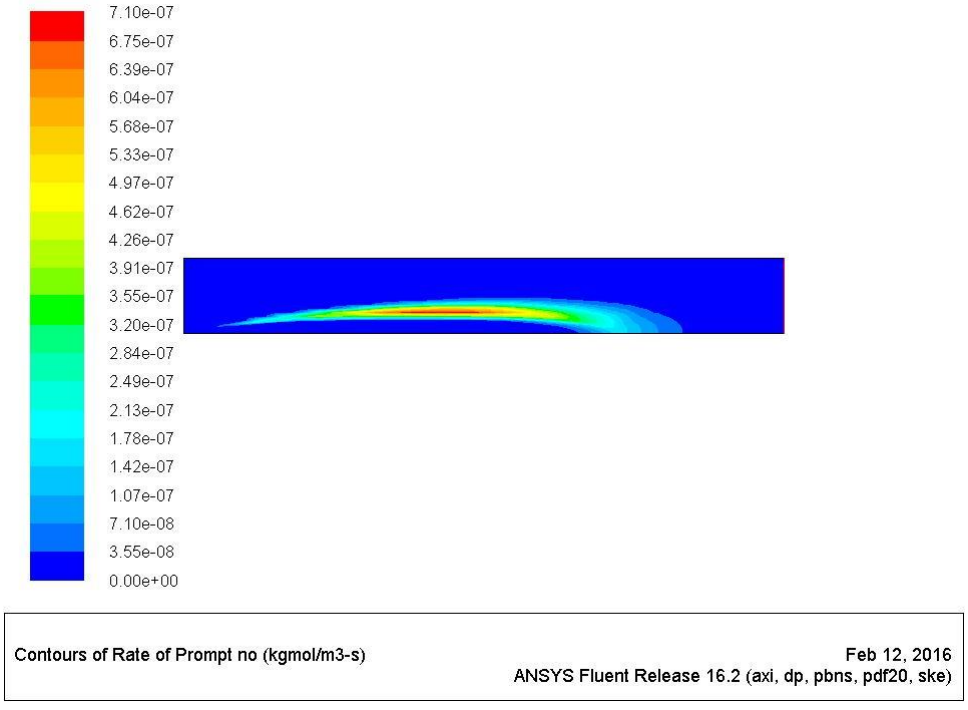

Figure 45: 5% WF prompt NOx

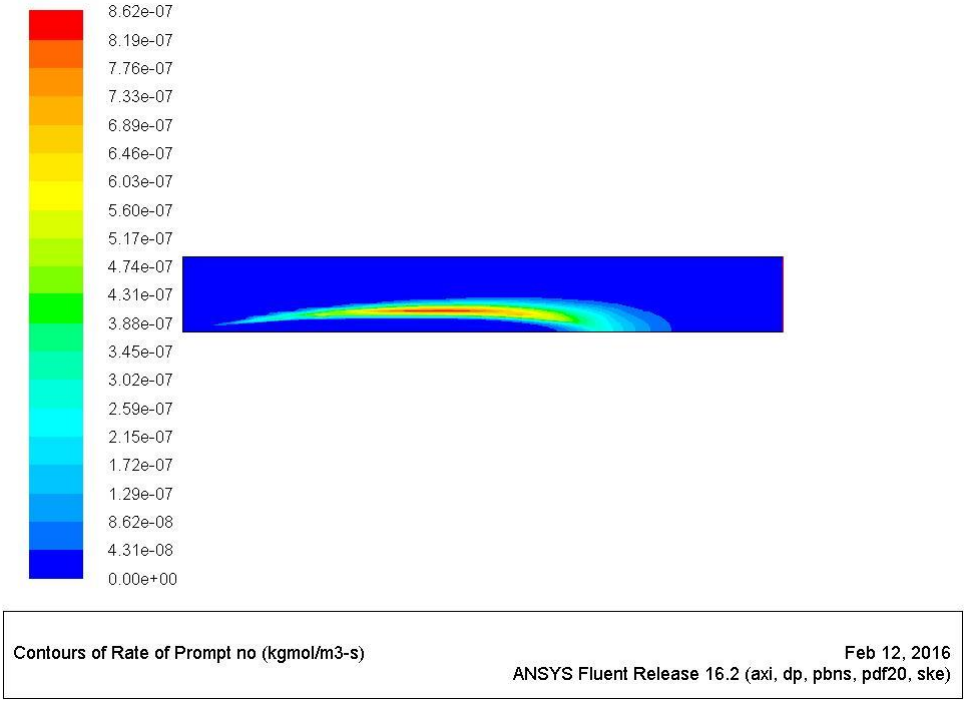

Figure 46: 10% WF prompt NOx

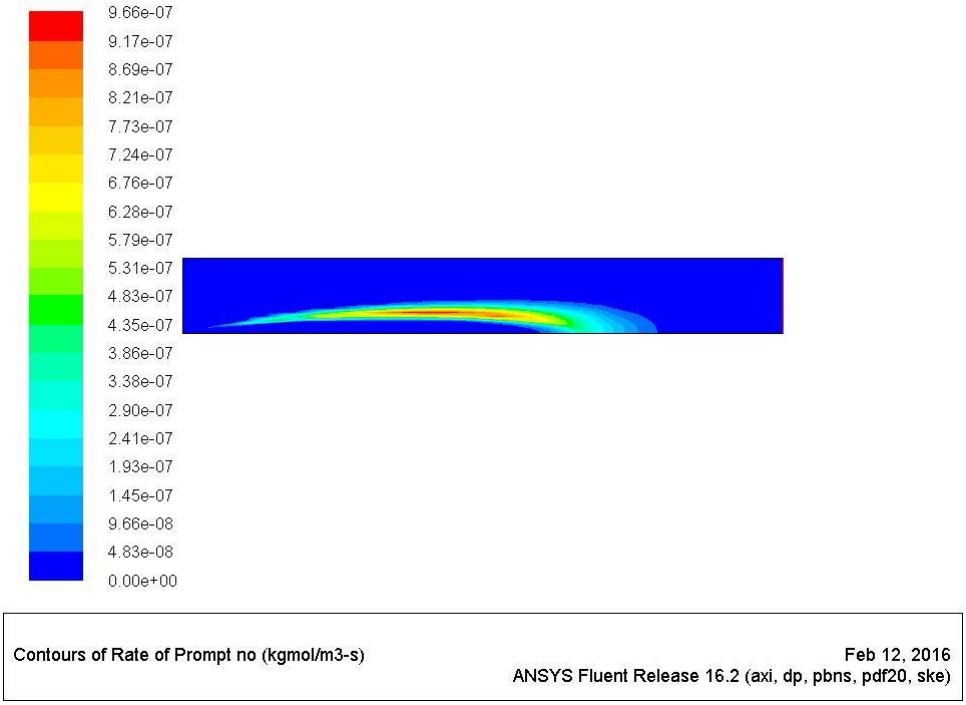

Figure 47: 15% WF prompt NOx

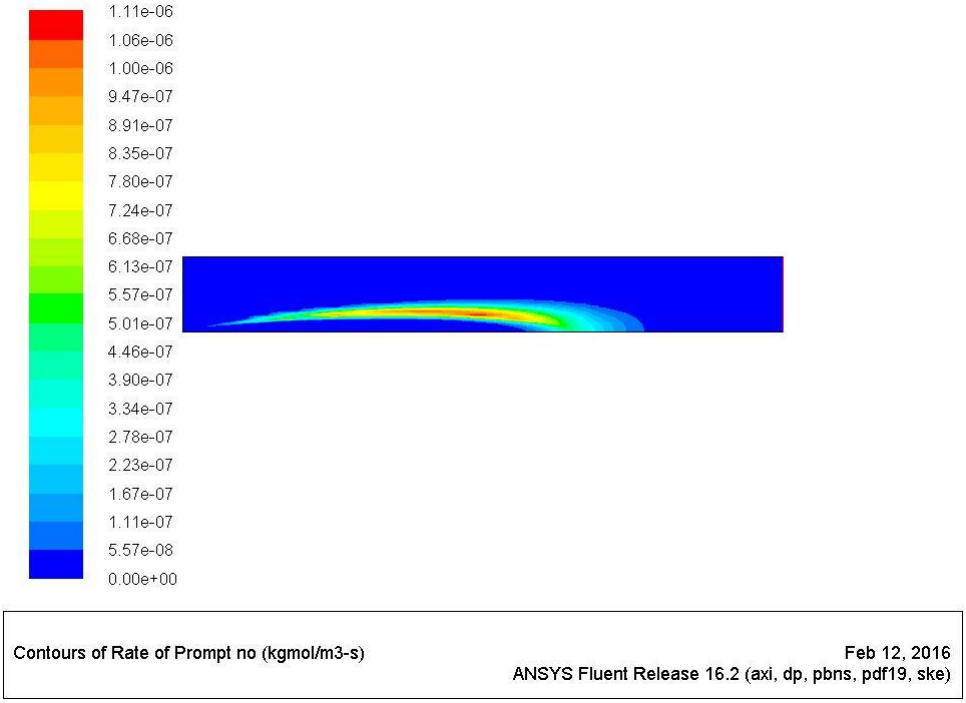

Figure 48: 20% WF prompt NOx

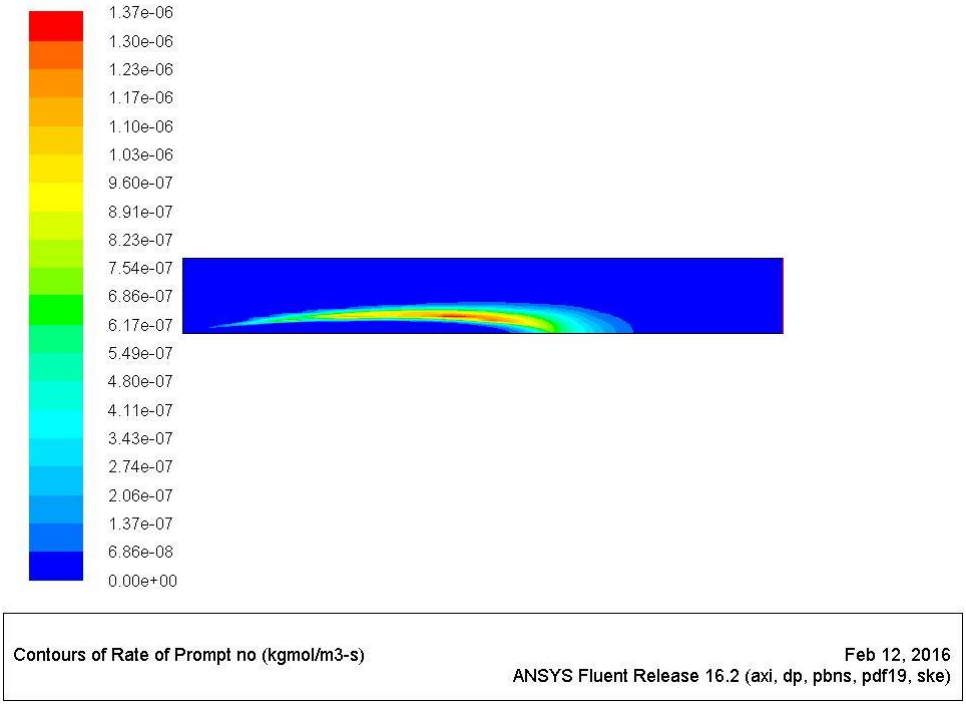

Figure 49: 25% WF prompt NOx

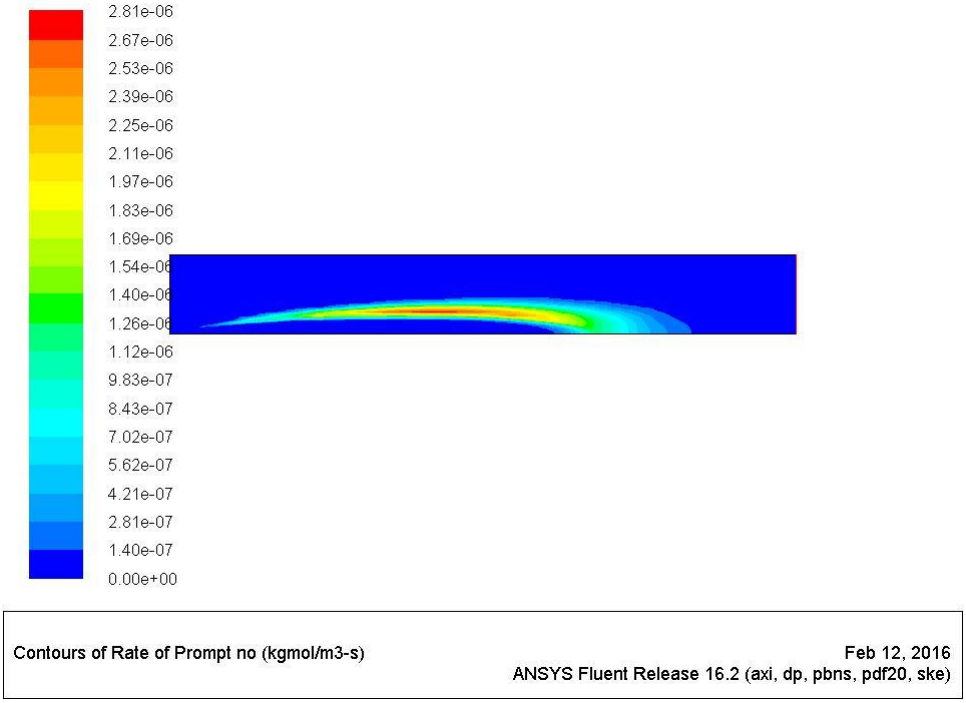

Figure 50: 5% WA prompt NOx

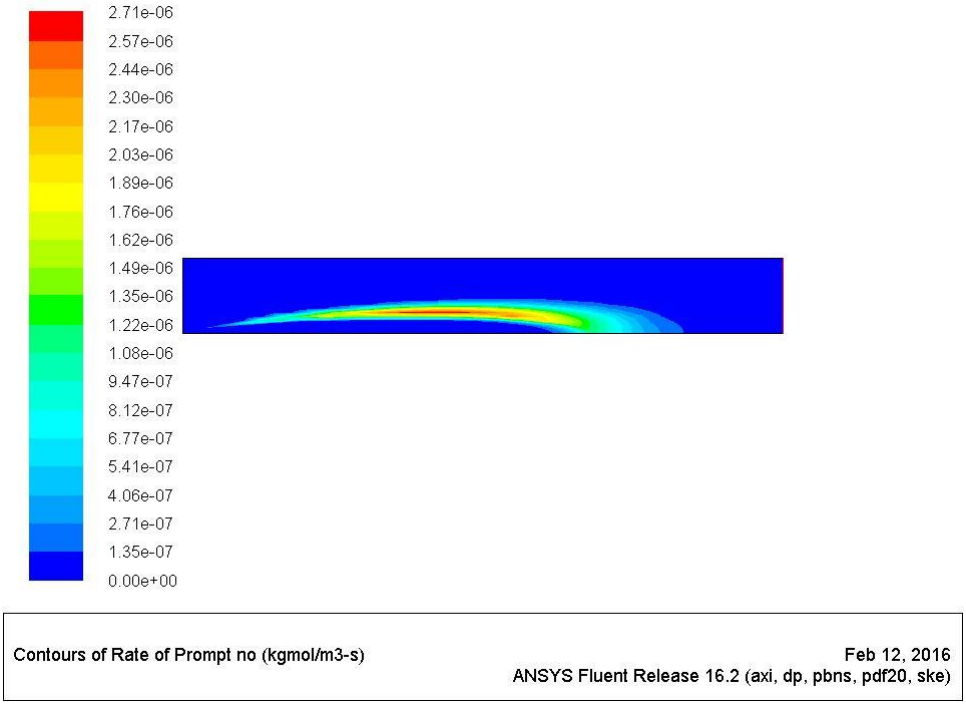

Figure 51: 10% WA prompt NOx

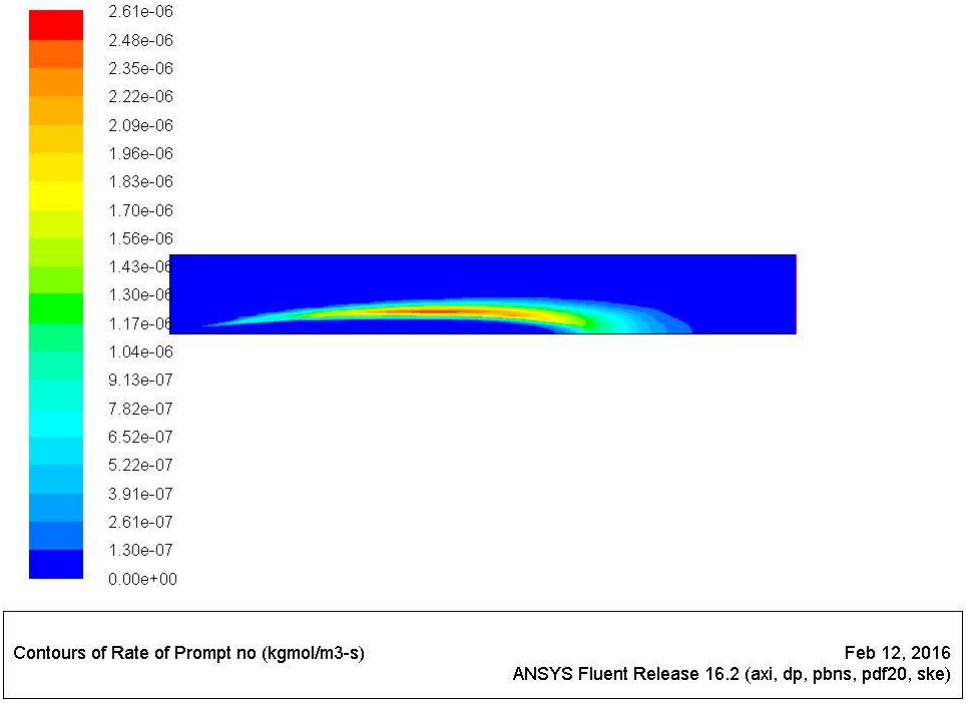

Figure 52: 15% WA prompt NOx

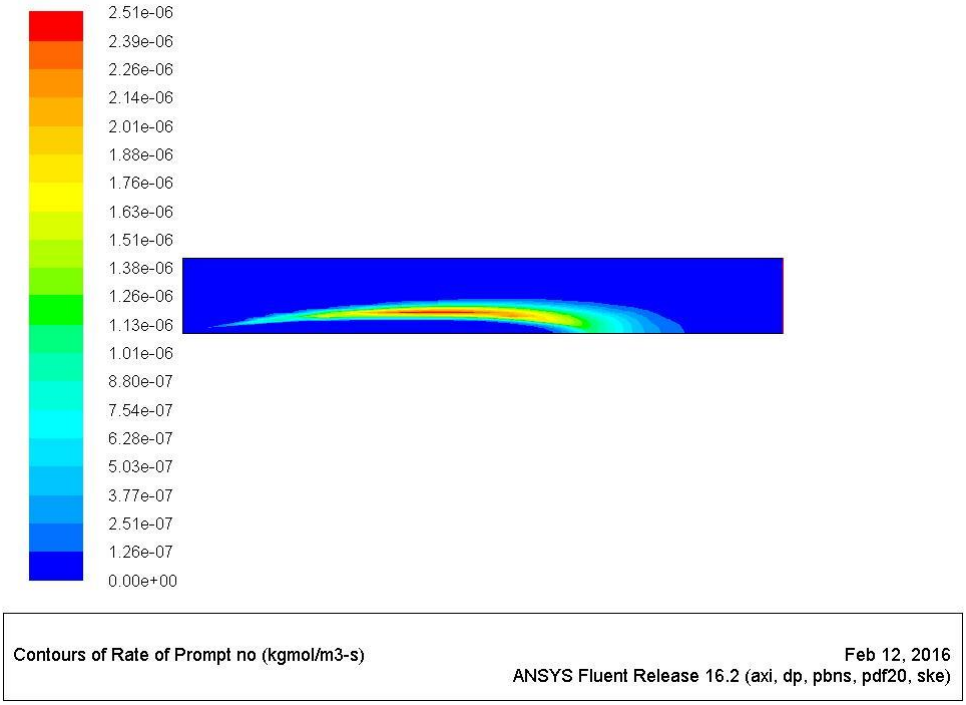

Figure 53: 20% WA prompt NOx

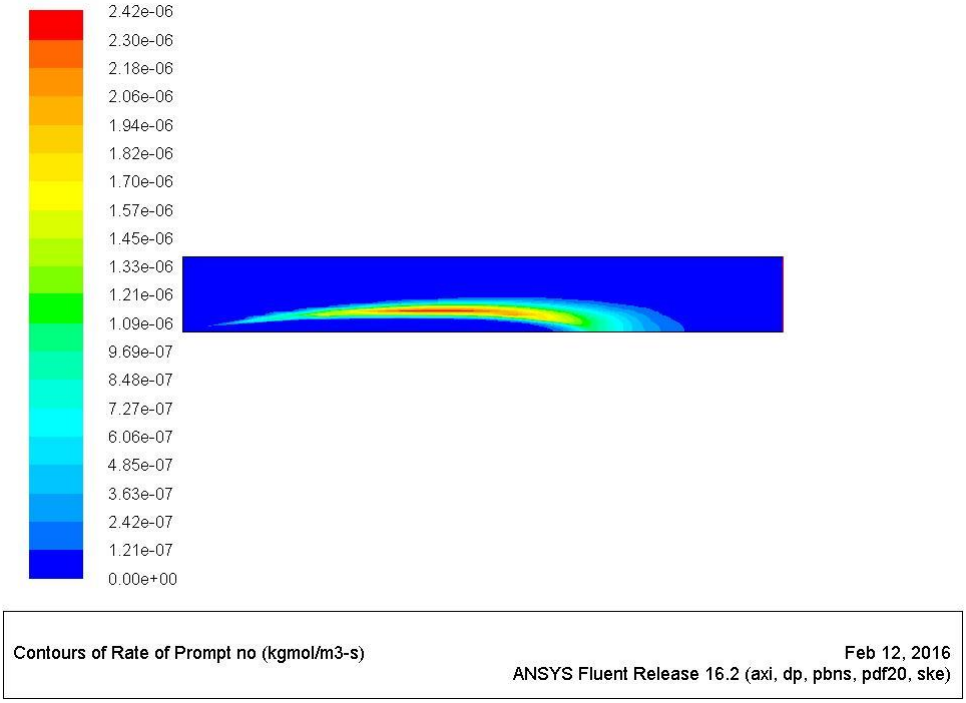

Figure 54: 25% WA prompt NOx

7.5. RADICAL [O] PROFILES

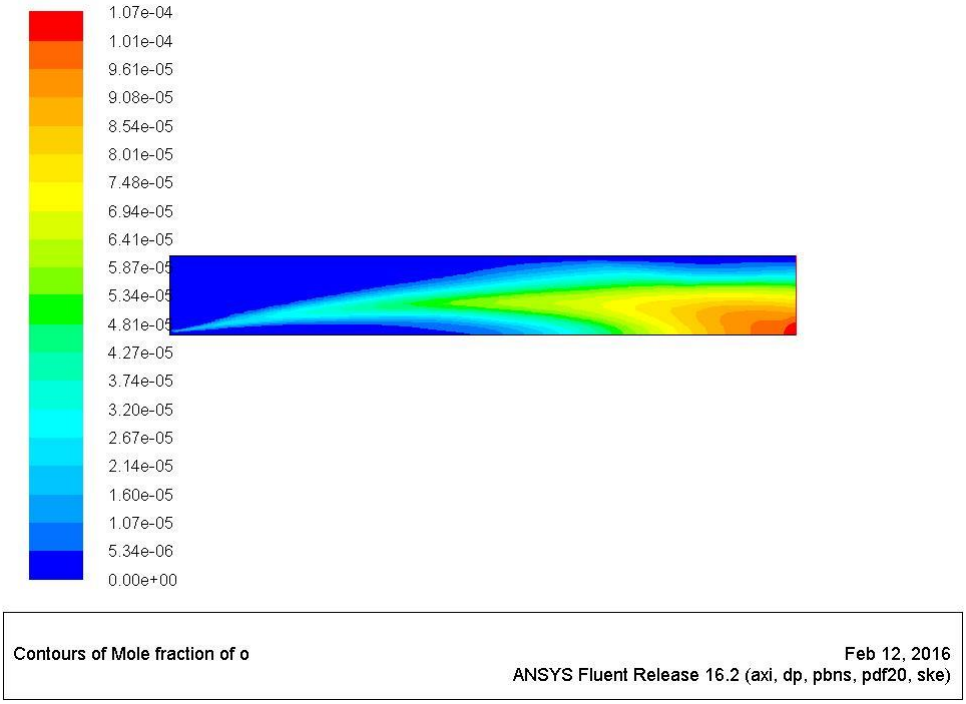

Figure 55: 0% water [O] mole fraction

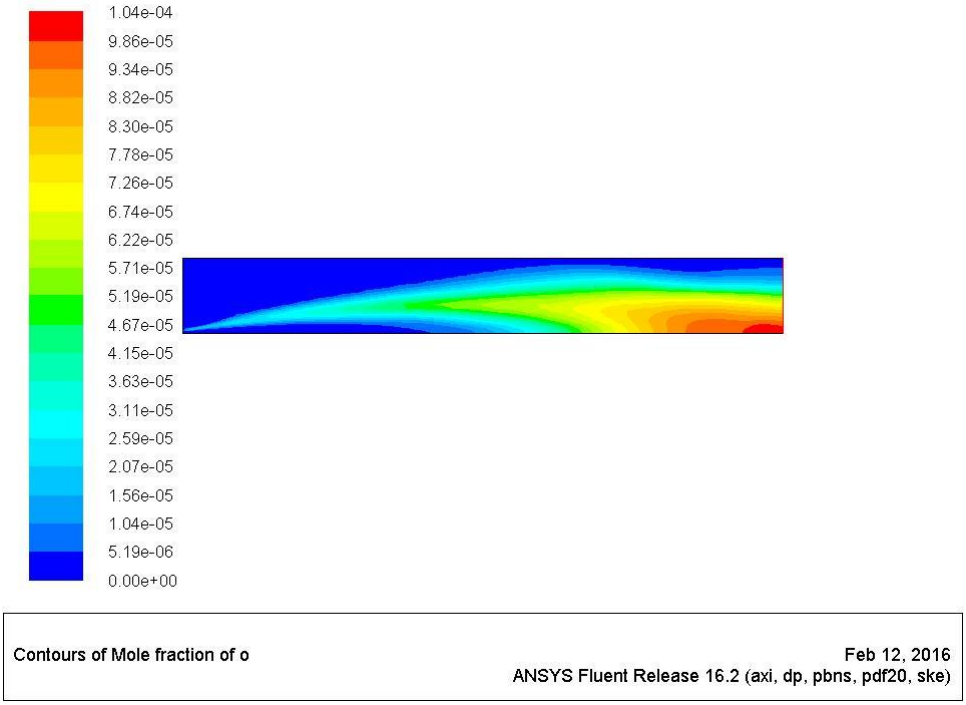

Figure 56: 5% WF [O] mole fraction

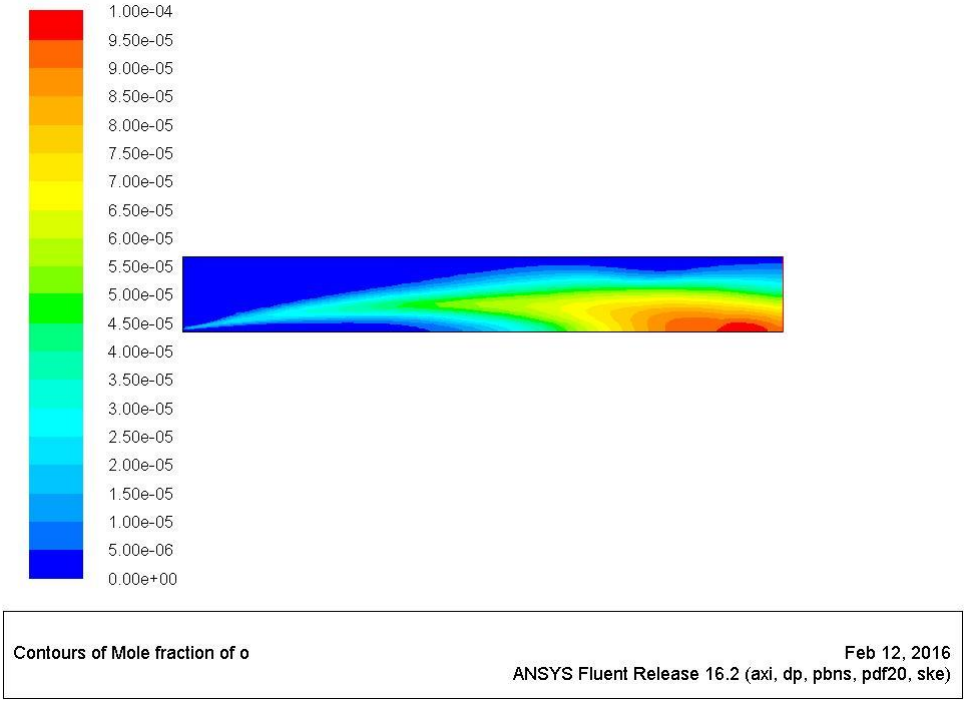

Figure 57: 10% WF [O] mole fraction

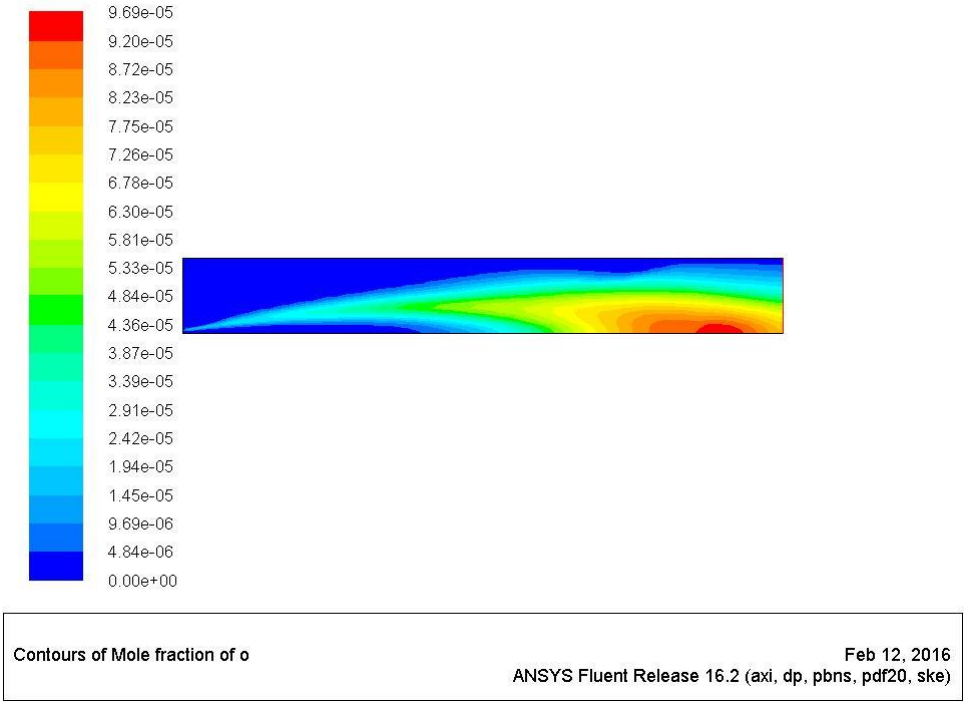

Figure 58: 15% WF [O] mole fraction

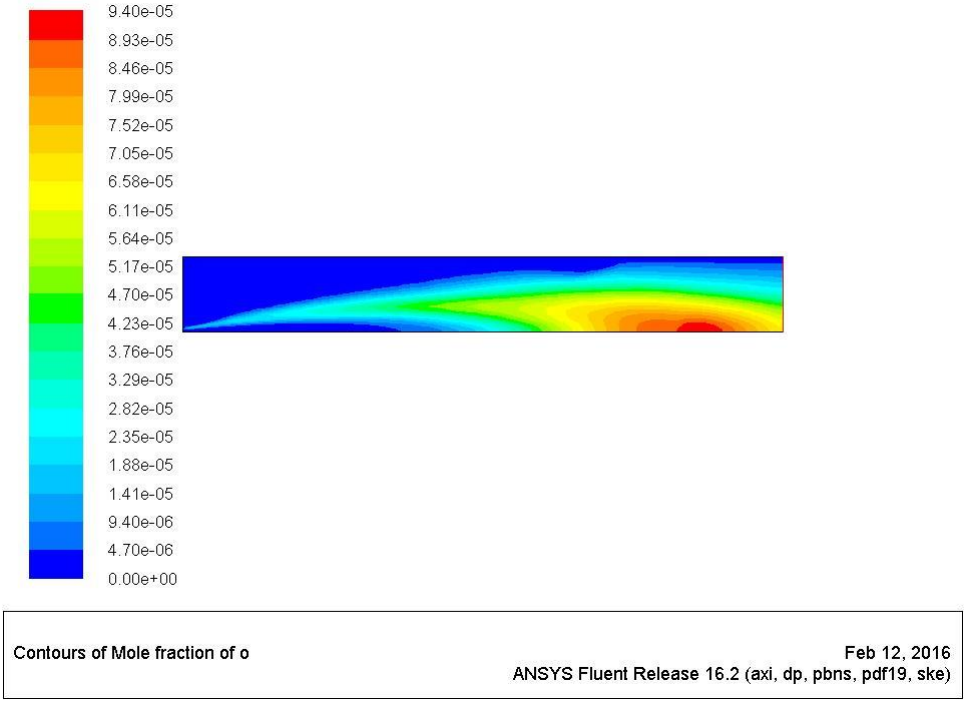

Figure 59: 20% WF [O] mole fraction

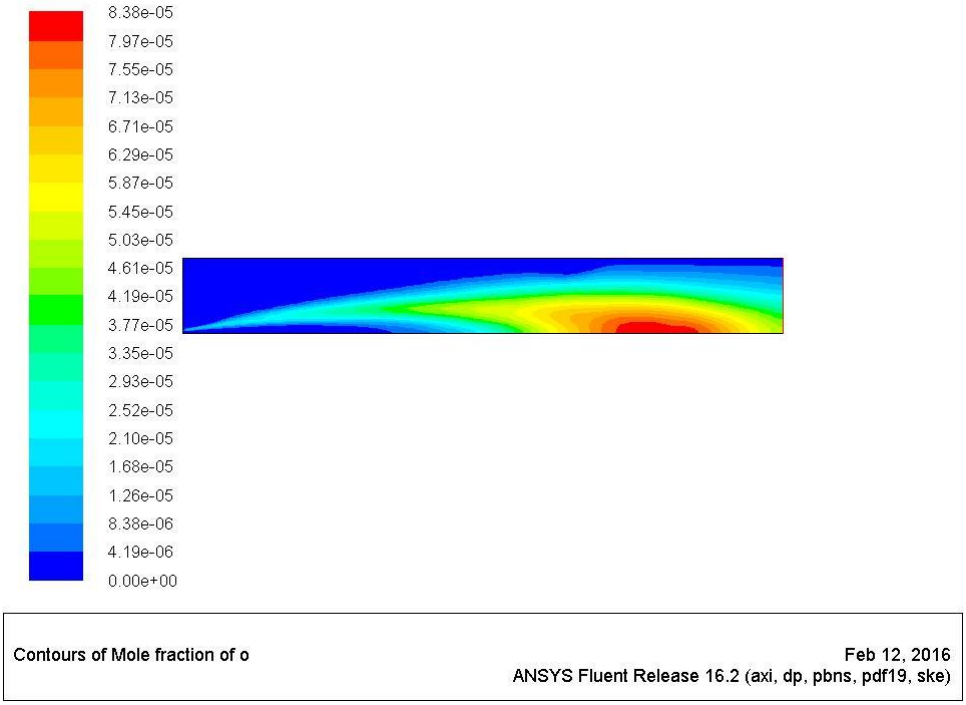

Figure 60: 25% WF [O] mole fraction

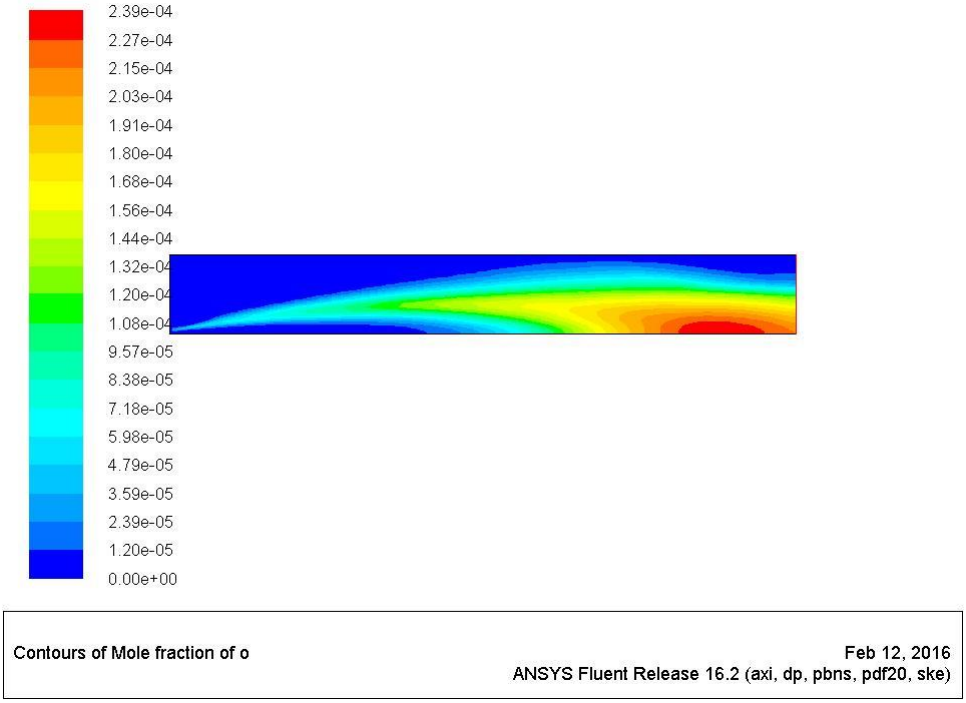

Figure 61: 5% WA [O] mole fraction

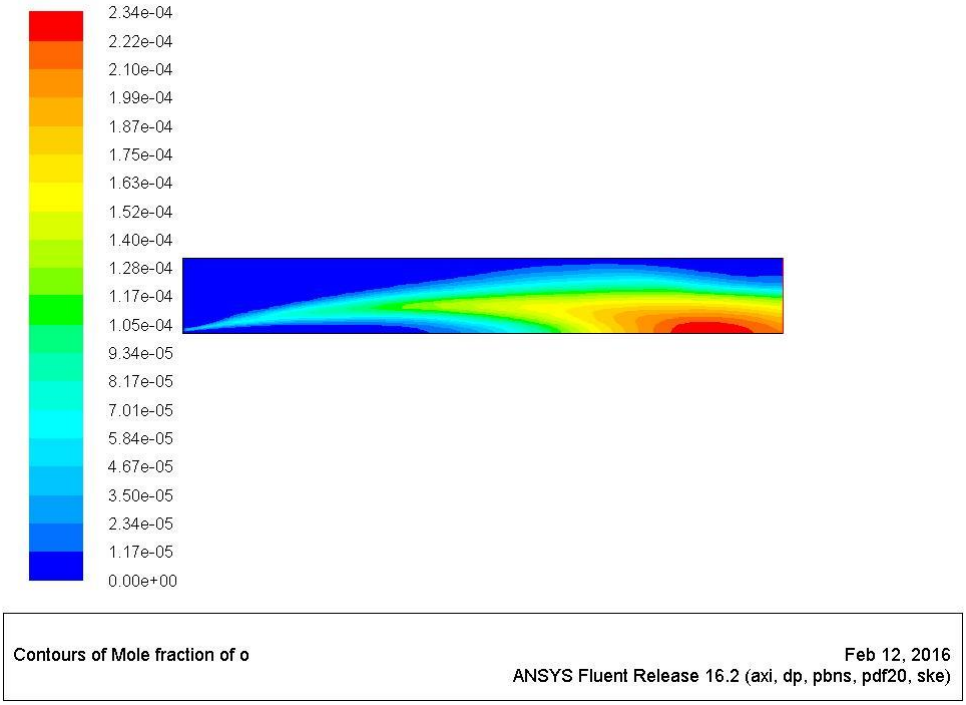

Figure 62: 10% WA [O] mole fraction

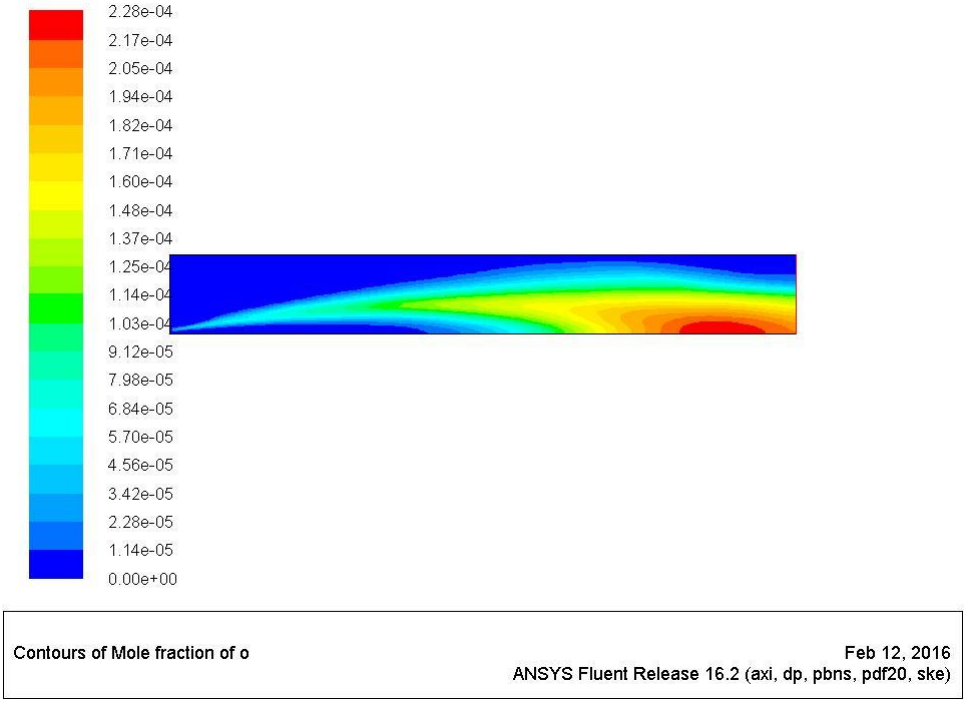

Figure 63: 15% WA [O] mole fraction

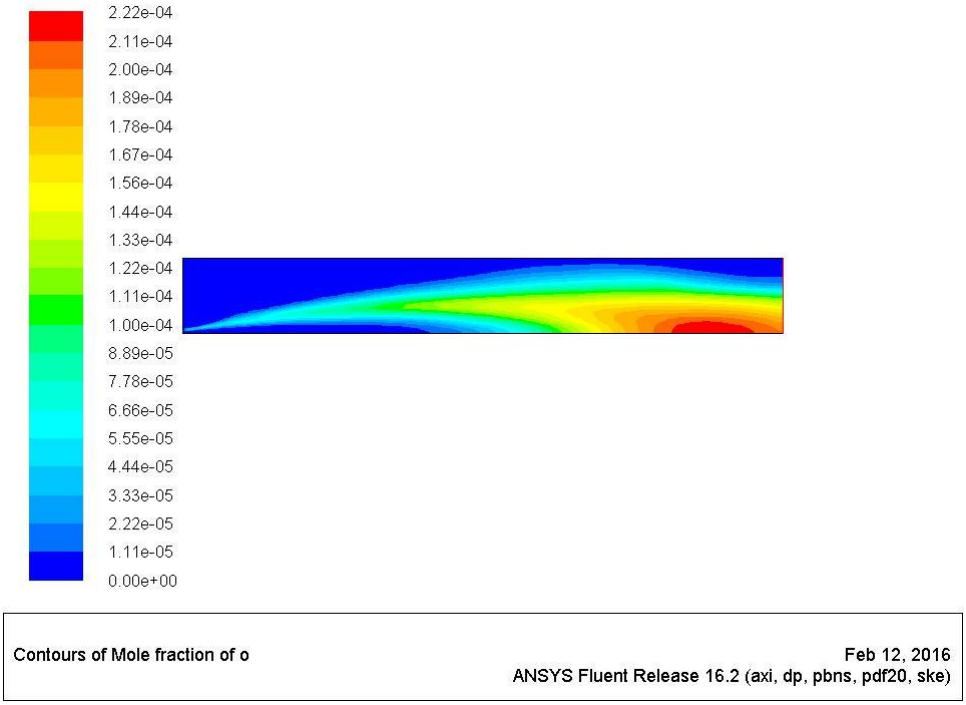

Figure 64: 20% WA [O] mole fraction

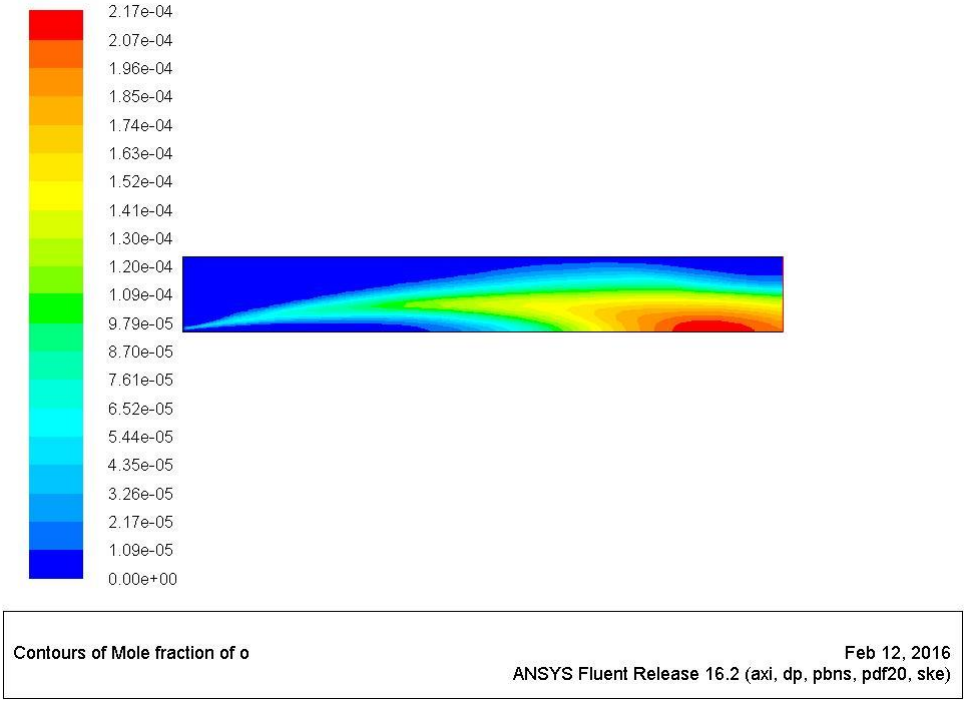

Figure 65: 25% WA [O] mole fraction

7.6. RADICAL [OH] PROFILES

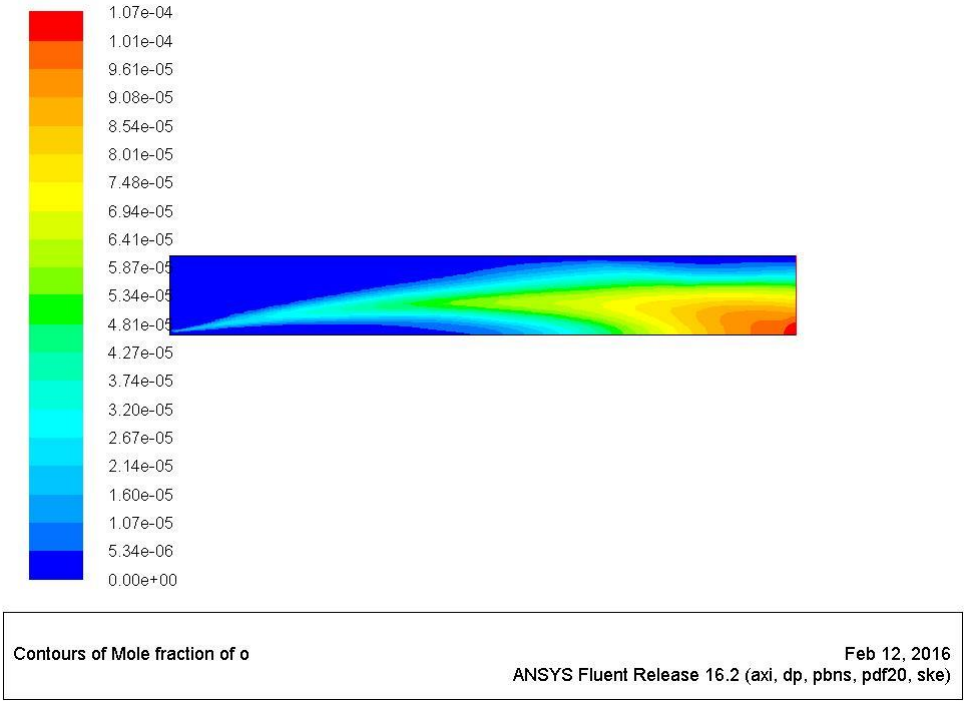

Figure 66: 0% water [OH] mole fraction

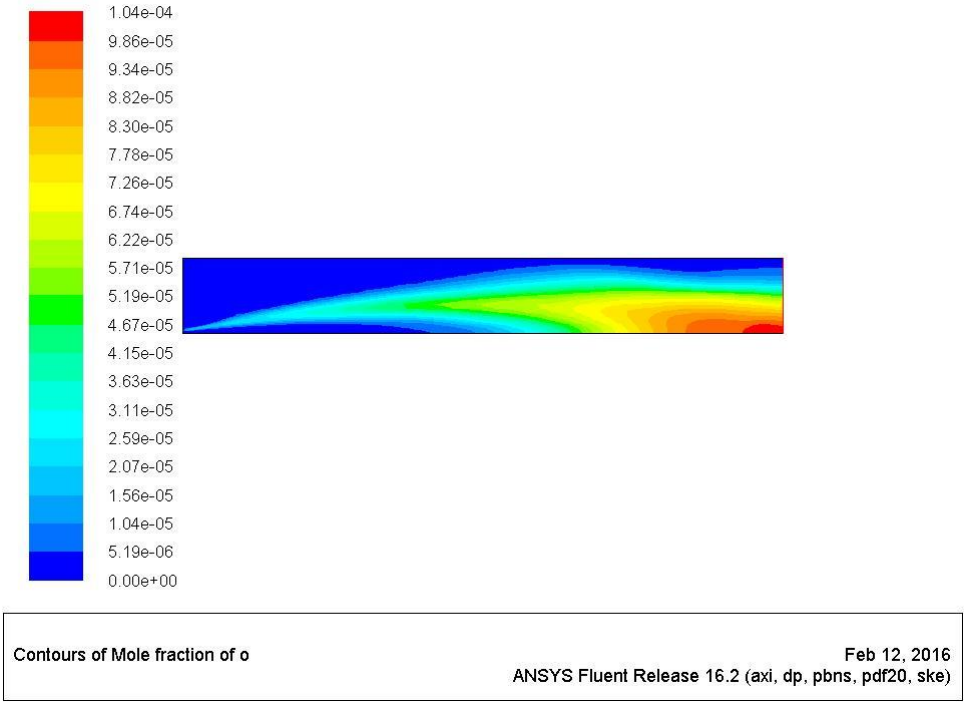

Figure 67: 5% WF [OH] mole fraction

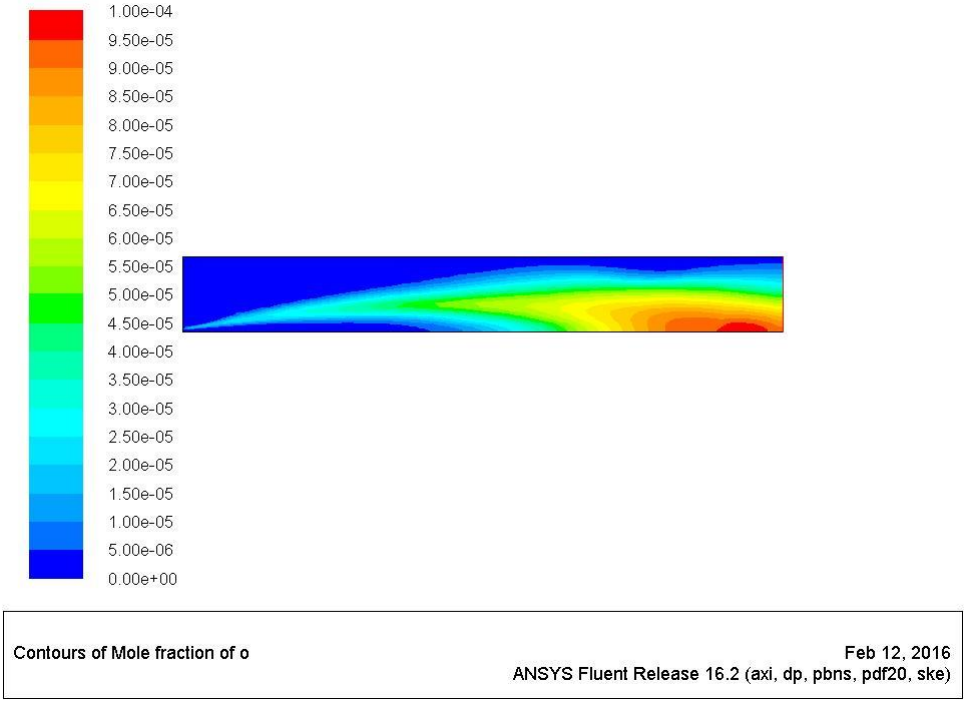

Figure 68: 10% WF [OH] mole fraction

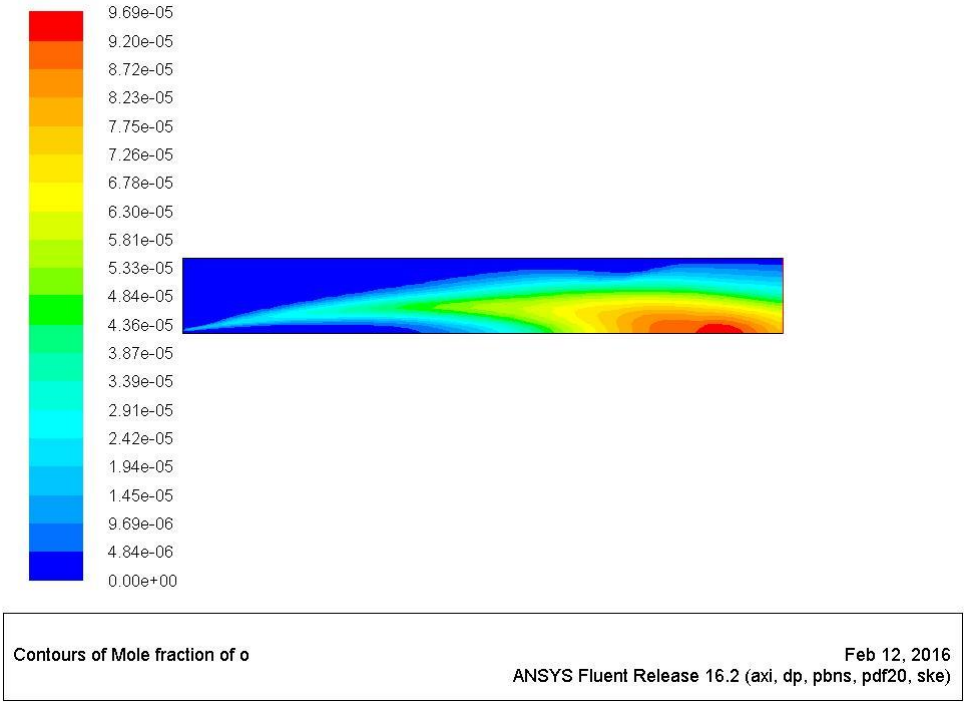

Figure 69: 15% WF [OH] mole fraction

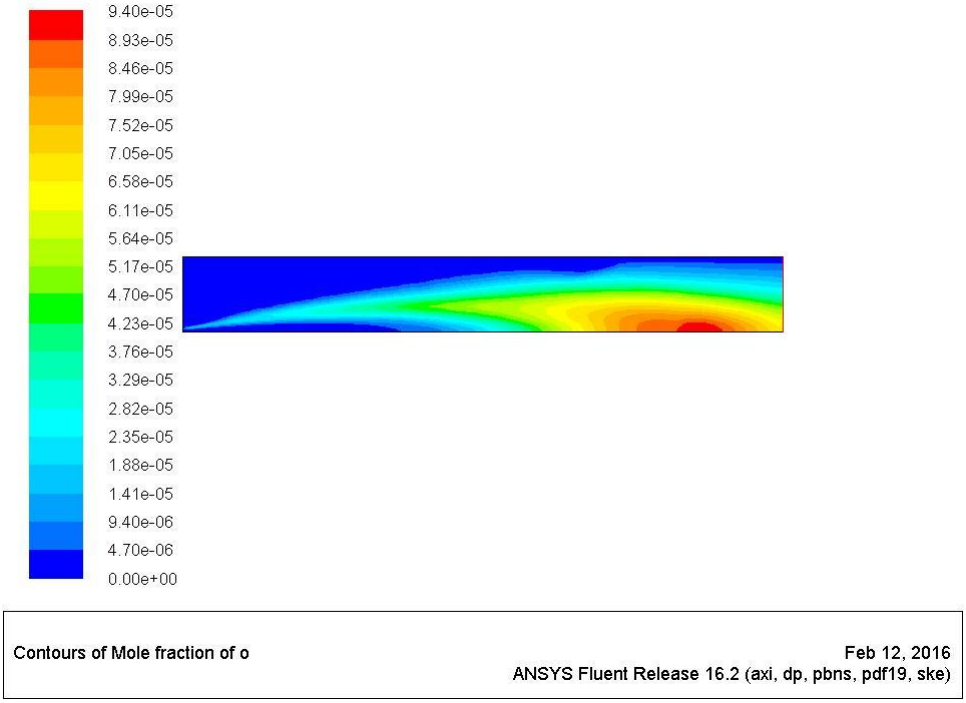

Figure 70: 20% WF [OH] mole fraction

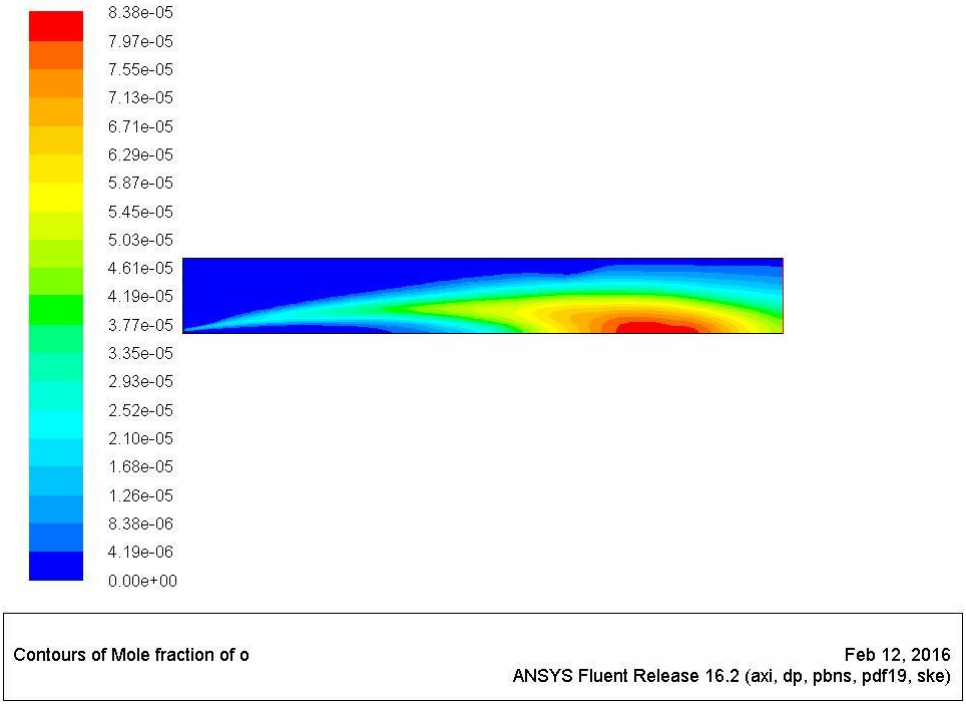

Figure 71: 25% WF [OH] mole fraction

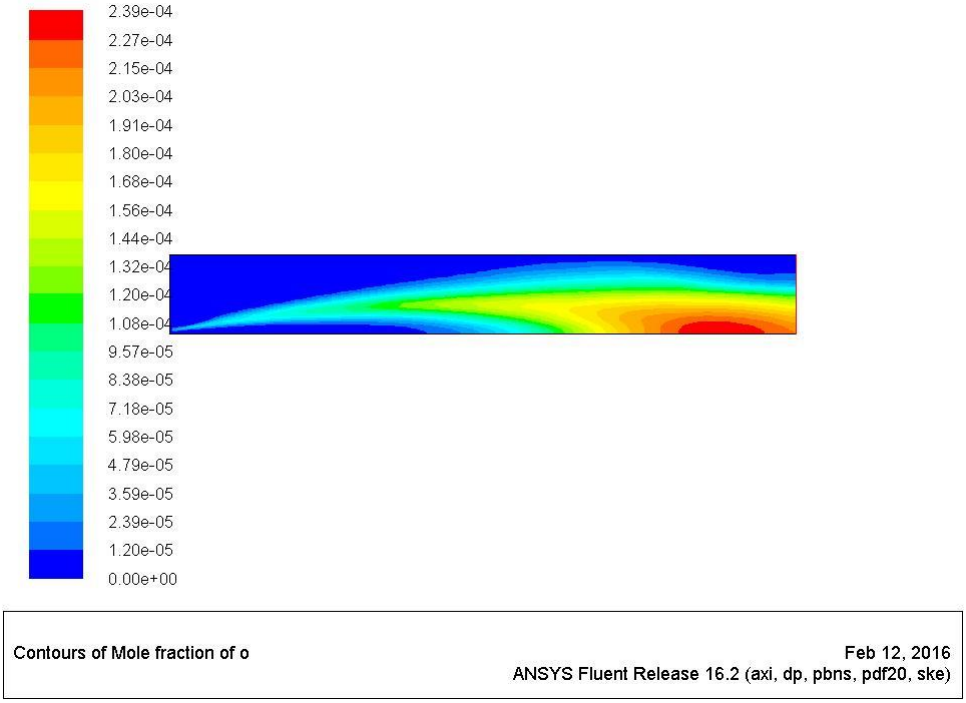

Figure 72: 5% WA [OH] mole fraction

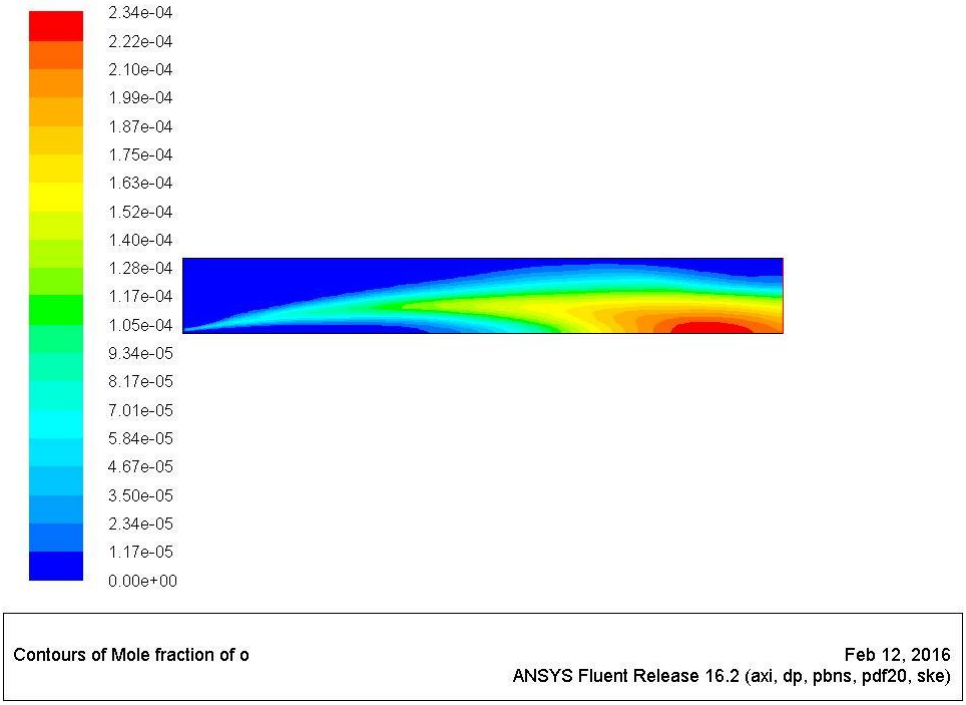

Figure 73: 10% WA [OH] mole fraction

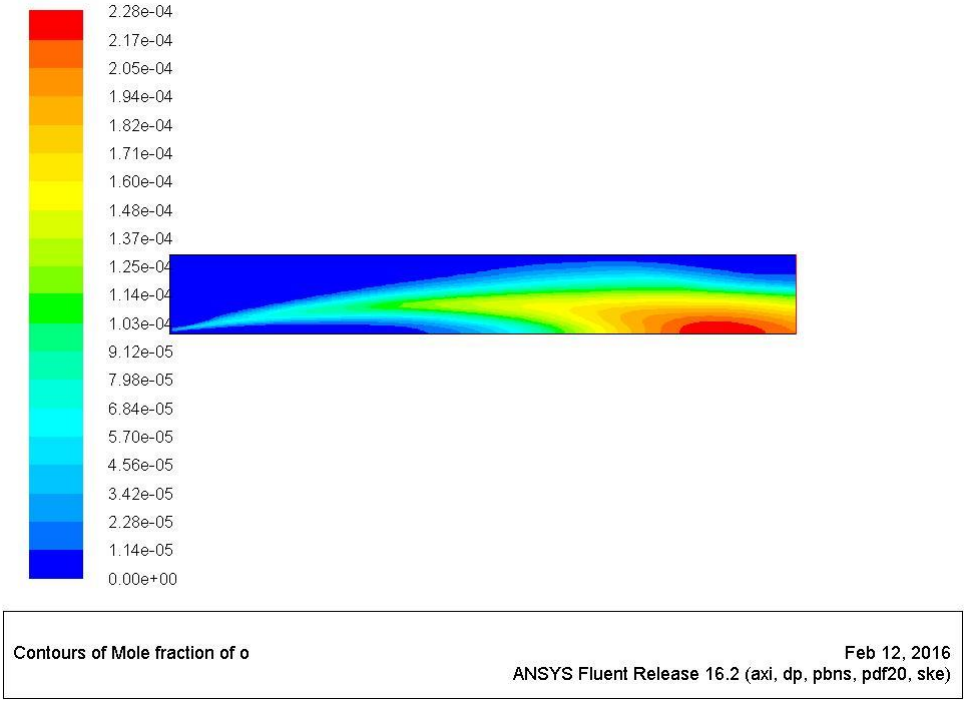

Figure 74: 15% WA [OH] mole fraction

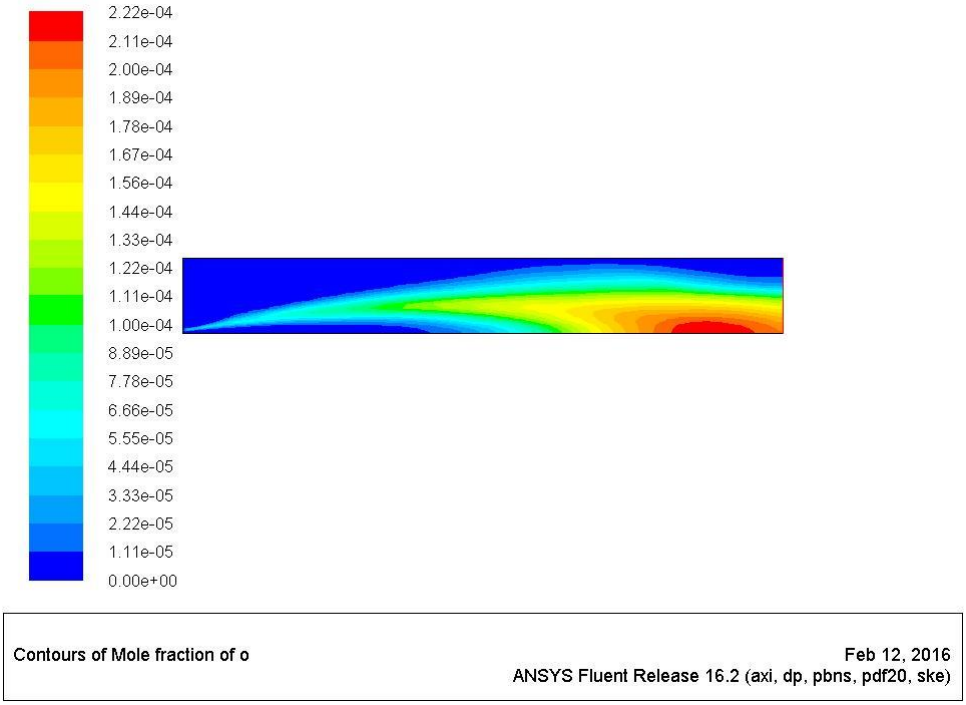

Figure 75: 20% WA [OH] mole fraction

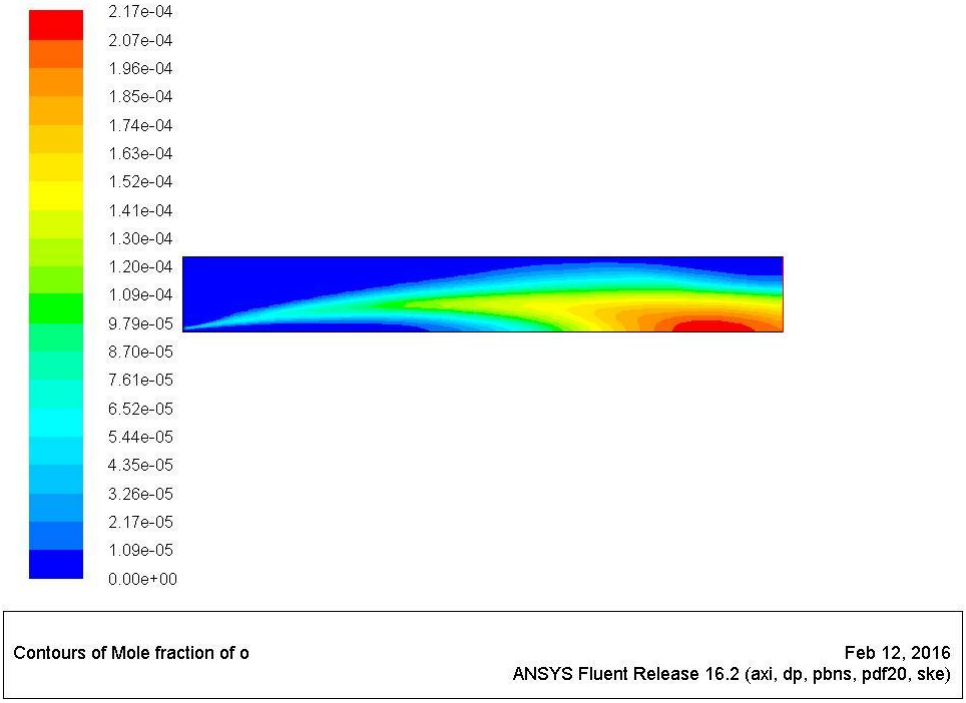

Figure 76: 25% WA [OH] mole fraction

8. CONCLUSIONS

After all the work done, the results show pretty interesting results. It is clear that the addition of water have a significant effect on the NOx formation. Independently of the contact mode, as more water is added to the system, less NOx are formed. This is supposed to be because of some reasons:

First, the addition of water has a direct effect in the temperature profile of the system. It reduce the peak temperature and also the average temperature of the system, what implies a reduction of the thermal NOx (which are the main contributors to the total NOx as can be observed from the profiles).

Secondly, as can be observed in the profiles, the concentration of both radicals [O] and [OH] is reduced as more water is added, what influences the equilibrium reactions implied in the formation of NO and NO_2.

Another interesting conclusion is that, if this process is not correctly done, the addition of water will have a detrimental effect of the system. This can be notice from the Figure 9, whereas the addition to the Fuel stream reduce the NOx formed in comparison with the non-water case, the addition of water to the Air stream causes an increment in the NOx formed in the system (it causes an increment of the average temperature and radicals concentration). This a clear example of how important it is the contact mode when performing any chemical reaction.

This work gives the tendency of the NOx formation when adding water to the system, but the reaction mechanism, the radiation model and other system' parameters used for the simulations are quite simple, so the results must be taken, as this is, a tendency.

9. FUTURE WORK

As commented in the conclusions, the models used for this work are very simple. For a more accurate study, it's recommended to implement more detailed models regarding to species transport, kinetics (for instance GRI 3.0(10)), radiation and contours (i.e. walls).

In addition, it would be very interesting to compare the simulations with an experimental assay to validate the models used in the study. However, one must take into account that this works implies much more time than the available for a master thesis, e.g. a PhD would be required. System selection and apparatus montage, and detailed modelling and calculations implies lots of time, but would be worth spent if these studies carry innovation and solutions for the problematic issue of NOx pollution.

REFERENCES

1. Byeonghun Yu; Seungro Lee; Chang-Eon Lee. Study of NOx emission characteristics in CH4/air non-premixed flames with exhaust gas recirculation. *ELSEVIER Energy*, Volume 91, November **2015**, pp 119-127.
2. Leszek Chybowski; Rafał Laskowski; Katarzyna Gawdzinska. An overview of systems supplying water into the combustion chamber of diesel engines to decrease the amount of nitrogen oxides in exhaust gas. *Japan society of Naval Architects and Ocean Engineers-Journal*, January **2015** Review
3. C.E.L. Pinho; J.M.P.Q. Delgado; R. Pilão; J. Conde; C. Pinho2, Numerical Study of Propane-Air Mixture Combustion in a Burner Element,*Defect and Diffusion Forum Vols*. 273-276 ,**2008** pp 144-149
4. Julio Rendón; Francisco Cadavid; Andrés Amell. Flame structure simulation in a methane/air co-flow partially premixed burner. *Fac. Ing. Univ. Antioquia* ,Junio **2008,** *N.° 44*. pp. 61-74.
5. M.M.Noor; Andrew P.Wandel1; Talal Yusaf. Detail guide for CFD on the Simulation of Biogas Combustion in Bluff-Body Mild Burner. *International Conference on Mechanical Engineering Research.* July **2013**. Paper ID: P342
6. ANSYS Tutorial (2015); FLUENT Tutorial guide. *ANSYS, Inc*. Release: 16.0, January **2015**
7. ANSYS Theory (2015) ANSYS FLUENT Theory guide. ANSYS, Inc. Release: 16.2, July **2015**
8. http://www.telegraph.co.uk/finance/newsbysector/transport/11463519/Car-industry-fumes-about-the-demonisation-of-diesel-engines.html (New about Europe concern in the NOx's pollution) Visited January **2016**
9. http://combustion.berkeley.edu/gri-mech/version30/text30.html (Combustion mechanism with NOx considerations: GRI 3.0). Visited: January **2016**
10. http://territori.gencat.cat/ca/01_departament/11_normativa_i_documentacio/ (Legislation website of Catalonia territory) Visited January **2016**