Comparison of NOx Predictions in Premixed & Non-premixed Laminar H2-air Flames- Detailed kinetics vs Inbuilt Fluent NOx Models

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Comparison of NOx Predictions in Premixed & Non-premixed Laminar H_2-air Flames- Detailed kinetics vs Inbuilt Fluent NOx Models

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ABSTRACT

The present study develops a computation strategy for accurately predicting NOx emissions in laminar H_2-air flames diluted with N_2 using commercially available Ansys-Fluent software. Reactive flow 2D-CFD computations were performed on 2D-axisymmetric opposed-jet counterflow configurations. Comparing these NO profiles generated from the fluent NOx model with the detailed chemistry (Gri-Mech 3.0) highlights the inconsistency of this inbuilt fluent NOx model. Hence, it is concluded that detailed kinetic models containing N species should be preferred over the inbuilt fluent NOx model for accurate NO predictions.

Keywords:- NOx predictions; opposed jet counterflow configuration, H_2-air premixed & non-premixed flames; Reactive flow 2D-CFD computations; NOx chemistry

INTRODUCTION

ISSUE

Gas turbine working on natural gas leads to CO_2 emissions leading to climate change.

SOLUTION

Use of Hydrogen as fuel instead natural gas eliminate CO_2 emissions completely.

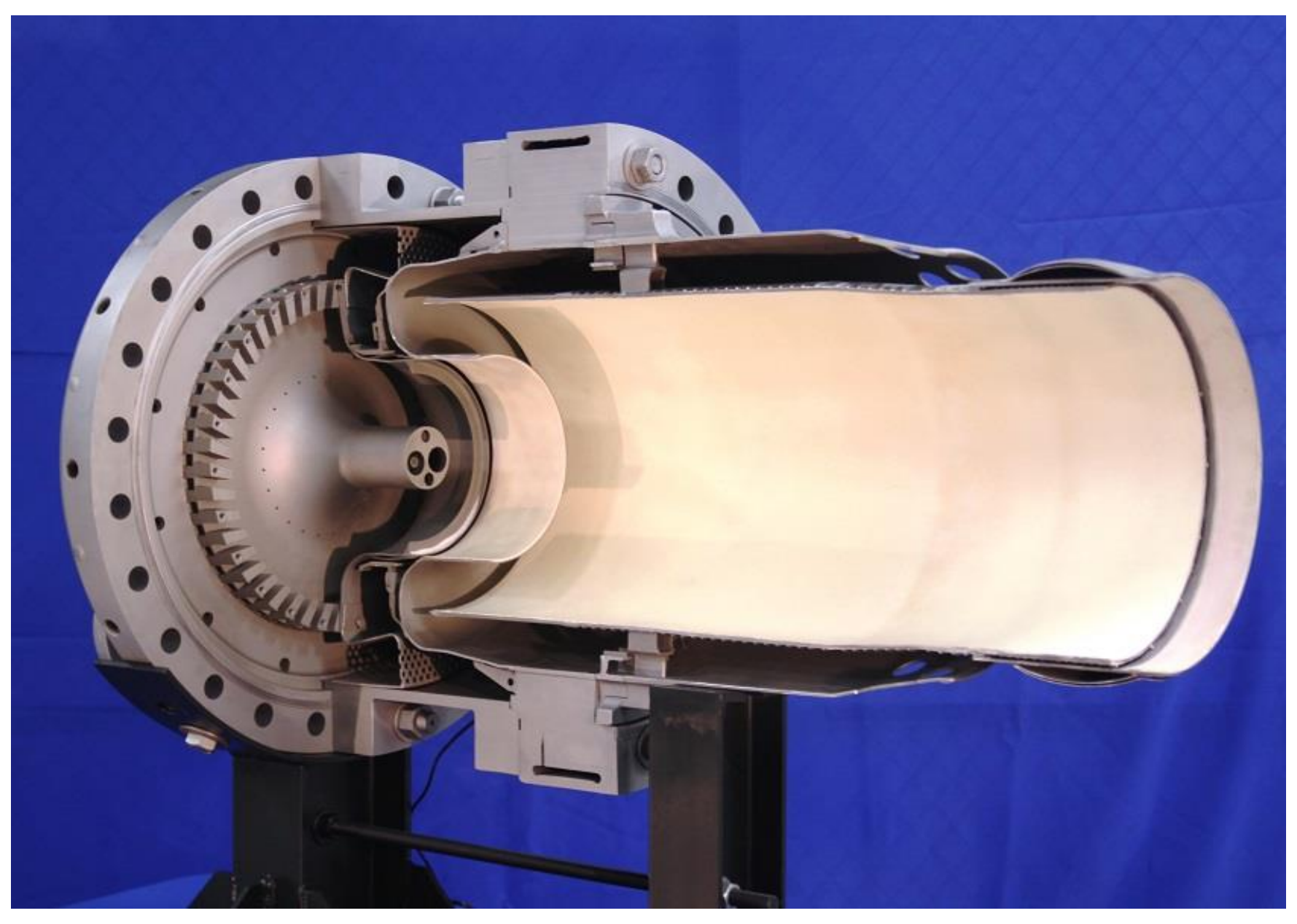


Fig. 1: Design of FlameSheet^{TM} combustion system by Thomassen Energy retrofitted for High Hydrogen Gas Turbine Retrofit Project [1,2]

Natural gas → Hydrogen

Figure 1 shows one such gas-turbine combustor design by Thomassen Energy working on pure hydrogen as a fuel.

Besides CO_2, NOx emission prediction and its reduction is the other focus for combustion researchers.

GOAL

Development of fast computational methodology for NOx prediction in Hydrogen GT Combustion.

COMPUTATIONAL METHODOLOGY

COMPUTATIONAL DOMAIN AND BOUNDARY CONDITIONS

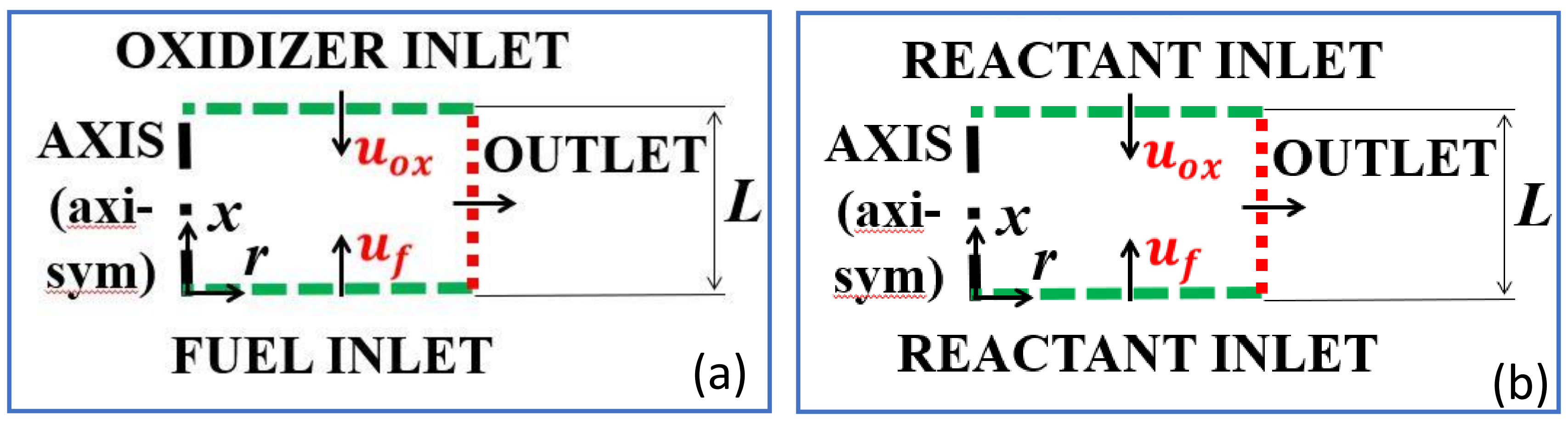


Fig. 2: Schematic of the computational domain with imposed boundary conditions (a) Non-premixed flame, (b) Premixed flame

SOLVER DETAILS FOR SIMULATION

- 2D axisymmetric domain constructed for opposed jet counterflow configuration.
- *Konnov (2019) kinetic* mechanism used.
- A fixed value of 100 s^{-1} of global strain rate (a_g) was used.
- Non-premixed combination of H_2/N_2 and air.
- Premixed mixture of H_2/Air at equivalence ratio of 0.25.

$$a_g = \frac{2u_{ox}}{L}\left[1 + \frac{u_f}{u_{ox}}\sqrt{\frac{\rho_f}{\rho_{ox}}}\right]$$

RESULT AND DISCUSSION

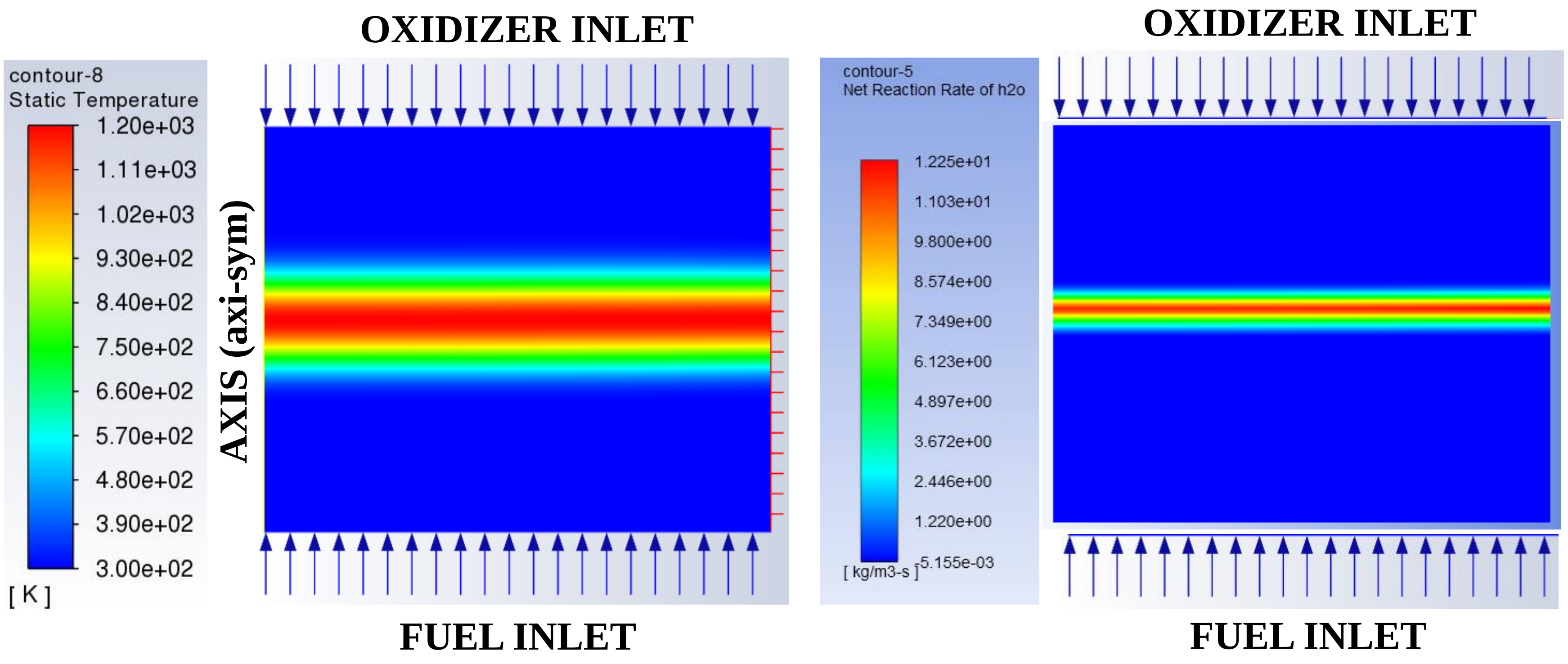


Fig. 3 Contour of temperature profile and H_2O net reaction rate for $12.5H_2/77.5N_2$-air diffusion flame at global strain of $100s^{-1}$

Figure 3 shows temperature profile and H_2O net reaction rate for $12.5H_2/77.5N_2$-air diffusion flame at global strain of $100s^{-1}$

A stable flame is obtained which is close to stagnation plane.

The contours in Figure 4 shows NO mole fraction production in the thermal zone.

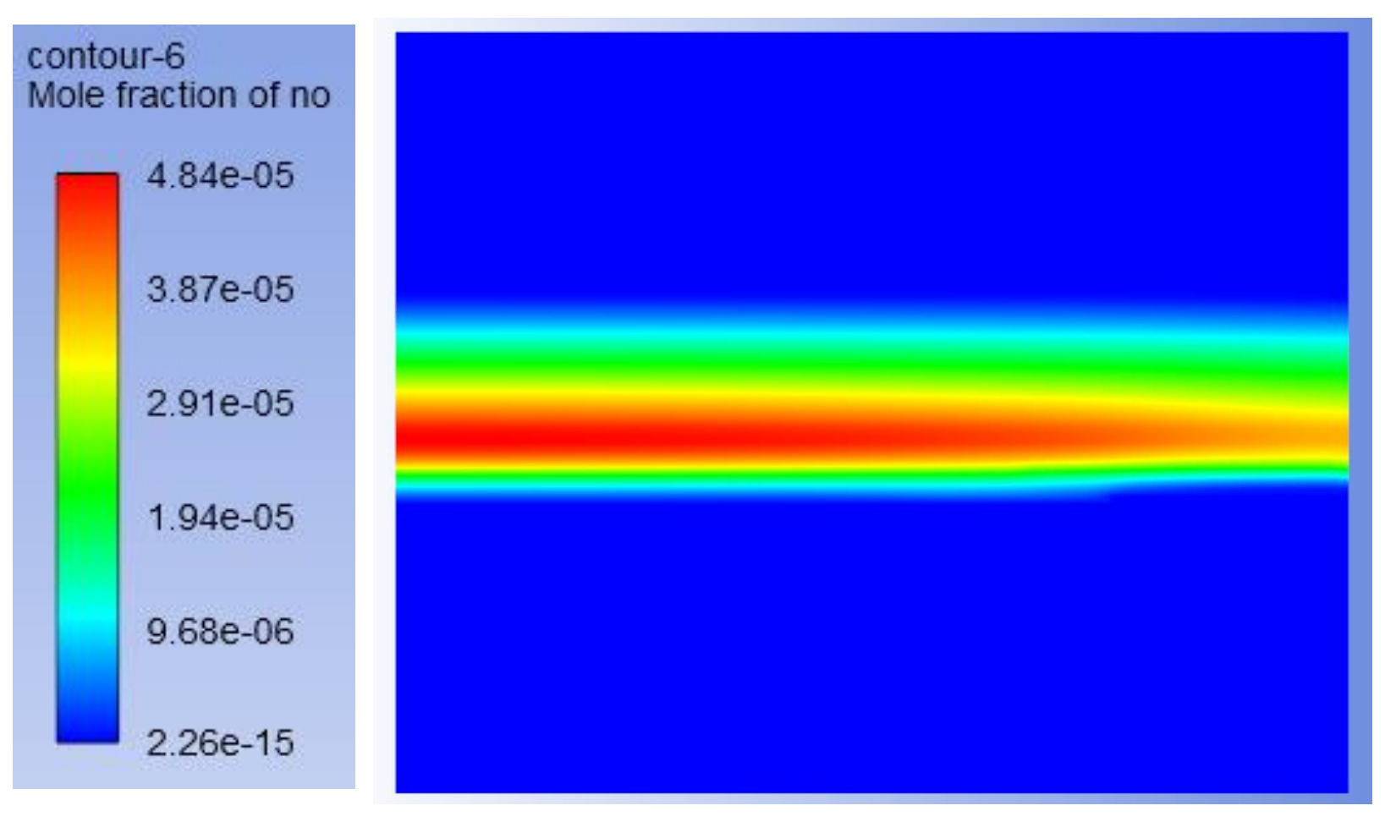


Fig. 4 Contour of NO mole fraction rate for $12.5H_2/77.5N_2$-air diffusion flame at global strain of $100s^{-1}$

RESULT AND DISCUSSION

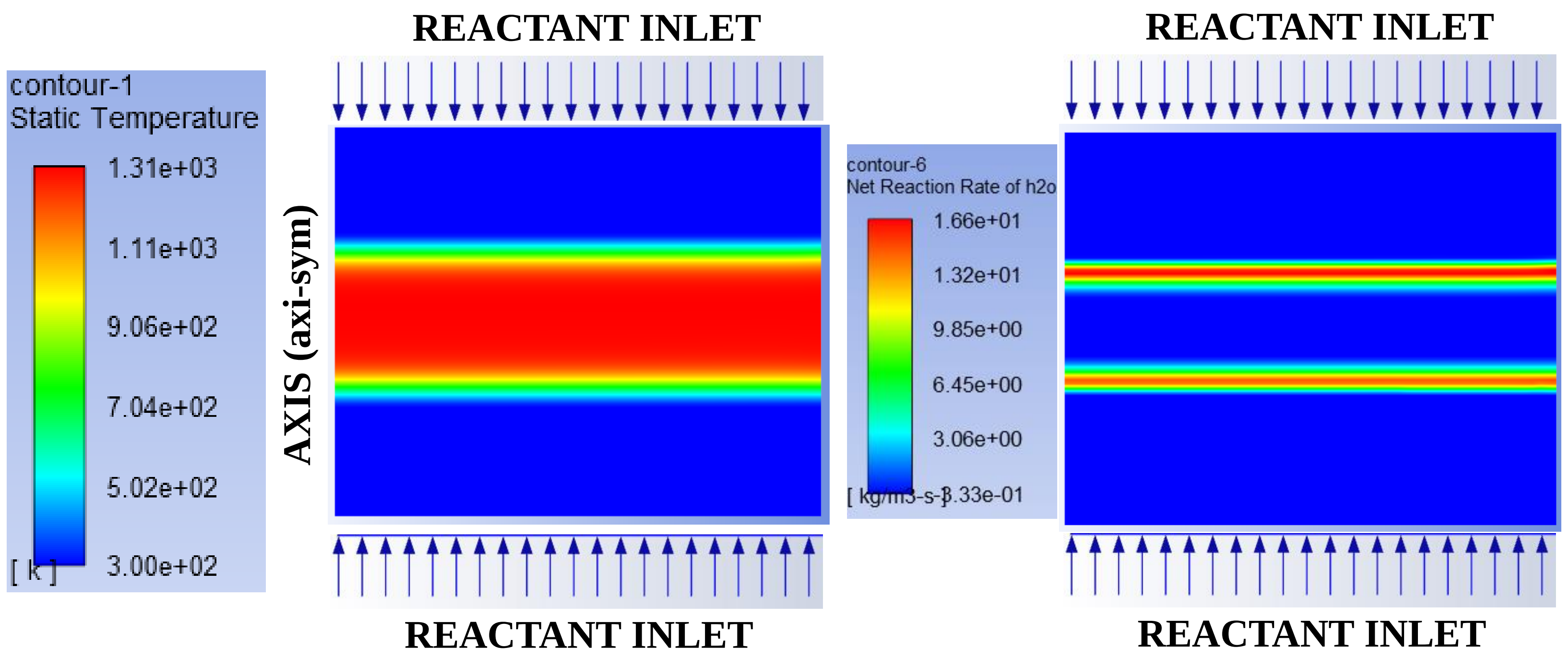


Fig. 5 Contour of temperature profile and H_2O net reaction rate for H_2-air premixed flame at global strain of $100s^{-1}$ at equivalence ratio of 0.25

Figure 5 shows temperature profile and H_2O net reaction rate for H_2-air premixed flame at global strain of $100s^{-1}$ at equivalence ratio of 0.25.

A twin H_2-air premixed flame is obtained as expected.

Premixed flames have 2 order of magnitude less NO production in comparison to non-premixed flames.

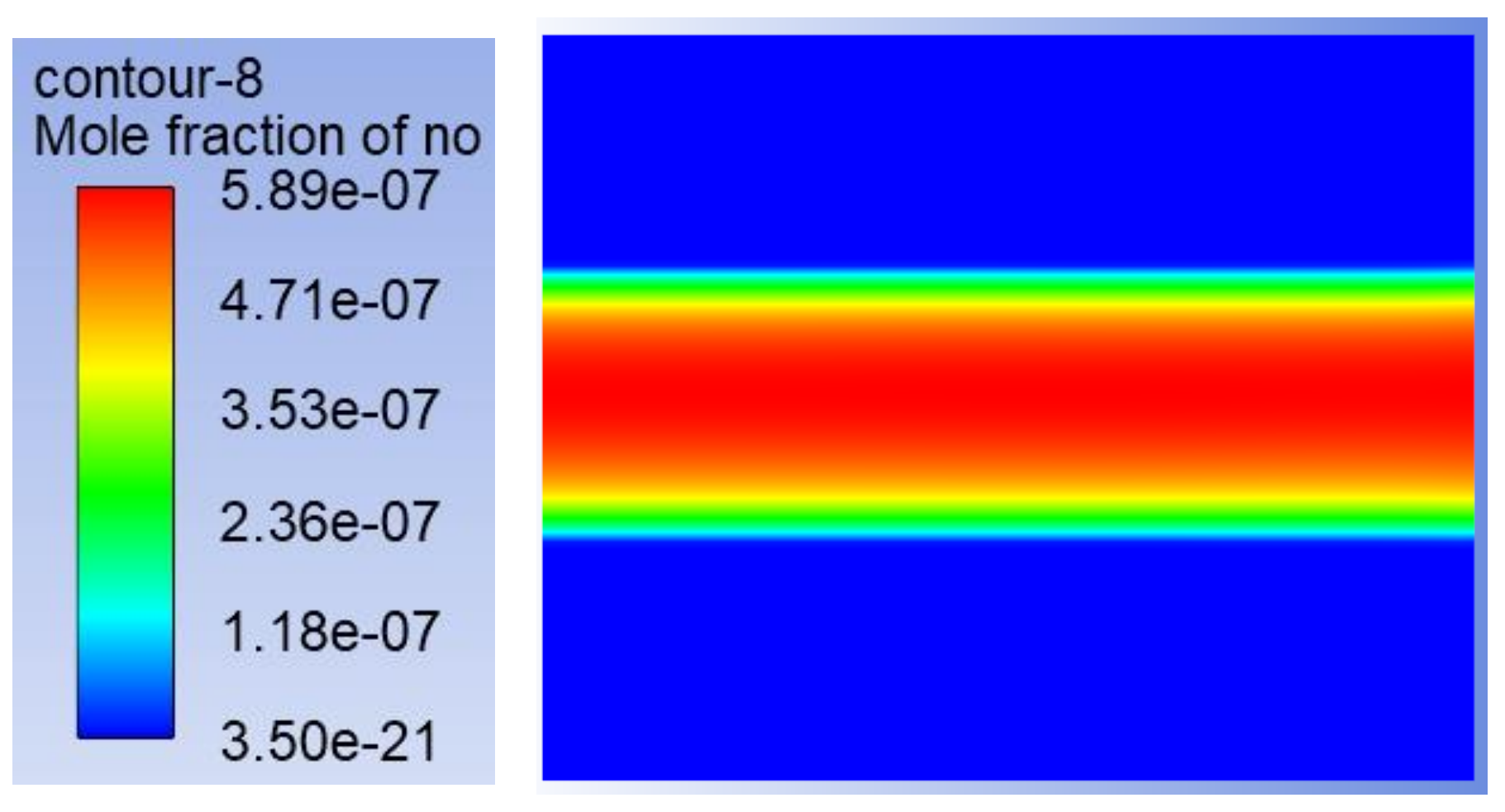
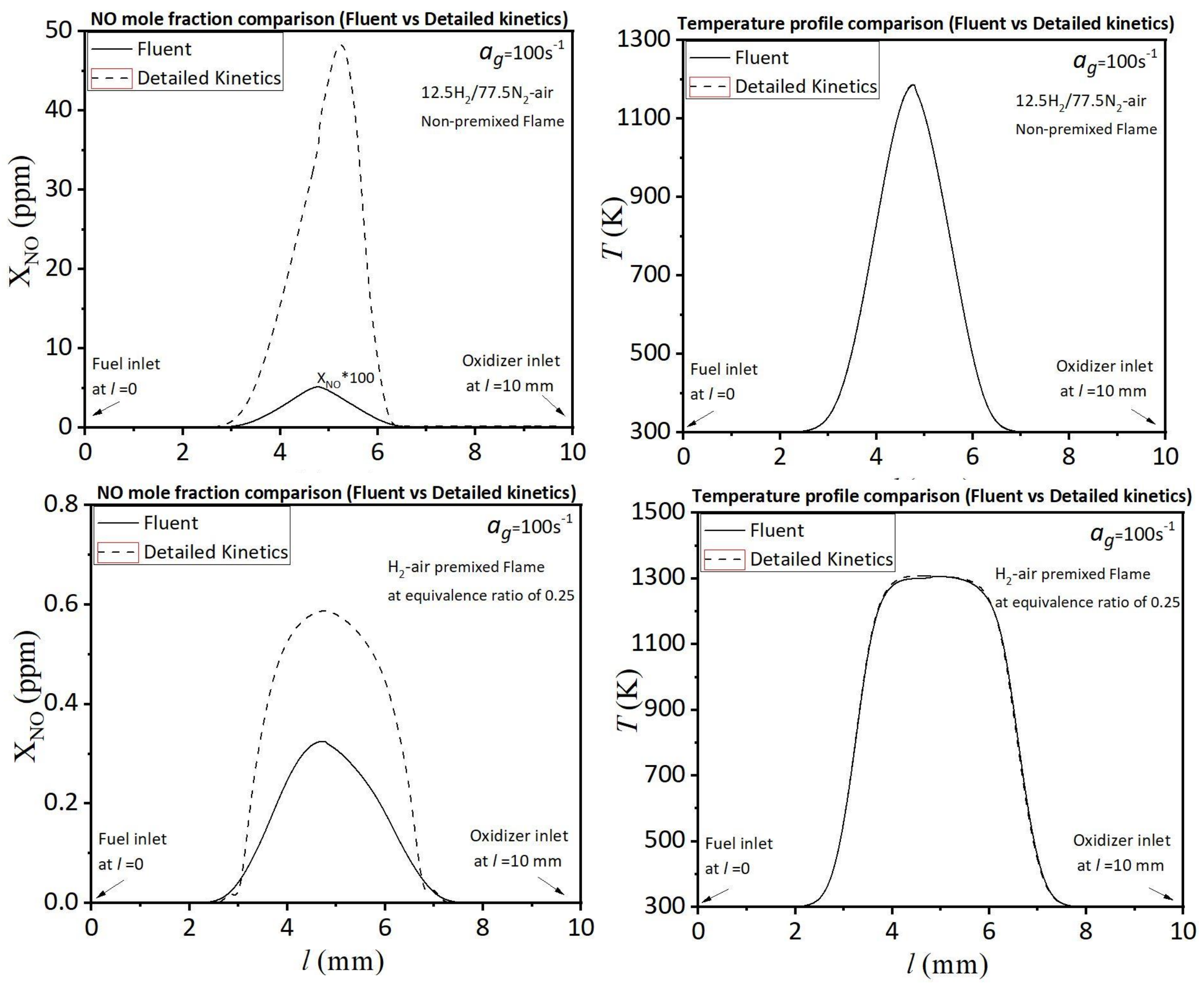


Fig. 5 Contour of NO mole fraction for H_2-air premixed flame at global strain of $100s^{-1}$ at equivalence ratio of 0.25

Fluent NO models are incapable for predicting NO mole fraction for H_2-air non-premixed flames (3 order of magnitude difference).

Identical temperature profile irrespective of NO models used.

Two order of magnitude less NOx production by H_2-air premixed flames in comparison to non-premixed flames.



Figs. 6(a,b,c,d) Comparison of NO and temperature profiles for Non-premixed and premixed flames- Detailed kinetics vs fluent NO model

CONCLUSION

- Inconsistency in the Fluent NO models with detailed kinetics is confirmed.
- This inconsistency is much larger for Non-premixed flames in comparison to premixed flames.
- The accuracy of the detailed kinetic model should also be established by comparing the results with experimental data.

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