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Numerical Analysis of Laminar Hydrogen Diffusion Flames

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Abstract

Hydrogen diffusion flames in the laminar flow regime are numerically analysed. Different global and detailed reaction mechanisms are considered and compared. Based on the published data of other authors, the presently considered mathematical and numerical models are assessed and validated.

Keywords: hydrogen, combustion, diffusion flame, reaction, validation, CFD.

1 Introduction

Parallel to new energy sources and recovery techniques [1], the energy conversion technology through the combustion process continues to play an important role in power generation. Within this context, hydrogen (H_2) and hydrogen blend fuels enable clean energy supply through combustion. On the one hand, hydrogen (H_2) represents an attractive alternative to storing excess energy in the renewable power generation [2] via wind turbines and photovoltaics [2]. On the other hand, instead of combustion [3,4] gasification [5] is a good possibility for clean power generation, since the synthesis gas contains significant amounts of H_2, in addition to carbon monoxide (CO) and small amounts or methane (CH_4). Additionally, there is a growing interest in hydrogen production using nuclear power plants [6].

The state-of-the-art technology for the combustors of the stationary gas turbines is the lean premixed combustion. A principal problem here is the so-called "flashback" [7]. This makes the use of H_2-blend fuels to a real challenge, since the high fuel reactivity due to H_2 increases the flashback propensity. To prevent flashback, many researchers started to revert to the more conventional non-premixed combustion technology and explore means of reducing nitrogen oxide (NO) emissions within this framework, with some success. In such applications that can be found in different areas, such as power generation [8], or domestic boilers [9], the main principle utilized to reduce the thermal NO formation has been the reduction of the residence time in the hot flame zone. Principally, this is achieved by such designs that utilize arrays of a large number of micro-scale diffusion flames. Due to the small sizes of the injectors, the resulting flames may turn out to be laminar, as, for example, observed in Ref. [9]. This brings the combustion in the laminar flow regime, again, in the focus of investigation as a relevant flow and combustion mode for certain types of applications. Thus, there is still a need for further studies on laminar hydrogen diffusion flames. This constitutes the focus of the present contribution.

In the present investigation, hydrogen diffusion flames in the laminar flow regime are numerically analysed for different Reynolds numbers. Different global and detailed reaction mechanisms are considered and compared with each other. The main purpose of the present study is the validation. Using the published data of other authors on H_2 flames [10], the presently considered mathematical and numerical models are assessed and validated.

2 Methods

The differential transport equations of the chemically reacting mixture are numerically solved, assuming a subsonic flow and an ideal gas behaviour [11], considering multi-component diffusion [12]. The isobaric specific heat capacities as function of temperature are obtained using a pair of fourth order polynomials [11], for low and high temperature ranges. The transport properties are obtained from the kinetic theory [11]. The chemical kinetics rate coefficients are modelled by the Arrhenius expressions [12]. Laminar diffusion jet flames in generic co-axial configurations are considered. Thus, the modelling errors with respect to the modelling of turbulence [13] and turbulence-chemistry interactions [14,15] do not occur. For the numerical simulations, the finite volume method (FVM) based general purpose computational fluid dynamics (CFD) software ANSYS Fluent 19.0 [16] is employed. As the Navier-Stokes solution method, the SIMPLEC [16] scheme is used. For the discretization of the convective terms, the QUICK upwind scheme [16] is utilized, which has a formal accuracy of third order. The chemical kinetics software Cantera [17], is also used for verification purposes.

As the reaction mechanism for the H_2 combustion with air, the detailed mechanism of Conaire et al. [18] is used. For comparison purposes, the global mechanism of Marinov et al. [19] has also been considered. The role of the radiative heat transfer is also investigated. Calculations by neglecting the radiative heat loss are compared by simulations where the radiative heat transfer is modelled by the spherical harmonics P1 and Discrete Ordinates (DO) methods [20]. Doing so, the radiation properties of the gas mixture are approximated based on the weighted sum of gray gases model [21], neglecting the carbon dioxide (CO_2) contribution. The grid independence is ensured in all considered cases. For coping with the high grid resolution requirements dictated by the small length scales of the flame front, adaptive gridding techniques are used.

3 Results

The first test case chosen for validation is the laminar axisymmetric hydrogen-air diffusion flame of Toro et al. [10]. A 2D-axissymmetric modelling is applied. The rectangular solution domain is enclosed, in the axial (main flow) direction, by the inlet boundaries for the central fuel and co-axial air jets on the upstream, and an outlet boundary on the downstream. The outlet boundary is placed at a distance of 60 cm from the inlet (sufficiently far for not to influence the results). In the radial direction, the domain extends from the symmetry axis to a boundary at the radial position of the outer edge of the co-flow annulus.

At the fuel inlet, a fully-developed pipe velocity profile is prescribed. For the air inlet, a uni-directional homogeneous velocity is assumed. The area-averaged velocities at both inlets are equal to each other. For the energy equation, the ambient temperature is prescribed as boundary condition at both inlets. For species transport equations, the corresponding Dirichlet conditions apply at inlets. At the exit, zero-gradient boundary conditions apply, along with a prescribed static pressure. On the symmetry axis and the enclosing radial boundary, symmetry conditions are applied.

The contour plots of the velocity magnitude (V), temperature (T) and mole fractions of H_2, O_2 and H_2O as predicted by the global [19] and detailed [18] reaction mechanisms are displayed in Figures 1-5.

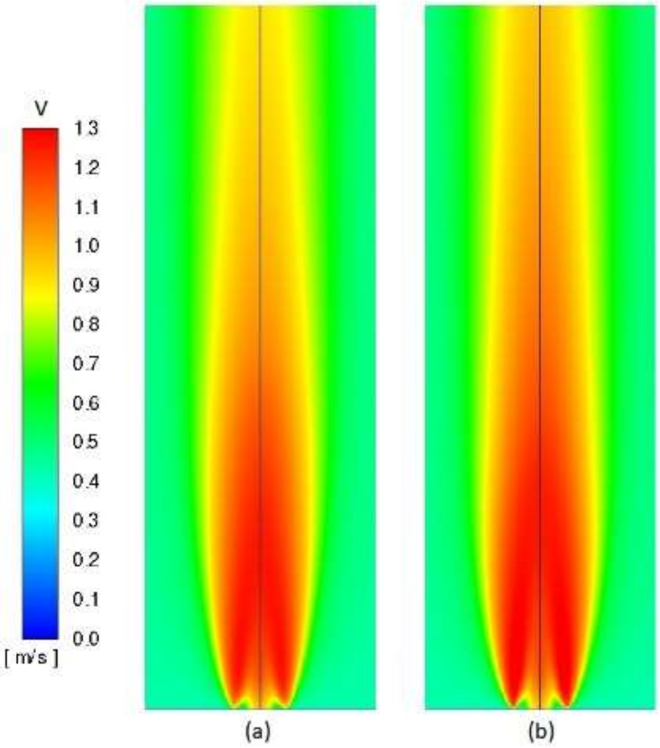

Figure 1: Velocity magnitude, (a) global mechanism, (b) detailed mechanism.

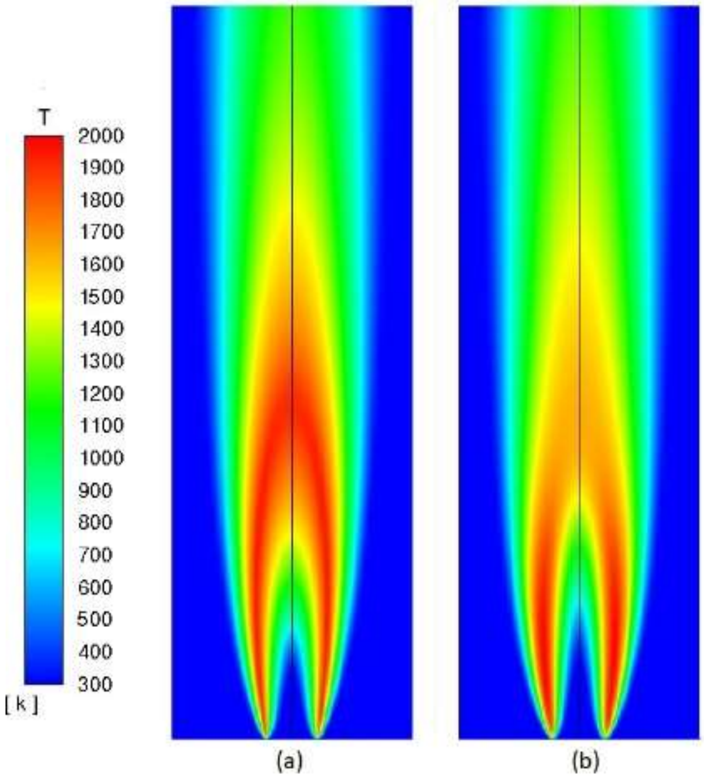

Figure 2: Temperature, (a) global mechanism, (b) detailed mechanism.

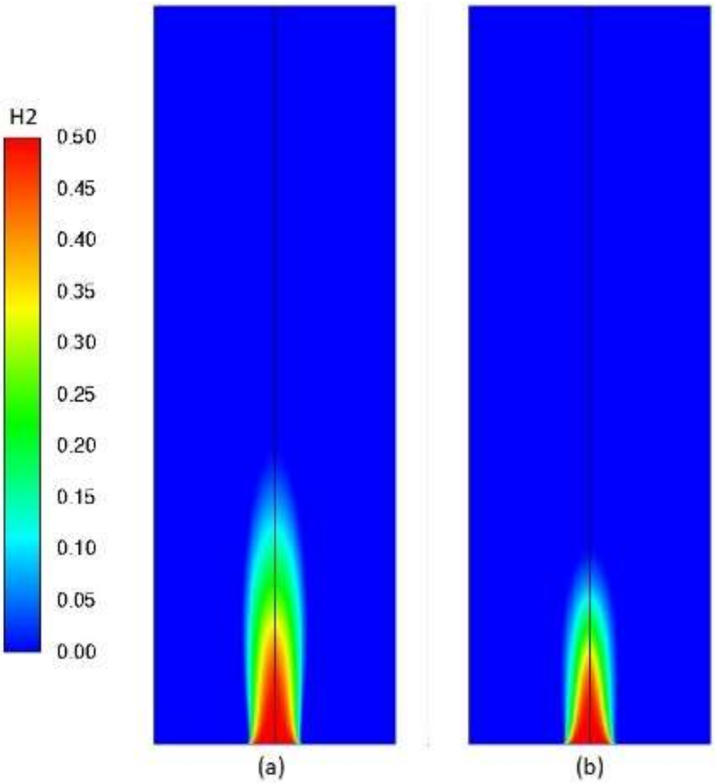

Figure 3: H_2 mole fraction, (a) global mechanism, (b) detailed mechanism.

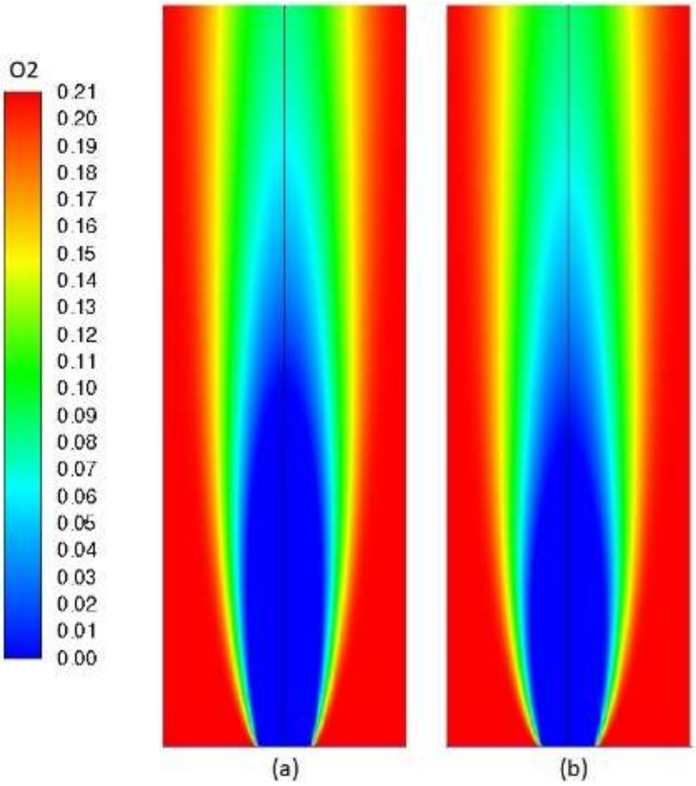

Figure 4: O_2 mole fraction, (a) global mechanism, (b) detailed mechanism.

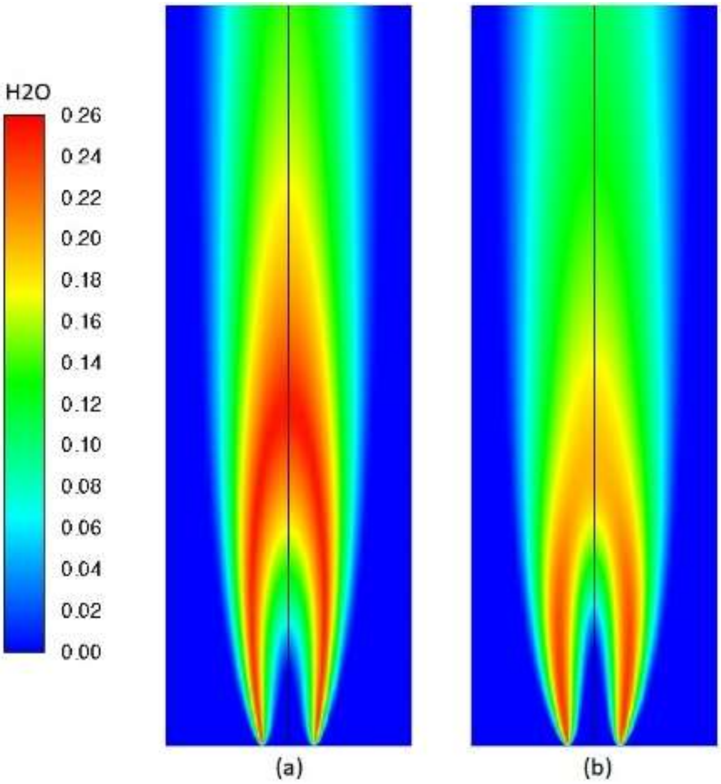

Figure 5: H_2O mole fraction, (a) global mechanism, (b) detailed mechanism.

Figure 6 shows the H, O and OH mole fraction contours predicted by the detailed mechanism [18].

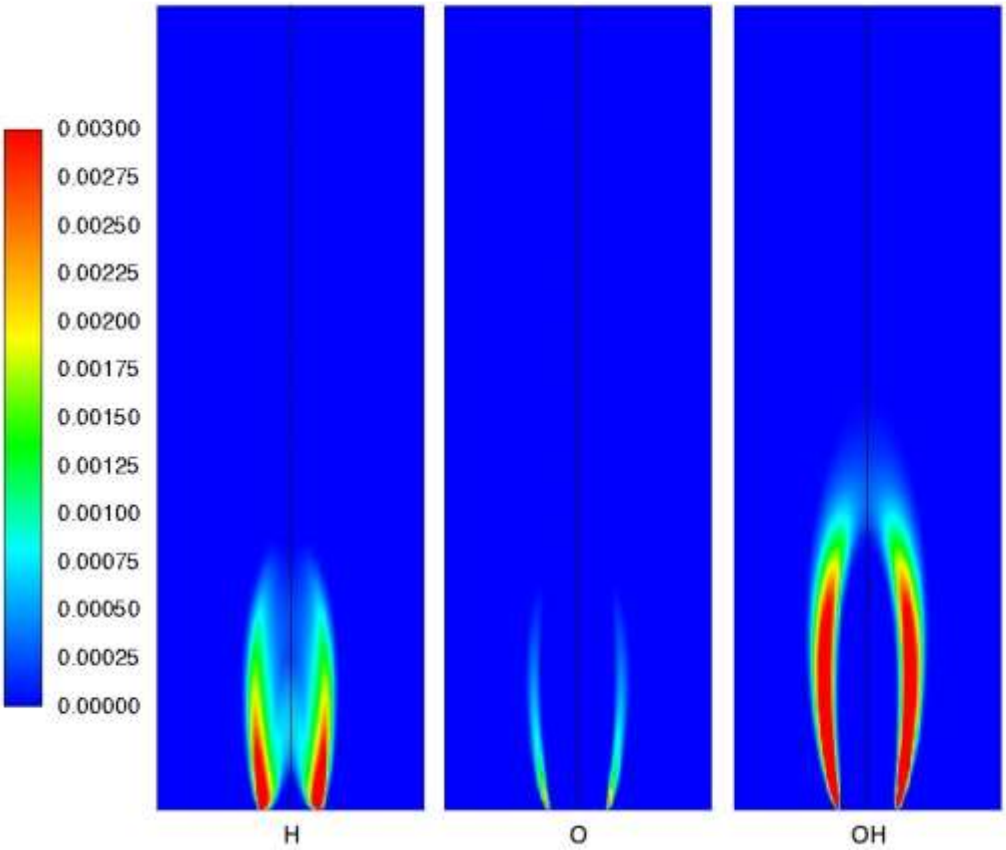

Figure 6: H, O, OH mole fractions (detailed mechanism).

The predicted radial profiles of temperature and H_2, O_2 and H_2O mole fractions are compared with the experimental values in Figures 7-10.

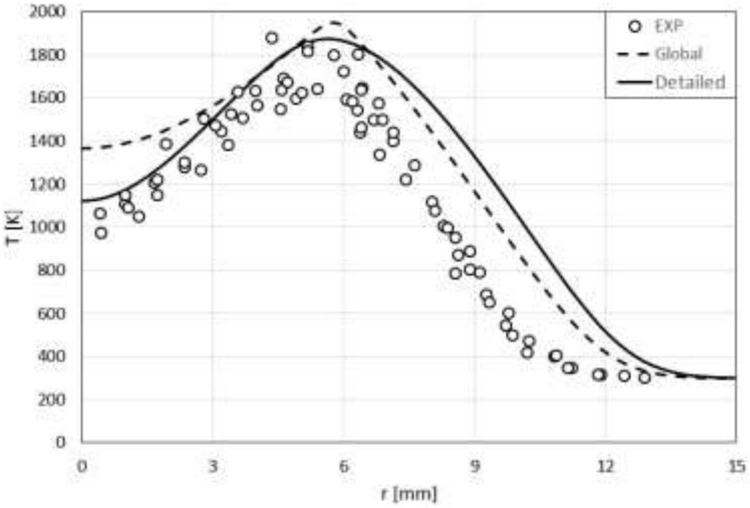

Figure 7: Radial profile of temperature at x=30mm.

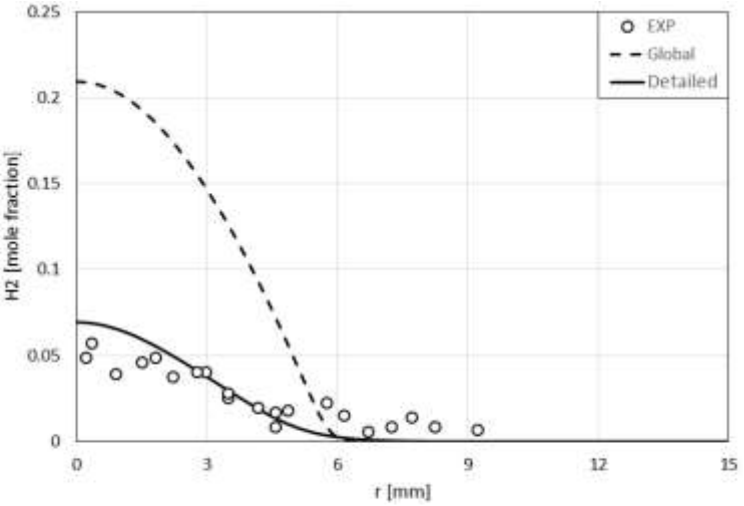

Figure 8: Radial profile of H_2 mole fraction at x=30mm.

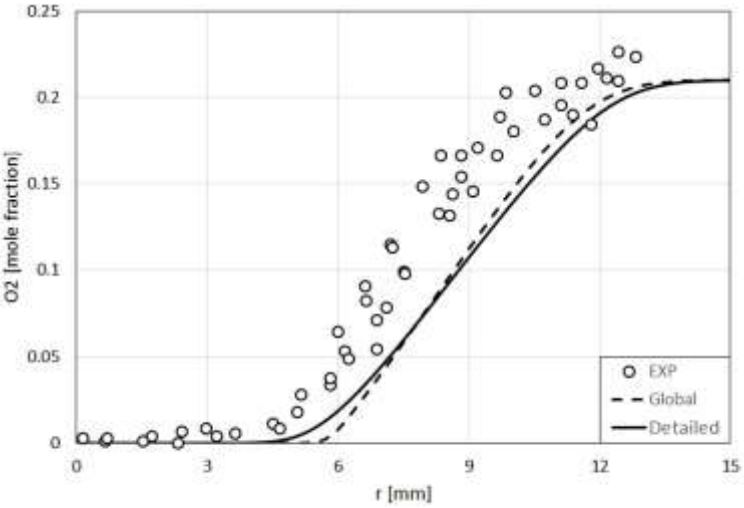

Figure 9: Radial profile of O_2 mole fraction at x=30mm.

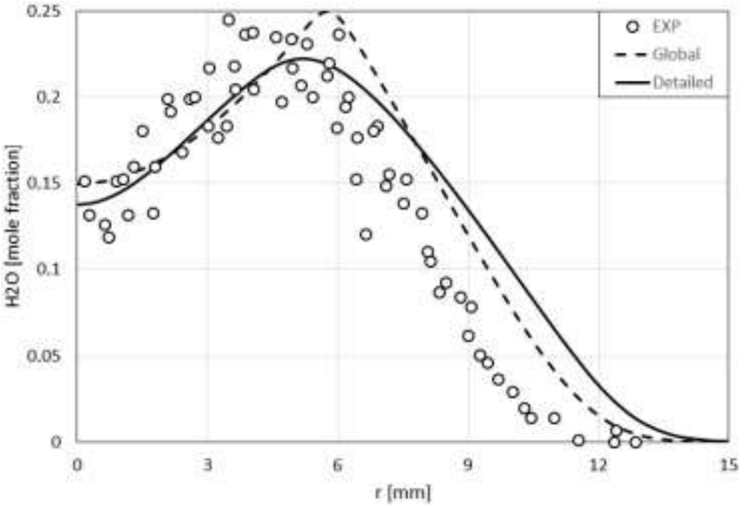

Figure 10. Radial profile of H_2O mole fraction at x=30mm.

4 Conclusions and Contributions

The velocity magnitudes predicted by global [19] and detailed [18] reaction mechanisms (Figure 1) similar. One can see that the detailed mechanism indicates a slightly larger radial expansion.

Comparing the predicted temperatures (Fig. 2), larger differences can be observed. One can see that the achieved maximum temperatures by the both mechanisms are similar. One can also see that regions of high temperature predicted by the detailed mechanism are smaller compared to the global mechanism. This is expected to make a difference in the NO prediction, although maximum temperatures are similar.

For predicted mole fractions of major species (Figures 3-5), noticeable differences can be observed especially in H_2 (Fig. 3) and H_2O (Fig. 5) distributions. The difference in H_2O (Fig. 5) is compatible with the observed temperature fields (Fig. 2). The predicted “core” of the H_2 jet in terms of mole fractions is smaller in the detailed mechanism compared to the global one (Fig. 3). This is partly due to the conversion of H_2 into intermediate species, which are not represented by the global mechanism. Predicted distributions of such species are displayed in Figure 6 for H, O and OH mole fractions.

Comparing the results with the experiments of [10] in terms of the radial temperature profile at x=30mm (x: axial distance from the inlet) (Figure 7), one can see that the maximum temperature predicted by the detailed mechanism agrees slightly better with the experimental value, compared to the global mechanism. One can also observe that experimental values are predicted better by the detailed mechanism in inner parts of the jet, whereas the global mechanism performs better in outer parts. For radial profiles of O_2 (Figure 9) and H_2O (Figure 10), the overall prediction performance of both mechanisms can be observed to be similar. However, a much better performance of the detailed mechanism can be observed for the H_2 profile (Figure 8).

As the NO formation is strongly temperature dependent, the differences in the temperature fields (Figs. 2, 7) are expected to lead to a substantial difference in the NO predictions. Since the NO formation depends on O, OH concentrations [12] the availability of the latter in the detailed mechanism would allow a consistent formulation, whereas this would need to be approximated by equilibrium assumptions using global mechanism. The predictive capabilities of the both approaches will be assessed in the continuation of the present work, by comparisons with the measured NO values.

References

[1] B. Pfeiffelmann, A. C. Benim, F. Joos. “A finite volume analysis of thermoelectric generators”, Heat Transfer Engineering, 40(17-18), 1442-1450, 2019.

[2] M. Götz, J. Lefebvre, F. Mörs, A McDaniel Koch, F. Graf, S. Bajohr, R. Reimert, Th. Kolb, “Renewable power-to-gas: a technological and economic review”, Renewable Energy, 85, 1371-139, 2016.

[3] A. C. Benim, B. Epple, B. Krohmer, “Modelling of pulverised coal combustion by a Eulerian-Eulerian two-phase flow formulation”, Progress in Computational Fluid Dynamics – An International Journal, 5(6), 345-361, 2005.

[4] B. Epple, W. Fiveland, B. Krohmer, G. Richards, A. C. Benim, “Assessment of two-phase flow models for the simulation of pulverized coal combustion”, International Journal of Energy for a Clean Environment, 6(3), 267-287, 2005.

[5] A. C. Benim, K. Kuppa, “Modeling of entrained-flow coal gasification by an equilibrium Eulerian-Eulerian two-phase flow formulation”, Isi Bilimi ve Teknigi Dergisi / Journal of Thermal Science and Technology”, 36(2), 93-102, 2016.

[6] IAEA, “Hydrogen Production Using Nuclear Energy”, IAEA Nuclear Energy Series, No. NP-T-4.2, International Atomic Energy Agency, Vienna, Austria, 2013.

[7] A. C. Benim, K. J. Syed, “Flashback Mechanisms in Lean Premixed Gas Turbine Combustion”, Academic Press, Cambridge, UK, 2015.

[8] A. Haj Ayed, K. Kusterer, H. H. W. Funke, J. Keinz, D. Bohn, “CFD based exploration of the dry-low-NOx hydrogen micromix combustion technology at increased energy densities”, Propulsion and Power Research, 6(1), 15-24, 2017.

[9] G. Lopez-Ruiz, A. R. Fernandez-Akarregi, L. Diaz, I. Urresti, I. Alava, J. M. Blanco, “Numerical study of a laminar hydrogen diffusion flame based on the non-premixed finite-rate chemistry model; thermal NO_X assessment”, International Journal of Hydrogen Energy, 44(36), 20426-20439, 2019.

[10] V. V. Toro, A. V. Mokhov, H. B. Levinsky, M. D. Smooke, “Combined experimental and computational study of laminar, axisymmetric hydrogen-air diffusion flames”, Proceedings of the Combustion Institute, 30, 485-492, 2005.

[11] S. R. Turns, “An Introduction to Combustion”, 3rd ed., McGraw-Hill, New York, USA, 2012.

[12] R. B. Bird, W. E. Stewart, E. N. Lightfoot, “Transport Phenomena”, 2nd ed., Wiley, New York, USA, 2002

[13] A. C. Benim, M. Cagan, A. Nahavandi, E. Pasqualotto, “RANS predictions of turbulent flow past a circular cylinder over the critical regime”, Proceedings of the 5th IASME/WSEAS International Conference on Fluid Mechanics and Aerodynamics, August 25-27, 2007, Athens, Greece, 232-237, 2007.

[14] A. C. Benim, A. Nahavandi, P. Stopford, K. J. Syed, “DES LES and URANS investigation of turbulent swirling flows in gas turbine combustors”, WSEAS Transactions on Fluid Mechanics, 5(1), 465-472, 2006.

[15] S. Iqbal, A. C. Benim, S. Fischer, F. Joos, D. Kluß, A. Wiedermann, “Experimental and numerical analysis of natural bio and syngas swirl flames in a model gas turbine combustor”, Journal of Thermal Science, 25(5), 460-469, 2016.

[16] www.ansys.com. Accessed on December 2, 2020.

[17] www.cantera.org. Accessed on November 6, 2020.

[18] C. O. Conaire, H. J Curran, J. M. Simmie, W. J. Pitz, C. K. Westbrook, “A comprehensive modeling study of hydrogen oxidation”, International Journal of Chemical Kinetics, 36, 603-622, 2004.

[19] N. M. Marinov, C. K. Westbrook, W. Pitz, “Detailed and global chemical kinetics model for hydrogen”, Report No. UCRL-JC-120677, Lawrence Livermore National Laboratory, CA, USA, 1995.

[20] M. N. Özisik, “Radiative Transfer and Interactions with Conduction and Convection”, Wiley, Hoboken, NJ, USA, 1973.

[21] T. F. Smith, Z. F. Shen, J. N. Friedman, “Evaluation of coefficients for the weighted sum of gray gases model”, Journal of Heat Transfer, 104, 602-608, 1982.