

ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL

**MULTI-OBJECTIVE OPTIMIZATION OF SWIRL BURNER WITH
PREMIXED AMMONIA/HYDROGEN FLAME**



Ph.D. THESIS

Mehmet Anıl GÜLŞAN

Department of Mechanical Engineering

Mechanical Engineering Programme

FEBRUARY 2026

ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL

**MULTI-OBJECTIVE OPTIMIZATION OF SWIRL BURNER WITH
PREMIXED AMMONIA/HYDROGEN FLAME**

Ph.D. THESIS

**Mehmet Anıl GÜLŞAN
(503182037)**

Department of Mechanical Engineering

Mechanical Engineering Programme

Thesis Advisor: Prof. Dr. Yakup Erhan BÖKE

FEBRUARY 2026

İSTANBUL TEKNİK ÜNİVERSİTESİ ★ LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

**ÖN KARIŞIMLI AMONYAK/HİDROJEN ALEVİNE SAHİP GİRDAPLI
YAKICININ ÇOK HEDEFLİ OPTİMİZASYONU**

DOKTORA TEZİ

**Mehmet Anıl GÜLŞAN
503182037**

Makina Mühendisliği Anabilim Dalı

Makina Mühendisliği Programı

Tez Danışmanı: Prof. Dr. Yakup Erhan BÖKE

ŞUBAT 2026

Mehmet Anıl GÜLŞAN, a Ph.D. student of İTÜ Graduate School student ID 503182037, successfully defended the thesis entitled “MULTI-OBJECTIVE OPTIMIZATION OF SWIRL BURNER WITH PREMIXED AMMONIA/HYDROGEN FLAME”, which he prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below.

Thesis Advisor : **Prof. Dr. Yakup Erhan BÖKE**
Istanbul Technical University

Jury Members : **Assis. Prof. Dr. İsmail Yalçın URALCAN**
Istanbul Technical University

Assoc. Prof. Dr. Abdussamet SUBAŞI
Istanbul Technical University

Prof. Dr. Şevket Özgür ATAYILMAZ
Yıldız Technical University

Prof. Dr. Özden AĞRA
Yıldız Technical University

Date of Submission : 13 December 2025
Date of Defense : 03 February 2026





To my family,



FOREWORD

First and foremost, I would like to express my sincere respect and gratitude to my supervisor, Prof. Dr. Yakup Erhan BÖKE, who has guided me throughout my doctoral studies with his knowledge and experience, and who has supported this thesis with his valuable suggestions and constructive feedback. I would also like to extend my respectful thanks to Prof. Dr. İsmail Yalçın URALCAN and Prof. Dr. Şevket Özgür ATAYILMAZ, whose insightful comments and guidance have greatly contributed to this work during the thesis process. I am deeply thankful to my master's thesis advisor, Prof. Dr. Seyhan UYGUR ONBAŞIOĞLU, who has always guided me and whose support throughout my doctoral studies enabled me to carry out the analysis work.

I am deeply grateful to Prof. Dr. Agustin VALERA-MEDINA and Dr. Syed MASHRUK for providing the experimental data which formed the basis for this study.

I would like to extend my heartfelt thanks to my family, especially my mother and father, who have played the most important role in bringing me to where I am today. They have always provided unwavering material and emotional support and given me strength during challenging times. Their understanding during the periods when I unintentionally had to neglect them due to my studies means a great deal to me. I am truly grateful to have you.

My deepest appreciation goes to my dear wife, Eda BİLGİN GÜLŞAN, who has been my greatest source of motivation and resilience. Her patience, kindness, and unshakeable support have illuminated even the most challenging periods of this process. Without her encouragement and her unwavering presence, completing this work would not have been possible. I am profoundly grateful to walk this path with her.

My son Göktürk Kutay GÜLŞAN; you are the greatest gift I could ever receive. These days you are busy discovering life, while we watch you grow with excitement. You entered the doors of ITU Faculty of Mechanical Engineering when you were only six months old, the same doors I first walked through at the age of eighteen. I hope you will turn this into a beautiful advantage, and may your path and your future always be bright.

December 2025

Mehmet Anıl GÜLŞAN
Mechanical Engineer (M.Sc.)



TABLE OF CONTENTS

	<u>Page</u>
FOREWORD	ix
TABLE OF CONTENTS	xi
ABBREVIATIONS	xiii
SYMBOLS	xv
LIST OF TABLES	xix
LIST OF FIGURES	xxi
SUMMARY	xxv
ÖZET	xxix
1. INTRODUCTION	1
1.1 Literature Review	1
1.1.1 Importance of ammonia as a fuel	2
1.1.2 Combustion properties of ammonia	4
1.1.3 Challenges of ammonia combustion	6
1.1.4 Parametric studies about the ammonia	7
1.1.5 Experimental studies of ammonia combustion	13
1.1.6 CFD Simulation of ammonia combustion	17
1.1.7 Kinetic mechanism studies	31
1.1.8 Burner optimization studies	33
1.2 Purpose and Scope of the Thesis	35
1.3 Unique Aspect	36
1.4 Impact	37
2. COLD FLOW	39
2.1 Experimental Setup	39
2.2 Numerical Model	41
2.3 Governing Equations	43
2.3.1 Conservation of mass	43
2.3.2 Conservation of momentum	43
2.3.3 Turbulence models	44
2.3.3.1 RNG k- ϵ turbulence model	44
2.3.3.2 Realizable k- ϵ turbulence model	44
2.3.3.3 k- ω SST turbulence model	44
2.3.3.4 Spalart-Allmaras turbulence model	44
2.3.3.5 RSM-SSG turbulence model	45
2.3.3.6 RSM-LRR turbulence model	45
2.4 Results	45
2.5 Conclusions	51
3. REACTING FLOW	53
3.1 Experimental Setup	53
3.2 Numerical Model	55
3.3 Governing Equations	60
3.3.1 Conservation of energy	60
3.3.2 Species transport	60

3.4 Results	61
3.5 Conclusions	72
4. OPTIMIZATION	75
4.1 Mathematical Definition of the Optimization Problem.....	75
4.1.1 Objective functions	76
4.1.2 Constraints.....	76
4.2 Optimization Methods	77
4.2.1 Genetic algorithm (GA)	77
4.2.2 Multi-objective particle swarm optimization (MOPSO).....	77
4.2.3 Multi-objective simulated annealing (MOSA).....	78
4.2.4 Non-dominated sorting genetic algorithm (NSGA-II).....	78
4.2.5 Differential evolution (DE)	79
4.3 Normalization.....	80
4.4 Optimization Tool and Coupled Optimization Model.....	81
4.4.1 Dakota optimization tool.....	81
4.4.2 Non-dominated sorting genetic algorithm (NSGA-II).....	81
4.4.3 Coupled optimization model	82
4.5 Parametric CFD Model and Initial Population.....	83
5. RESULTS AND DISCUSSION.....	87
5.1 Initial Population and Generation Results.....	87
5.1.1 Specific heat release	93
5.1.2 NO ₂ emission.....	94
5.1.3 H ₂ mass flow rate	95
5.2 Relationships Between Objectives and Parameters.....	96
5.3 Parametric Study with Inlet Conditions	106
6. CONCLUSIONS AND RECOMMENDATIONS	109
REFERENCES	113
APPENDICES	123
APPENDIX A	125
CURRICULUM VITAE	133

ABBREVIATIONS

3D	: Three Dimensional
AI	: Artificial Intelligence
AFR	: Air-Fuel Ratio
AMR	: Adaptive Mesh Refinement
CAD	: Computer Aided Design
CFD	: Computational Fluid Dynamics
CFL	: Courant Number
CNG	: Compressed Natural Gas
DE	: Differential Evolution
DNS	: Direct Numerical Simulation
DOE	: Design of Experiment
Dxxx	: Design Identifier Used for Individual Optimization Cases
FGM	: Flamelet Generated Manifold
GA	: Genetic Algorithm
GRI	: Gas Research Institute
HVAC	: Heating, Ventilating and Air Conditioning
LDA	: Laser Doppler Anemometry
LES	: Large Eddy Simulation
LPG	: Liquefied Petroleum Gas
MOPSO	: Multi-Objective Particle Swarm Optimization
MOSA	: Multi-Objective Simulated Annealing
NSGA	: Non-Dominated Sorting Genetic Algorithm
NURBS	: Non-uniform Rational B-spline
PIV	: Particle Image Velocimetry
PPM	: Parts Per Million
ppmV	: Parts Per Million by Volume
RANS	: Reynold Averaged Navier-Stokes
RNG	: Renormalization Group
RSM	: Reynolds Stress Model
RSM-LRR	: Reynolds Stress Model - Launder, Reece and Rodi

RSM-SSG : Reynolds Stress Model - Speziale-Sarkar-Gatski
SAGE : Stochastic Acceleration by Gradient Estimation
SST : Shear Stress Transport
TRL : Technology Readiness Level



SYMBOLS

Φ	: Equivalence Ratio [-]
Φ_{global}	: Global Equivalence Ratio [-]
Φ_{ij}	: Pressure-strain correlation term
α	: Optimization Weight [-]
α_{sst}	: Model constant [-]
α_v	: Vane Angle [°]
β, β^*	: Model constants [-]
ρ	: Fluid Density [kg/m ³]
δ_{ij}	: Kronecker Delta
$C_{\varepsilon 1}, C_{\varepsilon 2}$	: Model constants [-]
C_{b1}, C_{w1}	: Model constants [-]
CR	: Confinement Ratio [-]
d	: Distance to the nearest wall
D_{ij}	: Diffusion term of Reynolds stresses
D_m	: Diffusion Coefficient [-]
$D_{t,m}$	: Turbulent Diffusion Coefficient
e	: Specific Internal Energy
ε	: Turbulent kinetic energy dissipation rate
ε_{ij}	: Dissipation tensor of Reynolds stresses
F	: Flow Rate [kg/s]
F_{sst}	: SST blending function
$F(x)$	: Total Objective Function
F_s	: Exhaust Gas Sample Flow Rate
$F_{t,\text{in}}$	: Total inlet flow rate [-]
F_d	: Dilution flow rate [-]
f_1, f_2	: Objective Function
i, j, k	: Cartesian Coordinate Indices
K	: Thermal Conductivity
k	: Turbulent kinetic energy
K_t	: Turbulent Thermal Conductivity

$\dot{m}_{H_2}$	: H ₂ Mass Flow Rate
$\dot{m}_{H_2,ref}$	: Specific H ₂ Mass Flow Rate
$\dot{m}_{fuel}$	: Total Fuel Flow Rate
$\dot{m}_{fuel,ref}$	: Reference Total Fuel Flow Rate
N_v	: Number of Vanes [-]
NO_x	: NO _x formation
$NO_{x, ref}$	: Reference NO _x formation
O1, O2, O3	: Objective [-]
P	: Pressure [Bar]
P1, P2, P3, P4	: Parameter [-]
P_{ij}	: Production term of Reynolds stresses
P_k	: Production term of turbulent kinetic energy
R_{ij}	: Reynolds stress tensor
R_ϵ	: RNG correction term
$\dot{Q}$	: Heat Release [kJ/kg]
$\dot{Q}_{ref}$	: Reference Heat Release [kJ/kg]
$\dot{Q}_{spec}$	: Specific Heat Release [kJ/kg]
$\dot{Q}_{total}$	: Total Heat Release [kJ/kg]
r	: Radius [mm]
S	: Swirl Number [-]
S_e	: Volumetric Heat Release due to Chemical Reactions
S_g	: Geometric Swirl Number [-]
S_{st}	: Mean strain rate magnitude
$\tilde{S}$	: Modified vorticity magnitude
t	: time [s]
T	: Temperature [K]
$T_{Average}$	: Average Temperature [K]
u	: Velocity
U_{in}	: The Mixture Inlet Velocity
μ	: Dynamic Viscosity
μ_t	: Turbulent Viscosity
ν	: Kinematic Viscosity
$\tilde{\nu}$	: Modified Turbulent Viscosity variable
x	: Parameter Vector [-]

X_{NH_3}	: Molar Fraction of NH_3 in the Fuel
X_{NH_3/H_2}	: Volumetric NH_3/H_2 fuel blend ratio [-]
Y_m	: Mass Fraction of Species m
ω	: Specific Dissipation Rate
$\dot{\omega}_m$	: Net Chemical Source Term
σ_k	: Turbulent Prandtl number for k
σ_ε	: Turbulent Prandtl number for ε
σ_ω	: Turbulent Prandtl number for ω
σ_{ij}	: Viscous and turbulent stress tensor
$\sigma_{\omega 2}$	: Model constant [-]





LIST OF TABLES

	<u>Page</u>
Table 1.1 : Combustion properties of NH ₃ , H ₂ and other hydrocarbon fuels [2, 4, 5, 7].	5
Table 1.2 : Swirler specifications [8].	13
Table 1.3 : Experimental and numerical boundary conditions [34].	21
Table 1.4 : Boundary conditions; atmospheric conditions [35].	23
Table 1.5 : Boundary conditions; high pressure, high inlet temperature conditions [35].	23
Table 1.6 : Chemical kinetics model used in the Mikulcic et al. [39].	26
Table 1.7 : Simulated cases [39].	27
Table 1.8 : Inlet boundary conditions [58].	35
Table 2.1 : Turbulence models used in CFD simulations.	42
Table 2.2 : Mesh dependency metrics.	50
Table 3.1 : Simulated cases.	55
Table 3.2 : Compared reaction mechanisms.	59
Table 3.3 : Boundary conditions and parameters.	60
Table 4.1 : Optimization parameters and objectives.	75
Table 4.2 : Comparison of various optimization algorithms.	79
Table 4.3 : Comparison of GA and NSGA-II algorithms.	80
Table 4.4 : Parameters and initial population (parameters in red denote variables).	85
Table 5.1 : Initial population results.	88
Table 5.2 : Initial population results (normalized).	89
Table 5.3 : The first and second generation results.	90
Table 5.4 : The first and second generation results (normalized).	91
Table 5.5 : The third generation results.	92
Table 5.6 : The third generation results (normalized).	93
Table 5.7 : Comparison of base design and optimized design.	102
Table 5.8 : Parametric study results.	106



LIST OF FIGURES

	<u>Page</u>
Figure 1.1 : The amount of ammonia produced around the world [4].	3
Figure 1.2 : The number of publications per year that report novel research studies on ammonia as a fuel that have been published in the Journal Fuel since 2010 [1].	3
Figure 1.3 : Technology Readiness Level (TRL) of main technologies to be used in transportation and power industry with ammonia as a fuel [1].	4
Figure 1.4 : The gravimetric and volumetric densities of hydrogen, ammonia and other fuels based on lower heating values [2].	4
Figure 1.5 : Gravimetric and volumetric H ₂ density of hydrogen carriers [7].	5
Figure 1.6 : Simulated NO _x concentration versus H ₂ mole fraction in NH ₃ /H ₂ blends for stoichiometric mixtures at 1 bar and 298K [2, 16].	8
Figure 1.7 : CO ₂ and NO _x emissions for different ammonia fuel blends [4].	9
Figure 1.8 : Laminar burning velocity of ammonia flame with a function of equivalence ratio at 298 K and 1 atm [1, 5].	9
Figure 1.9 : Laminar burning velocity of ammonia flame with a function of equivalence ratio at various temperature [5].	10
Figure 1.10 : Laminar burning velocity of ammonia flame with a function of initial mixture pressure at $\phi=0.9$, 1 and 1.2 [5].	10
Figure 1.11 : Laminar burning velocity of ammonia flame with a function of equivalence ratio at various oxygen enrichment level [5].	11
Figure 1.12 : Laminar burning velocity of ammonia flame with a function of volumetric hydrogen fraction at 298K [5].	12
Figure 1.13 : Variation of the unstretched laminar burning velocity of pure ammonia versus hydrogen and other hydrocarbon fuels with mixture equivalence ratio at 0.1 MPa [2].	12
Figure 1.14 : Flames stabilized in the swirl burner with cylindrical liners: (a) ammonia/air flame, $\phi=1$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; (b) ammonia/air flame, $\phi=1.2$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; (c) ammonia/air flame, $\phi=1.2$, $h=100\text{mm}$, $U_{in}=3.35\text{ m/s}$; (d) methane/air flame, $\phi=1$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; (e) ammonia/air flame, $\phi=0.8$, $h=200\text{mm}$, $U_{in}=3.14\text{ m/s}$; (f) ammonia/air flame, $\phi=1$, $h=200\text{mm}$, $U_{in}=3.14\text{ m/s}$; (g) ammonia/air flame, $\phi=1.2$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; [8].	14
Figure 1.15 : Flame stability map of ammonia/air premixed flame in the swirl burner [8].	14
Figure 1.16 : (a) Schematic of the burner and (b) flame conditions [9].	15
Figure 1.17 : Predicted flow pattern for flame 5. (a) Contours of mean axial velocity; (b) contours of instantaneous gas temperature. [9].	15
Figure 1.18 : Axial profiles of mean O ₂ and NO _x concentrations and gas temperature for flames [9].	16
Figure 1.19 : Experimental setup [19].	16

Figure 1.20 : Flame temperature along the centerline of the burner at different distances from the burner exit plane for (a) $x_{\text{NH}_3}=0.7$ and (b) $x_{\text{NH}_3}=0.8$ [19].	17
Figure 1.21 : Burner geometry and mesh, boundary conditions [18].	20
Figure 1.22 : (a) Isothermal validation, (b) Comparison with previous experiments [18].	20
Figure 1.23 : Meshed geometry [34].	21
Figure 1.24 : Isothermal results at different axial positions. Experiments (solid, orange line) and numerical (dashed, black line) [34].	22
Figure 1.25 : Emission results. (a) CO (ppm); (b) CO ₂ (%); (c) NH ₃ (ppm) [34].	22
Figure 1.26 : Mesh used for modelling. (Top) Full mesh; (Bottom left) Details of the swirl vanes; (Bottom right) Close-up local mesh refinement [35].	23
Figure 1.27 : Validation using exhaust emissions profiles. Experiments as in [33, 37].	24
Figure 1.28 : Isothermal results. (Left) Experiments from [38]; (Right) numerical analysis (zone of interest is highlighted).	24
Figure 1.29 : (A) Temperature (K); (B) ammonia concentration (mol%); (C) NO concentration (mol%); (D) hydrogen concentration (mol%); (E) hydrogen rate of production (kg/m ³ s). Operating conditions: 101 kPa, 304K [35].	25
Figure 1.30 : (A) Temperature (K); (B) ammonia concentration (mol%); (C) NO concentration (mol%); (D) hydrogen concentration (mol%); (E) hydrogen rate of production (kg/m ³ s). Operating conditions: 900 kPa, 500K inlet temperature, 1800K quartz tube [35].	25
Figure 1.31 : Generic swirl burner at the Gas Turbine Research Centre [40].	26
Figure 1.32 : Computational domain: with swirler (left) and simplifies (right) [39].	26
Figure 1.33 : Comparison of the results in central cross section for $\phi=0.81$: a) temperature field, b) axial velocity field, c) CO ₂ concentration, d) CO molar concentration, e) NO molar concentration, f) O radical concentration, g) OH radical concentration [39].	27
Figure 1.34 : Emission comparison for various equivalence ratios: a) NO, b) CO ₂ , c) O ₂ , d) CO [39].	28
Figure 1.35 : a) Sketch of burner geometry with dimensions in mm; b) Measured blow-out curves for the NH ₃ /H ₂ /N ₂ blend [41].	28
Figure 1.36 : OH PLIF images of flames 1 s before blow-out. The intensity is normalized by the peak value [41].	28
Figure 1.37 : Time-averaged OH chemiluminescence images of flames from 1.1 s to 0.9 s before blow-out. The intensity is normalized by the peak value [41].	29
Figure 1.38 : NO distribution in turbulent non-premixed NH ₃ /air flames in terms of equivalence ratio, ϕ (the fuel and air stream inlet temperatures are 500K and the swirl numbers are 0.69 and 0.68, respectively. Combustor walls are adiabatic) [43].	29
Figure 1.39 : (a) NO; (b) OH; concentration distributions in turbulent premixed NH ₃ /air flames in terms of equivalence ratio and pressure [7].	30
Figure 1.40 : Space and time averaged emissions of NO, x_{NO} , NH ₃ , x_{NH_3} , and H ₂ , x_{H_2} in turbulent premixed NH ₃ /air flames in terms of equivalence ratio and pressure [7].	30
Figure 1.41 : Swirl burner and schematic diagram, respectively [58].	34

Figure 1.42 : Geometrical swirl number 1.5, 1.05 and various divergent angles nozzles, respectively [58].	35
Figure 1.43 : Comparison of the axial velocity of different angles [58].	35
Figure 2.1 : Tangential combustor with measuring techniques and control systems [59].	40
Figure 2.2 : Detailed geometrical view of the burner. Dimensions in meter (m) [62].	40
Figure 2.3 : Surface meshed burner model.	41
Figure 2.4 : Volume mesh of second order k-w SST model.	42
Figure 2.5 : Converting 3D data to 2D plane by using 2.5D method.	43
Figure 2.6 : Isothermal air flow velocity vector maps with axial velocity contours for the unconfined swirl burner [59].	46
Figure 2.7 : Comparison of LDA and first order CFD results: (a) 3mm, (b) 15 mm, (c) 24mm, (d) 30mm, (e) 36mm, (f) 60mm.	47
Figure 2.8 : Comparison of LDA and second order CFD results: (a) 3mm, (b) 15 mm, (c) 24mm, (d) 30mm, (e) 36mm, (f) 60mm.	48
Figure 2.9 : Comparison of the first and second order solver results: (a) 3mm, (b) 15 mm, (c) 24mm, (d) 30mm, (e) 36mm, (f) 60mm.	49
Figure 2.10 : Mesh dependency study at 15mm axial length.	50
Figure 3.1 : Tangential combustor with measuring techniques and control systems [59].	53
Figure 3.2 : Detailed geometrical view of the burner. Dimensions in meter (m) [62].	54
Figure 3.3 : Surface meshed burner model.	56
Figure 3.4 : Adaptive volume mesh of the model.	57
Figure 3.5 : Comparison of velocity profiles at various axial positions. LDA experiments (dashed red line-right side, dashed black line-left side) and numerical (solid orange line) [66].	57
Figure 3.6 : Thermocouple names and locations.	61
Figure 3.7 : Comparison of temperature data at various burner locations.	62
Figure 3.8 : Temperature distributions of simulated cases.	63
Figure 3.9 : OH distribution of experiments.	64
Figure 3.10 : OH distributions of simulated cases (<i>normalized with max 5.0e-4 mole fraction</i>).	65
Figure 3.11 : NH distribution of experiments.	66
Figure 3.12 : NH distributions of simulated cases (<i>normalized with max 3.0e-7 mole fraction</i>).	66
Figure 3.13 : NH ₂ distribution of experiments.	68
Figure 3.14 : NH ₂ distributions of simulated cases (<i>normalized with max 1.0e-6 mole fraction</i>).	68
Figure 3.15 : The comparison of reaction mechanisms with experiments for the exhaust emissions.	69
Figure 3.16 : NO ₂ distributions of simulated cases (<i>normalized with max 1.0e-5 mole fraction</i>).	70
Figure 3.17 : NO distributions of simulated cases (<i>normalized with max 3.0e-3 mole fraction</i>).	71
Figure 3.18 : NH ₃ distributions of simulated cases (<i>normalized with max 1.0e-3 mole fraction</i>).	72
Figure 4.1 : Effect of normalization on the Pareto front.	80
Figure 4.2 : Flow chart of the general genetic algorithms [70].	82

Figure 4.3 : The loosely-coupled or “black-box” interface between Dakota and a user-supplied simulation code [76].	83
Figure 4.4 : Confinement ratio. (a) base model, (b) x2 confinement ratio, (c) x0.5 confinement ratio.	84
Figure 4.5 : Number of vanes. (a) 9 vanes, (b) 6 vanes, (c) 12 vanes.	84
Figure 4.6 : Vane angle. (a) base model, (b) +30° rotated vanes, (c) -15° rotated vanes.	84
Figure 5.1 : Specific heat release of each design.	94
Figure 5.2 : Histogram of specific heat release.	94
Figure 5.3 : Histogram of NO ₂ emission.	95
Figure 5.4 : NO ₂ emission of each design.	95
Figure 5.5 : Histogram of H ₂ mass flow rate.	96
Figure 5.6 : H ₂ mass flow rate of each design.	96
Figure 5.7 : Relationship between O1 and O2.	97
Figure 5.8 : Relationship between O1 and O3.	97
Figure 5.9 : Relationship between O2 and O3.	97
Figure 5.10 : Relationship between O1, O2 and O3.	98
Figure 5.11 : Relationship between P1 and objectives.	99
Figure 5.12 : Relationship between P2 and objectives.	99
Figure 5.13 : Relationship between P3 and objectives.	100
Figure 5.14 : Relationship between P4 and objectives.	100
Figure 5.15 : Comparison of D000 and D052 – axial velocity.	103
Figure 5.16 : Comparison of D000 and D052 – static pressure.	104
Figure 5.17 : Comparison of D000 and D052 – total temperature.	104
Figure 5.18 : Comparison of D000 and D052 – NO ₂ emission.	105

MULTI-OBJECTIVE OPTIMIZATION OF SWIRL BURNER WITH PREMIXED AMMONIA/HYDROGEN FLAME

SUMMARY

In this thesis, the objective is to numerically investigate, validate, and optimize a premixed ammonia-hydrogen swirl burner. The fundamental goal is to establish the necessary design criteria that would allow ammonia, which is gaining prominence in the transition toward sustainable energy resources, to be used in industrial applications in an environmentally friendly, safe, and efficient manner. Although the literature includes numerous studies on the combustion characteristics of ammonia–hydrogen blends, most of these investigations remain either experimentally limited or constrained solely to numerical modeling. This study aims to fill this gap by combining a CFD-based approach, detailed validation with experimental data, and multi-objective optimization within a single unified framework. The originality of the work arises from the integration of CFD, validation, and optimization.

The role of ammonia in global energy strategies has increased significantly in recent years. Particularly in the processes of reducing carbon emissions and establishing the hydrogen economy chain, ammonia is considered a strategic energy carrier due to its transportability, ease of storage, and carbon-free nature. Its existing large-scale production infrastructure and transportation network help overcome many of the storage and logistical challenges associated with hydrogen. For this reason, ammonia has been positioned as an early-stage transition fuel in the hydrogen economy in many countries, playing a critical role in the shift toward carbon-neutral systems. When transported in liquid form, its high hydrogen content per unit volume and ease of storage make it an attractive option for various energy applications, especially industrial heating, boiler systems, and internal combustion engines. While hydrogen requires either cryogenic storage or high-pressure tanks, ammonia can be liquefied at temperatures close to atmospheric pressure, enabling a less costly and safer distribution infrastructure. However, ammonia's slow reaction rate, long ignition delay, high NO_x formation tendency, and unburned ammonia emissions constitute major drawbacks, particularly in pure ammonia flames, where they adversely affect flame stability and environmental performance. Therefore, burner systems that employ ammonia–hydrogen blends must be evaluated in detail with appropriate geometries, suitable mixing ratios, and validated kinetic mechanisms. In particular, NO_x formation is one of the most critical environmental parameters in ammonia-based combustion systems. NO_x is both a strong air pollutant and toxicologically hazardous. In ammonia combustion, NO_x formation intensifies especially in regions with high temperature and excess oxygen. Hence, controlling the flame shape and heat-release profile in ammonia–hydrogen blends is of great importance to meet environmental regulations.

The scope of this study is defined as the development of an integrated numerical approach involving cold-flow validation, reacting-flow analyses, kinetic mechanism comparisons, and multi-objective optimization. This integrated structure provides a unique contribution, as cold-flow validation, chemical mechanism evaluation, and

design optimization—typically treated separately in different studies—are applied together for the first time in the same ammonia–hydrogen swirl burner. All models and evaluations used throughout the study were conducted based on a real-scale industrial swirl burner, thereby increasing the practical relevance of the results.

In the first stage of the thesis, a laboratory-scale swirl burner system characterized experimentally in the literature was modeled numerically, aiming to validate the numerical results using cold-flow experiments. For this purpose, LDA measurements available in the literature and obtained at laboratory scale were used. The formation, location, and size of the central recirculation zone—one of the most important parameters determining flame stability in swirl burners—were examined using both experimental data and CFD solutions. The numerical analyses were performed using Converge CFD[®]. In the cold-flow CFD analyses, six different turbulence models were compared based on LDA measurements, and the second-order $k-\omega$ SST-based RANS approach was found to best represent the experimental data. The selected turbulence model accurately predicted axial velocity profiles near the center and successfully captured turbulence characteristics away from the center. Moreover, by applying an AMR strategy, the mesh was refined only in regions with complex flow features, improving accuracy while reducing computational cost. The results demonstrated that the cold-flow model provides a reliable foundation for the reacting-flow solutions.

In the reacting-flow analyses, three different reaction mechanisms—Duynslaegher, Nakamura, and Stagni—were examined based on temperature profiles and emission values to validate the model. Comparisons of these kinetic mechanisms were made alongside experimental literature. Among them, the Nakamura mechanism exhibited the highest agreement with experimental data in terms of both temperature distribution and product species profiles. Additionally, it produced more realistic predictions of NO_x compared to the Duynslaegher mechanism and yielded more consistent NH_3 slip predictions, particularly at low H_2 fractions. Therefore, the Nakamura mechanism was selected for the validated combustion analysis models used in the optimization phase. In summary, the validation of the optimization model was assessed under both cold-flow conditions (velocity comparison with LDA data) and reacting-flow conditions (comparison of flame location and temperature distribution), and good agreement with experimental measurements was achieved in both cases.

A multi-objective optimization model was developed to systematically explore the design space of the swirl burner using the validated CFD model. Different multi-objective optimization algorithms commonly used in the literature were evaluated. Considering the limited number of analyses, the high cost of validated CFD computations, and physical requirements, the NSGA-II algorithm was selected due to its advantages such as rapid convergence, balanced solution distribution, and low computational cost. Four design parameters were considered in the optimization: confinement ratio, vane number, vane angle, and fuel blend ratio. The optimization was based on three objective functions: increasing specific heat release per unit mass of fuel, reducing NO_2 formation, and minimizing hydrogen consumption. Since these three objectives conflict with one another, the best design is not represented by a single solution but rather by a family of solutions located along the Pareto front. The initial population consisted of 14 randomly selected individuals, each defined within the minimum and maximum allowable parameter limits. Evolutionary processes including crossover, mutation, and ranking were then applied. Due to limitations on the number of analyses, the population size and number of iterations were carefully balanced. In the fuel-mixing optimization, the equivalence ratio and total thermal power were kept

constant, while the volumetric ratio of ammonia–hydrogen was varied to evaluate combustion characteristics. With the integration of Converge CFD[®] and Dakota, CFD analyses for all candidate individuals were executed automatically. All individuals were normalized and compared, and the resulting Pareto fronts clearly illustrated the relationships between design variables and objective functions. The results showed that in some regions of the design space, increasing heat-release rate inevitably increased NO₂ levels, whereas in other regions, obtaining low NO₂ required higher hydrogen consumption. This clearly demonstrates that achieving a high-efficiency, low-emission, and low-hydrogen-consuming design in ammonia–hydrogen burners inherently requires multi-objective trade-offs.

Because the design parameters addressed in the optimization directly influence the physical behavior of the burner, the manner in which each parameter shaped the design space was also evaluated. The confinement ratio plays a critical role in flame stability and NO₂ formation because it determines swirl intensity and the size of the recirculation zone. Increasing the confinement ratio enhances the mass of hot products recirculated toward the burner center, raising temperatures in the flame root and influencing both specific heat release and NO₂ formation. The vane number and vane angle are fundamental geometric parameters that determine swirl strength and mixing quality. Particularly at high vane angles, an increase in swirl frequency promotes mixture homogenization but also broadens the reaction zone, which in turn affects heat release and NO₂ emissions.

The role of the fuel blend ratio in the optimization is also one of the significant findings of the study. Increasing the hydrogen fraction in ammonia–hydrogen blends typically elevates reaction rates and stabilizes combustion. However, this also increases hydrogen consumption, posing disadvantages from economic and sustainability standpoints. Therefore, optimizing the hydrogen fraction is essential not only for performance but also for operational cost. The optimization results revealed that a performance-oriented approach and an approach targeting reduced hydrogen consumption correspond to substantially different regions of the design space. Thus, the presence of a Pareto front provides flexibility to select a solution based on user-defined priorities.

According to the optimization results, the best physically feasible solution was identified as D052. It offers high performance in terms of specific heat release while keeping NO₂ emissions at acceptable levels and ensuring reasonable hydrogen consumption.

In the final part, the effects of boundary conditions such as inlet temperature and inlet pressure on D052 were evaluated. These analyses are critical for understanding how flame behavior changes under varying operating conditions in industrial systems. Increasing inlet temperature strengthened flame stability, expanded the reaction zone, and elevated heat release. In contrast, increasing inlet pressure significantly increased NO₂ formation, indicating that ammonia–hydrogen blends in high-pressure systems require more careful control. The parametric studies confirmed that the low-emission and stable characteristics of D052 make it a suitable reference geometry for such analyses. The results demonstrate that system design must carefully consider not only geometry and fuel composition but also boundary conditions. The observation that NO_x formation increases beyond a certain inlet temperature suggests the need for determining an optimal inlet temperature in future studies.

The influence of inlet pressure exhibited an even more pronounced chemical sensitivity than temperature. Pressure increase accelerated NO_2 formation mechanisms, as higher pressure increases molecular collision rates and elevates reaction rates of intermediate species that convert to NO_x . Therefore, even mixtures with nominally low hydrogen content tend to produce substantial NO_2 under high-pressure conditions. This finding indicates that ammonia–hydrogen blends must be optimized particularly carefully for systems operating at elevated pressures. Moreover, increasing pressure narrowed the reaction zone, significantly altering turbulence–chemistry interactions. The accurate numerical capture of this physical behavior demonstrates the reliability of the combustion model under high-pressure conditions.

Another important outcome of these analyses is the observation that operating conditions are as critical as geometric optimization. Focusing solely on geometry or fuel composition during design is insufficient; inlet pressure, inlet temperature, and the overall operating window must also be optimized simultaneously to achieve minimum NO_2 , high stability, and high efficiency. Therefore, future industrial applications of ammonia–hydrogen blends may require adaptive control strategies and feedback-based combustion control systems tailored to operating conditions.

In conclusion, this thesis presents a unique numerical framework that holistically examines the combustion behavior of ammonia–hydrogen blends in swirl burners. Cold-flow validation showed strong agreement with experimental data; reacting-flow analyses demonstrated accurate prediction of temperature profiles; and multi-objective optimization generated new design recommendations for various applications. The insights provided by the model may contribute to the design of future ammonia-fueled systems that are more efficient, lower in emissions, and safer. Controlling NO_2 formation is a critical requirement for sustainable combustion technologies, and the findings of this study provide an important foundation in this regard. Overall, the proposed approach constitutes a concrete step toward integrating ammonia into low-carbon energy systems, paving the way for high-performance and environmentally friendly combustion solutions through appropriate blending strategies, balanced geometry, and carefully managed operational conditions.

This study also highlights the need for further development of kinetic mechanisms used for ammonia–hydrogen burners, as well as the limitations of existing RANS-based turbulence models, which may be insufficient in certain cases. Advanced turbulence models may yield more accurate results. In the future, the use of AI-assisted optimization methods may allow faster evaluation of complex mechanisms and more efficient exploration of intricate design spaces. Moreover, the application of LES, DNS, or hybrid models may contribute to a deeper understanding of turbulence–chemistry interactions. In the long term, the development of high-fidelity numerical models may accelerate the industrial adoption of ammonia-based combustion systems and significantly contribute to carbon reduction in the energy sector.

ÖN KARIŞIMLI AMONYAK/HİDROJEN ALEVİNE SAHİP GİRDAPLI YAKICININ ÇOK HEDEFLİ OPTİMİZASYONU

ÖZET

Bu tez çalışmasında, karbon içermeyen bir enerji taşıyıcısı olarak öne çıkan amonyağın hidrojenle karıştırılarak yakıldığı bir ön karışimli girdaplı yakıcının sayısal olarak incelenmesi, doğrulanması ve optimize edilmesi amaçlanmıştır. Temel hedef; sürdürülebilir enerji kaynaklarına geçiş sürecinde öne çıkan amonyağın, endüstriyel uygulamalarda çevre dostu, güvenli ve verimli şekilde kullanılabilmesi için gerekli tasarım kriterlerini ortaya koymaktır. Literatürde amonyak-hidrojen karışımlarının yanma özelliklerine dair birçok çalışma bulunmaktadır. Ancak bu çalışmaların çoğu ya yalnızca deneysel sınırlarda kalmış ya da sayısal modelleme ile kısıtlanmıştır. Bu çalışma, HAD temelli yaklaşımı, deneysel verilerle detaylı validasyonu ve çok hedefli optimizasyonu aynı çatı altında birleştirerek literatürdeki boşluğu doldurmayı hedeflemektedir. Çalışmanın özgünlüğü HAD, validasyon ve optimizasyon entegrasyonu ile ortaya konulmaktadır.

Amonyağın küresel enerji stratejilerindeki rolü son yıllarda belirgin şekilde artmıştır. Özellikle karbon emisyonlarının azaltılması ve hidrojen ekonomi zincirinin oluşturulması aşamalarında amonyak taşınabilirlik, depolama kolaylığı ve karbon içermemesi nedeniyle stratejik bir enerji taşıyıcısı olarak değerlendirilmektedir. Amonyağın mevcut ticari ölçeğe ulaşmış üretim altyapısı ve taşımacılık sistemleri, hidrojenin karşılaştığı depolama ve lojistik engellerin önemli bir kısmını ortadan kaldırmaktadır. Bu nedenle birçok ülkede amonyak, hidrojen ekonomisinin erken dönem geçiş yakıtı olarak konumlandırılmakta ve karbon-nötr sistemlere geçişte kritik bir rol üstlenmektedir. Likit halde taşındığında birim hacimde yüksek hidrojen içeriği sunması ve kolay depolanabilir olması, onu özellikle endüstriyel ısıtma, kazan sistemleri ve içten yanmalı motorlar gibi çeşitli enerji uygulamaları için çekici bir seçenek haline getirmektedir. Hidrojenin kriyojenik koşullarda depolanması veya yüksek basınçlı tanklar gerektirmesi önemli bir mühendislik zorluğu iken, amonyak atmosfer basıncına yakın düşük sıcaklıklarda sıvılaştırılabildiği için daha düşük maliyetli ve daha güvenli bir dağıtım altyapısı sunmaktadır. Bununla birlikte, amonyağın düşük reaksiyon hızı, uzun tutuşma gecikmesi, yüksek NO_x oluşumu ve yanmamış amonyak salınımı gibi dezavantajları, özellikle saf amonyak alevlerinde kararlılığı ve çevresel performansı olumsuz etkileyen önemli sınırlamalardır. Bu nedenle, amonyak-hidrojen karışımlarının kullanıldığı yakıcı sistemlerinin uygun geometriler, uygun karışım oranları ve doğrulanmış kinetik mekanizmalar ile detaylı olarak değerlendirilmesi gerekmektedir. Özellikle NO_x oluşumu, amonyak temelli yanma sistemlerinde en kritik çevresel parametrelerden biridir. NO_x hem güçlü bir hava kirleticidir hem de toksikolojik açıdan tehlikeli bir bileşiktir. Amonyak yakıldığında özellikle yüksek sıcaklık ve oksijen fazlalığı içeren bölgelerde NO_x oluşumunu hızlanmaktadır. Bu nedenle amonyak-hidrojen karışımlarında hem alev şeklinin hem de ısı salınımının kontrol edilmesi, çevresel regülasyonların karşılanması açısından büyük önem taşımaktadır.

Bu çalışmanın kapsamı, soğuk akış doğrulaması, reaksiyonlu akış analizleri, kinetik mekanizma karşılaştırmaları ve çok amaçlı optimizasyon süreçlerini içeren bütünlük bir sayısal yaklaşımın geliştirilmesi olarak belirlenmiştir. Bu bütünlük yapı, literatürde farklı çalışmalarda ayrı ayrı ele alınan akış doğrulaması, kimyasal mekanizma değerlendirmesi ve tasarım optimizasyonunun ilk kez aynı amonyak-hidrojen girdaplı yakıcısında birlikte uygulanması açısından özgün bir katkı sunmaktadır. Çalışma boyunca kullanılan tüm modeller ve değerlendirmeler, gerçek ölçekli endüstriyel bir girdaplı yakıcı temel alınarak gerçekleştirilmiş olup sonuçların uygulamaya yönelik geçerliliği artırılmıştır.

Tezin ilk aşamasında, literatürde deneysel olarak karakterize edilmiş laboratuvar tipi bir girdaplı yakıcı sistemi sayısal olarak modellenmiş; soğuk akış deneyleri ile sayısal sonuçların doğrulanması hedeflenmiştir. Bu amaçla, halihazırda literatürde de bulunan ve laboratuvar ölçeğinde gerçekleştirilmiş LDA ölçümleri kullanılmıştır. Girdaplı yakıcılarda alev kararlılığını belirleyen en önemli parametrelerden biri olan merkezi resirkülasyon bölgesinin oluşumu, konumu ve büyüklüğü hem deneysel ölçümlerle hem de HAD çözümleri ile incelenmiştir. Sayısal analizler Converge CFD® yazılımı kullanılarak gerçekleştirilmiştir. Soğuk akış HAD analizlerinde, LDA ölçümleri temel alınarak altı farklı türbülans modeli karşılaştırılmış ve ikinci mertebeden k- ω SST tabanlı RANS yaklaşımının deneysel veriyi en iyi şekilde temsil ettiği görülmüştür. Seçilen türbülans modeli, özellikle merkezdeki eksenel hız profillerini doğru tahmin etmekte ve merkez dışındaki türbülans etkilerini başarılı şekilde yansıtmaktadır. Ayrıca, AMR stratejisi kullanılarak çözüm bölgesinde yalnızca akışın karmaşık olduğu bölgelerde çözüm ağı detaylandırılmış, böylece hem çözüm doğruluğu artırılmış hem de hesaplama maliyeti optimize edilmiştir. Elde edilen sonuçlar, soğuk akış modelinin reaksiyonlu çözümler için güvenilir bir temel oluşturduğunu göstermiştir.

Reaksiyonlu akış analizlerinde, modelin validasyonunu gerçekleştirmek için, sıcaklık profilleri ve emisyon değerleri referans alınarak Duynslaegher, Nakamura ve Stagni'ye ait üç farklı reaksiyon mekanizması incelenmiştir. Üç farklı kinetik mekanizma test edilmiş ve sonuçlar deneysel literatür ile birlikte değerlendirilmiştir. Karşılaştırmalar sonucunda, Nakamura mekanizması hem sıcaklık dağılımı hem de yanma sonucunda açığa çıkan ürünlerin dağılımı açısından deneysel verilerle en yüksek uyumu sağlamıştır. Ayrıca NO_x tahminlerinde Duynslaegher mekanizmasına kıyasla daha gerçekçi sonuçlar üretmiş, NH₃ slip oranlarının tahmininde ise özellikle düşük H₂ oranlarında daha tutarlı değerler elde edilmiştir. Bu nedenle optimizasyon çalışmasındaki valide yanma analizi modellerinde Nakamura mekanizmasının kullanılması tercih edilmiştir. Özetle optimizasyon modelinin validasyonu hem soğuk akış koşullarında (LDA verileri ile hız karşılaştırması) hem de reaksiyonlu akış koşullarında (alev konumu ve sıcaklık dağılımı karşılaştırması) incelenmiş; her iki durumda da deneysel verilerle iyi uyum sağlandığı görülmüştür.

Validasyonu sağlanmış HAD modeli ile girdaplı yakıcının tasarım uzayını sistematik olarak araştırabilmek amacıyla çok amaçlı optimizasyon modeli geliştirilmiştir. Optimizasyon sürecinde literatürde yaygın olarak kullanılan farklı çok amaçlı optimizasyon algoritmaları değerlendirilmiştir. Ancak sınırlı analiz imkanı, doğrulanmış HAD çalışmalarının yüksek maliyeti ve fiziksel gereklilikler dikkate alındığında; hızlı yakınsama, dengeli çözüm dağılımı ve düşük hesaplama maliyeti gibi avantajları nedeniyle NSGA-II algoritması tercih edilmiştir. Optimizasyon sürecinde dört tasarım parametresi esas alınmıştır: daralma oranı (confinement ratio), kanat sayısı, kanat açısı ve yakıt karışım oranı. Optimizasyon üç farklı amaç

fonksiyonu üzerine kurulmuştur: birim kütle yakıt başına düşen özel ısı salınımının artırılması, NO₂ oluşumunun azaltılması ve hidrojen tüketiminin minimize edilmesi. Bu üç hedef birbirleriyle çelişkili olduğundan, en iyi çözümün tek bir tasarım değil, Pareto eğrisi üzerinde yer alan bir çözüm ailesi şeklinde ifade edilmiştir. Başlangıç popülasyonu, incelenecek parametreleri minimum ve maksimum değer aralıklarında kapsayan, rastgele seçilmiş 14 farklı bireyden oluşturulmuştur. Ardından çaprazlama, mutasyon ve sıralama işlemleriyle evrimsel süreç yürütülmüştür. Analiz sayısındaki kısıtlar nedeniyle popülasyon boyutu ve iterasyon sayısı dikkatle dengelenmiştir. Yakıt karışımı optimizasyonunda eşdeğerlik oranı ve toplam termal güç sabit tutulmuş, amonyak-hidrojen hacimsel oranı değiştirilerek yanma karakteristikleri değerlendirilmiştir. Converge CFD® ve Dakota yazılımlarının entegrasyonu sayesinde her aday bireyin HAD analizi otomatik olarak gerçekleştirilmiştir. Tüm bireyler normalize edilerek karşılaştırılmış ve elde edilen Pareto eğrileri tasarım değişkenleri ile hedef fonksiyonlar arasındaki ilişkileri açıkça göstermiştir. Elde edilen sonuçlar, tasarım uzayının bazı bölgelerinde ısı salınımının artırılmasının NO₂ oluşumunu kaçınılmaz olarak yükselttiğini; bazı bölgelerde ise düşük NO₂ elde edilebilmesi için hidrojen tüketiminin arttığını ortaya koymuştur. Bu durum, amonyak-hidrojen yakıcılar da yüksek verimli, düşük emisyonlu ve düşük hidrojen tüketimli bir tasarım elde etmenin doğası gereği çok amaçlı bir dengeleme gerektirdiğini açıkça göstermektedir.

Optimizasyonda ele alınan tasarım parametreleri yakıcının fiziksel davranışı üzerinde doğrudan etkili olduğundan, her bir değişkenin tasarım uzayını nasıl şekillendirdiği ayrıca değerlendirilmiştir. Daralma oranı (confinement ratio), özellikle girdap yoğunluğunu ve resirkülasyon bölgesinin büyüklüğünü belirlediği için alev stabilitesi ve NO₂ oluşumu üzerinde kritik rol oynamaktadır. Daralma oranının artması, akışın merkezine geri dönen sıcak ürün miktarını artırarak alev kökünde daha yüksek sıcaklıklar oluşturmakta; bu durum spesifik ısı salınımını ve NO₂ oluşumunu etkileyebilmektedir. Kanat sayısı ve kanat açısı ise girdap yoğunluğunu ve karışım kalitesini belirleyen temel geometrik parametrelerdir. Özellikle yüksek kanat açılarında girdap sayısının artması, karışımın homojenleşmesini kolaylaştırırken aynı zamanda reaksiyon zonunun daha geniş bir alana yayılmasına sebep olabilmektedir. Bu etki ısı salınımını ve NO₂ miktarını değiştiren bir mekanizma olarak da ortaya çıkmaktadır.

Yakıt karışım oranının optimizasyon sürecindeki rolü de çalışmanın önemli bulgularından biridir. Amonyak-hidrojen karışımlarında hidrojen oranının artırılması genellikle reaksiyon hızlarını yükseltmekte ve yanmayı kararlı hale getirmektedir. Ancak bu durum hidrojen tüketimini artırarak ekonomik ve sürdürülebilirlik açısından dezavantaj yaratabilmektedir. Bu nedenle hidrojen oranının optimize edilmesi, yalnızca performans açısından değil, aynı zamanda sistemin operasyonel maliyeti açısından da önem taşımaktadır. Optimizasyon bulguları, yalnızca performans odaklı bir yaklaşım ile hidrojen tüketiminin azaltılmasına yönelik bir yaklaşımın tasarım uzayında oldukça farklı bölgeleri işaret ettiğini göstermiştir. Bu nedenle Pareto front elde edilmesi, hedef önceliklerine göre seçim yapma özgürlüğü sağlamaktadır.

Optimizasyon sonuçlarına göre fiziksel olarak uygulanabilir en iyi çözüm D052 olarak belirlenmiştir. D052, spesifik ısı salınımı açısından yüksek performans sunarken NO₂ oluşumunu da kabul edilebilir seviyelerde tutmakta ve makul düzeyde hidrojen tüketimi sağlamaktadır. Çalışmanın sonraki adımlarında gerçekleştirilen sıcaklık ve basınç parametre incelemeleri de bu tasarım üzerinden yürütülmüştür.

Son kısımda giriş sıcaklığı ve giriş basıncı gibi sınır koşullarının D052 üzerindeki etkileri değerlendirilmiştir. Bu analizler endüstriyel sistemlerde değişken sınır koşulları altında alev davranışının nasıl değiştiğini anlamak açısından kritiktir. Giriş sıcaklığının artırılması alev kararlılığını güçlendirmiş, reaksiyon bölgesini genişletmiş ve ısı salınımını yükseltmiştir. Buna karşın giriş basıncının artırılması NO₂ oluşumunu belirgin şekilde artırmış; bu durum yüksek basınçlı sistemlerde amonyak-hidrojen karışımlarının daha dikkatli kontrol edilmesi gerektiğini göstermiştir. Ayrıca bu parametre çalışmalarında seçilen D052 geometrisinin düşük emisyonlu ve kararlı yapısının bu tür analizler için uygun bir temel oluşturduğu bir kez daha doğrulanmıştır. Elde edilen sonuçlar, sistem tasarımı sırasında yalnızca geometri ve yakıt değil, sınır koşullarının da dikkatle kontrol edilmesi gerektiğini ortaya koymaktadır. Sıcaklık artışının belli bir değerden sonra NO_x oluşumunu arttırması gelecek çalışmalarda optimum giriş sıcaklığının belirlenmesi gerektiğini göstermiştir.

Giriş basıncının etkisi ise sıcaklık parametresinden daha belirgin bir kimyasal hassasiyet göstermiştir. Basınç artışı özellikle NO₂ oluşum mekanizmalarını hızlandırmış; çünkü basınç arttıkça moleküller arası çarpışma sıklığı artmakta ve NO_x'e dönüşen ara türlerin reaksiyon hızları yükselmektedir. Bu nedenle yüksek basınçlı sistemlerde nominal olarak düşük hidrojen içeren karışımlar bile belirgin düzeyde NO₂ üretme eğilimindedir. Bu bulgu, özellikle yüksek basınçta çalışan ekipmanlarda amonyak-hidrojen karışımlarının dikkatle optimize edilmesi gerektiğini göstermektedir. Ayrıca basınç artışı, reaksiyon zonunun daha dar bir alanda oluşmasına neden olmuş ve bu durum türbülans-kimya etkileşimlerini önemli ölçüde değiştirmiştir. Bu fiziksel davranışın sayısal sonuçlarla tutarlı şekilde yakalanması, kullanılan yanma modelinin yüksek basınç koşullarındaki güvenilirliğini de ortaya koymuştur.

Bu analizlerin bir diğer önemli çıktısı, işletme koşullarının geometrik optimizasyon kadar kritik olduğunun görülmesidir. Tasarım sürecinin yalnızca geometri veya yakıt karışımına odaklanması yeterli değildir; giriş basıncı, sıcaklığı ve genel işletme penceresi de minimum NO₂, yüksek kararlılık ve yüksek verim için mutlaka eş zamanlı optimize edilmelidir. Bu nedenle amonyak-hidrojen karışımlarının gelecekteki endüstriyel uygulamalarında adaptif kontrol stratejilerinin ve işlem koşuluna bağlı çalışan geri beslemeli yanma kontrol sistemlerinin gerekli olabileceği öngörülmektedir.

Sonuç olarak bu tez amonyak-hidrojen karışımlarının girdaplı yakıcılardaki yanma davranışını bütünsel bir şekilde ele alan özgün bir sayısal çerçeve sunmaktadır. Soğuk akış doğrulaması, deneysel veriler ile yüksek uyum göstermiş; reaksiyonlu akış analizleri sıcaklık profilinin doğru temsil edildiğini ortaya koymuş; çok amaçlı optimizasyon ise farklı uygulamalara yönelik yeni tasarım önerileri sunmuştur. Modelin sağladığı bilgiler, gelecekteki amonyak yakıtlı sistemlerin daha verimli, daha düşük emisyonlu ve daha güvenli şekilde tasarlanmasına katkıda bulunabilir. Özellikle NO₂ oluşumunun kontrol edilebilmesi, sürdürülebilir yanma teknolojileri açısından kritik bir gereklilik olup, bu çalışmada elde edilen bulgular bu konuda önemli bir zemin sunmaktadır. Toplamda ortaya konan yaklaşım, amonyakın düşük karbonlu enerji sistemlerine entegrasyonunda somut bir adım olup; uygun karışım, dengeli geometri ve dikkatli işletme stratejileriyle yüksek performanslı, çevre dostu yanma çözümlerine giden yolu açmaktadır.

Bu çalışma ayrıca amonyak-hidrojen yakıcıları için kullanılan kinetik mekanizmaların geliştirilmesi gerektiğini, mevcut RANS tabanlı türbülans modellerinin bazı

durumlarda yetersiz kalabileceğini ve ileri seviye türbülans modellerinin daha doğru sonuçlar sağlayabileceğini göstermiştir. Gelecekte yapay zeka destekli optimizasyon yöntemlerinin kullanımı, kompleks mekanizmaların daha hızlı çözülmesine ve karmaşık tasarım uzaylarının daha verimli şekilde araştırılmasına olanak sağlayabilir. Ayrıca LES, DNS veya hibrit modellerin uygulanması, türbülans-kimya etkileşimlerinin daha ayrıntılı incelenmesine katkıda bulunacaktır. Uzun vadede geliştirilecek yüksek doğruluklu sayısal modeller, amonyak temelli yanma sistemlerinin endüstriyel ölçekte yaygınlaşmasını hızlandırabilir ve enerji sektöründe karbon azaltımına önemli bir katkı sağlayabilir.



1. INTRODUCTION

This study presents the multi-objective optimization of a swirl burner and effects of various inlet conditions on combustion performance of $\text{NH}_3/\text{H}_2/\text{N}_2/\text{O}_2$ fuel blends using CFD techniques. Ammonia studies accelerate nowadays, but there is still a gap about the optimization of ammonia burners. In this thesis it is aimed to find a pathway to optimize current burners as an efficient ammonia burner by changing the geometrical features. The combustion performance, emissions and flame characteristics were investigated for different fuel blends and inlet conditions. An efficient burner geometry and suitable flame were obtained with optimizations. By using the techniques in this thesis; other burners those already in use can be transformed to a desired form for $\text{NH}_3/\text{H}_2/\text{N}_2/\text{O}_2$ fuel blends.

1.1 Literature Review

Combustion always plays a crucial role in scientific research due to its complex and diverse nature. In recent years, the global trend towards decarbonization has accelerated interest in carbon-free combustion technologies. Additionally, the increasing demand for energy has led researchers to find alternative energy sources beyond hydrocarbons. Among these, ammonia has emerged as a promising carbon-free fuel due to its favorable thermo-chemical properties and well-established supply chain infrastructure. While extensive experimental research has been conducted on ammonia combustion, investigating all relevant parameters remains challenging due to the need for advanced measurement technologies. Meanwhile, improvements in computational power have significantly enhanced the capabilities of numerical simulations.

In this section, the previous literature studies about ammonia and ammonia blends were summarized. The importance of ammonia and its improving popularity were presented in the first section. Combustion properties of ammonia was explained and compared with the hydrocarbon fuels in the second section. The challenges and disadvantages of the ammonia use was investigated in the third section. Parametric

studies were listed in the fourth section. The experimental studies about the ammonia combustion was summarized in the fifth part. At the next step; the CFD studies are presented in the section six. Finally, the burner optimization studies are explained in the last section.

1.1.1 Importance of ammonia as a fuel

Ammonia can be a key solution to reduce the carbon emissions by changing the hydrocarbon combustion systems into hydrogen ones. Although the pure H_2 is the desired fuel on the way of zero-emissions, there are several technical difficulties on the applications. Bigger chemical storage will be required for many applications due to the extremely low volumetric energy density of pure H_2 . The safety and infrastructure issues associated with its distribution on a global scale are another problem [1]. Utilizing ammonia as a fuel directly, partly decomposed, or blended with other fuels, have many remarkable benefits to facilitate the decarbonization of the energy sector and promote the market penetration of hydrogen [2]. At this point, ammonia steps forward as an energy vector with the carbon-free molecular structure (NH_3) and its several advantages compared to the hydrogen:

- It can easily be produced from conventional or renewable resources.
- It is cost-effective and economically feasible for applications [1-4].
- It is a potential hydrogen storage and carrier [1-4].
- Transportation and distribution of ammonia is much safer compared to hydrogen [1].
- When liquefied, it contains approximately 48% more hydrogen by volume.
- It can be easily detectable with its distinctive smell when any leakage occurs.
- It can be utilized for a wide range of applications as a fuel, working fluid, refrigerant, hydrogen carrier, fertilizer, feedstock, chemical, cleaning agent, nitric acid, explosive production and many more [4-5].
- A strong fuel candidate for internal combustion engines, power generators, and burners. The performance of ammonia can be comparable with conventional fuels [5]. Modifications needed for such engines are relatively small also.

The production volume of ammonia rises exponentially due to its increasing usage and the realization of its potential as a clean fuel (Figure 1.1) [4]. It will play an important role in the future energy economy [1].

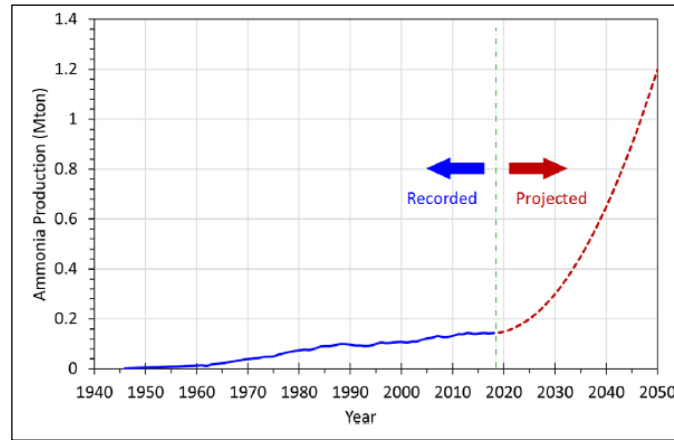


Figure 1.1 : The amount of ammonia produced around the world [4].

In recent years, the number of scientific publications increase with the popularity of zero-emission combustion strategies. Change of the number of publications can be seen in Figure 1.2.

Technology readiness level (TRL) is a method for measuring the maturity level of technologies [6]. There are nine different levels, starting from the lowest (TRL 1) to the highest (TRL 9). Based on that, the importance of ammonia as a fuel for naval transportation can be seen in Figure 1.3, which is mainly due to the technologies developed by Mann Energy Solutions and in particular the dual fuel naval engine designed to be fueled with “green” ammonia. On the other hand, alkaline fuel cells and solid oxide fuel cells running on ammonia have a TRL between 3 and 4 [1].

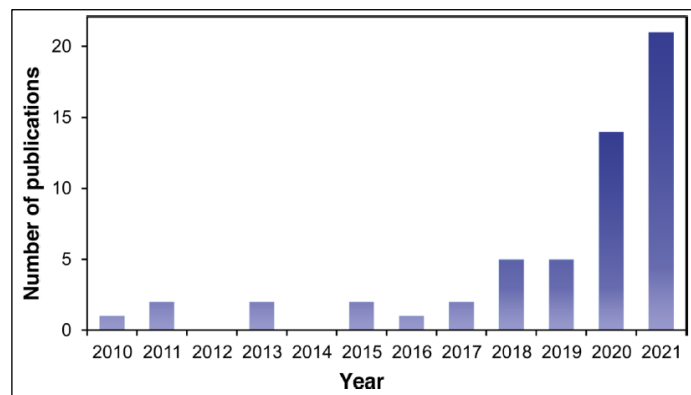


Figure 1.2 : The number of publications per year that report novel research studies on ammonia as a fuel that have been published in the Journal Fuel since 2010 [1].

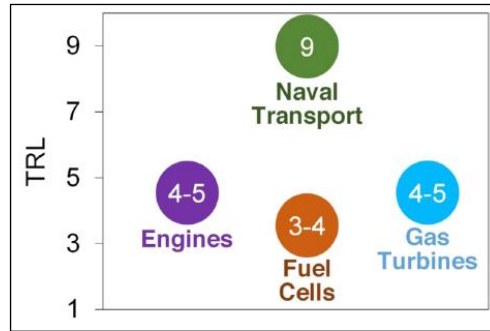


Figure 1.3 : Technology Readiness Level (TRL) of main technologies to be used in transportation and power industry with ammonia as a fuel [1].

1.1.2 Combustion properties of ammonia

Some characteristics of ammonia and the common fuels those are used in many applications can be seen in Table 1.1. Despite the fuel and energy densities of ammonia are lower than gasoline, diesel and LPG, the fuel density of ammonia is three times higher than CNG and the energy density is also much higher than CNG. Ammonia exhibits higher minimum ignition energy than gasoline, which can be improved through some methods like co-firing with hydrogen. The lower heating value and the maximum laminar burning velocity of ammonia-air flame are very low compared to the typical hydrocarbon fuels. The radiation properties of ammonia flame are low relative to the hydrocarbon flames due to the absence of CO_2 in the ammonia combustion products [2, 4, 5, 7].

Figure 1.4 shows a comparison of energy densities of a variety of fuels. The volumetric energy density of liquid ammonia is higher than that of liquid hydrogen, which is one of the properties that make it attractive for energy storage and transport [7].

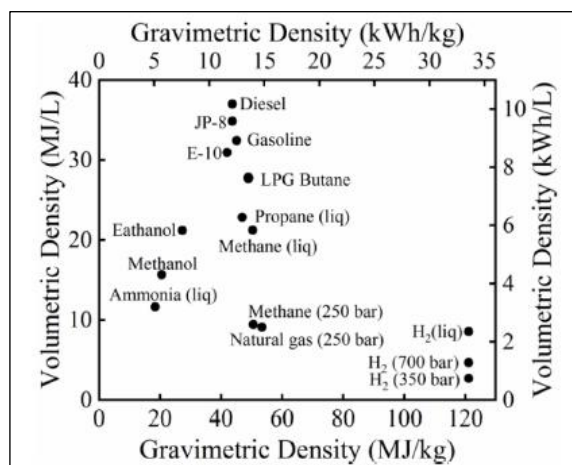


Figure 1.4 : The gravimetric and volumetric densities of hydrogen, ammonia and other fuels based on lower heating values [2].

Table 1.1 : Combustion properties of NH₃, H₂ and other hydrocarbon fuels [2, 4, 5, 7].

Properties	Units	Gasoline	Diesel	LPG	CNG	Gaseous Hydrogen	Liquid Hydrogen	Ammonia
Formula		C ₈ H ₁₈	C ₁₂ H ₂₃	C ₃ H ₈	CH ₄	H ₂	H ₂	NH ₃
Lower Heating Value	MJ/kg	44.5	43.5	46.4	50	120.1	120.1	18.8
Latent Heat of Vaporization	MJ/kg	0.0718	0.0478	0.0444	0.1048	0	N/A	1.369
Flammability Limits, Gas in Air	Vol. %	1.4-7.6	0.6-5.5	1.81-8.86	5.0-15.0	4-75	4-75	16.25
Flame Speed	m/s	0.58	0.87	0.83	8.45	3.51	3.51	0.15
Maximum Laminar Burning Velocity	m/s	N/A	N/A	0.43	0.37	N/A	2.91	0.07
Octane		90-98	N/A	112	107	>130	>130	110
Fuel Density	kg/m ³	698.3	838.8	1898	187.2	17.5	71.1	602.8
Energy Density	MJ/m ³	31074	36403	86487	7132	2101	8539	11333
Storage Method		Liquid	Liquid	Comp. liquid	Comp. gas	Comp. gas	Comp. liquid	Comp. liquid
Storage Pressure	kPa	101.3	101.3	850	24821	24821	102	1030
Condensation Pressure at 25°C	kPa	N/A	N/A	952	N/A	N/A	N/A	1003
Storage Temperature	°C	25	25	25	25	25	-253	25
Auto-Ignition Temperature	°C	300	230	466	540	571	571	651
Flash Point	°C	-42.7	73.8	-87.7	-184.4	N/A	N/A	-33.4
Boiling Temperature at 1 atm	°C	N/A	N/A	-42.1	-161	N/A	-253	-33.4
Adiabatic Flame Temperature	°C	N/A	N/A	2000	1950	N/A	2110	1800
Minimum Ignition Energy	MJ	0.14	N/A	N/A	N/A	0.018	N/A	8
Molecular Weight	kg/kmol	N/A	N/A	N/A	N/A	N/A	2.02	17

In Figure 1.5; the gravimetric and volumetric hydrogen (H₂) densities for various hydrogen carriers were shown. Ammonia has a very high hydrogen density and can either be used as a fuel for combustion systems without additional hydrogen extraction process, or as a fuel in applications [7].

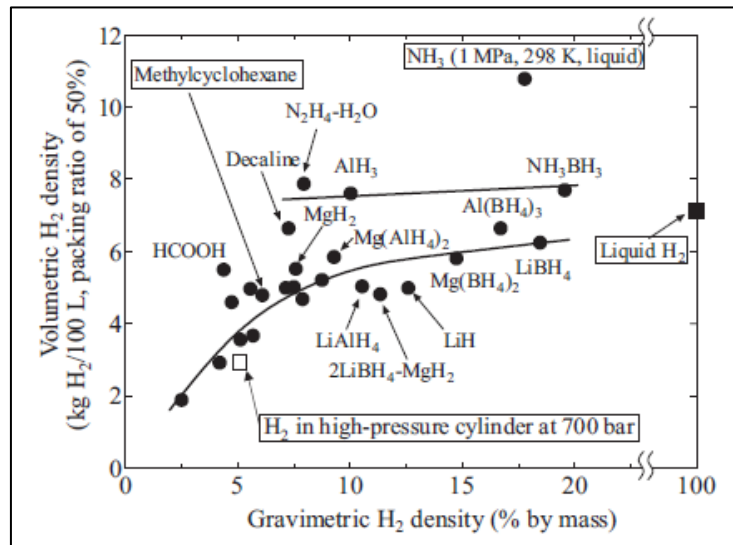


Figure 1.5 : Gravimetric and volumetric H₂ density of hydrogen carriers [7].

1.1.3 Challenges of ammonia combustion

As a carbon-free fuel, ammonia is a promising candidate for the future [3]. The use of ammonia has a long history, but even today, it is not a common technology and in general, ammonia has not been considered for use as a fuel [8]. Although the ammonia has many advantages when compared with other hydrocarbon fuels and hydrogen, it has some challenges also. The less understanding of the NH_3 combustion characteristics, research gaps, methods of combustion enhancement and optimization of NO_x formation restrict the utilization of NH_3 [2]. Thus, the practical application of NH_3 is still unsatisfying. Despite of the progressive usage of ammonia in practical applications, NO_x reduction and optimization of flame stability are still main challenges [2]. The comprehensive understanding of combustion and emission characteristics are necessary for the pure ammonia and ammonia blended fuels [3, 5].

According to Erdemir and Dincer [4]; high ignition temperature, low flame velocity and slow chemical kinetics is three main challenges in ammonia combustion. Blending ammonia with traditional fuels can help to solve these problems. Also, preheated ammonia and higher ambient pressure can help to improve flame velocity and auto-ignition.

Herbinet et al. [1] categorized ammonia combustion challenges into a relatively low reactivity and its nitrogenous emissions (NO_x and NH_3 residuals). The relatively low reactivity results in a low laminar burning velocity, a long ignition delay, a low heat release rate and a flame instability. They suggest a dual-fuel strategy to overcome some of these challenges. They suggest possible ammonia combustion promoters such as hydrogen, syngas, methane, alkanes, dimethyl ether, diethyl ether, alcohols, kerosene or diesel, coal and biofuels/biomass.

Franco et al. [9] stated that the ammonia combustion shows a numerous challenges because of the low reactivity, poor flame stability, very low flame speed and high NO_x emissions. They stated that device modifications and new device developments are required to adopt ammonia into existing systems.

According to the Li et al. [5]; one of the main challenges in the investigation of ammonia-based fuel is the validation of numerical simulations. Due to the reaction mechanisms, the numerical results usually overpredict or underpredict when compared with those obtained from the actual combustion process. Thus, it is necessary to

develop accurate reaction mechanism to fully understand the combustion characteristics of ammonia-based flames. Ammonia does not produce NO_x as a final product when it is completely combusted and it only turns to nitrogen and water. The overall reaction of ammonia is $4\text{NH}_3 + 3\text{O}_2 \rightarrow 2\text{N}_2 + 6\text{H}_2\text{O}$ when considering the Gibbs free energy of the combustion products [7]. However, it generates relatively high NO_x emissions in practical combustion applications. Therefore, detailed reaction mechanism is required to understand and reduce the NO_x production [5].

1.1.4 Parametric studies about the ammonia

NO_x is mainly composed of thermal NO_x and fuel NO_x , which is the major pollution of ammonia combustion. Thermal NO_x is usually produced by the oxidation of N_2 at temperature up to 1800 K. Controlling the temperature is an effective way to reduce thermal NO_x production. Fuel NO_x is mainly generated by the oxidation of NH_3 and it is widely studied by researchers [5].

Equivalence ratio and pressure are also important parameters for NO_x emissions. The main component of NO_x is NO. According to Kobayashi et al. [7]; it was found that with an increase of the equivalence ratio, the mole fraction of NO in NH_3 /air flame firstly increased before the equivalence ratio reaches 0.9 and then rapidly decreased when the equivalence ratio is large than 0.9. NO production is extremely low after the equivalence ratio up to 1.3. Therefore, it seems that burning under fuel rich condition is an effective way to reduce NO_x emission. Lee et al. [10] also found that both NO_x and N_2O emissions are low in fuel rich condition when compared to those under lean condition.

Li et al. [11] experimentally measured the NO_x concentration of NH_3/H_2 /air flames, covering the NH_3 concentration from 0.440 to 0.544 at the equivalence ratios from 1.0 to 1.25. According to the results; NO_x emission decreases when the equivalence ratio increases from 1.00 to 1.25 under various NH_3 contents. The significant change is observed when the equivalence ratio increased from 1.0 to 1.10, while the change is small between 1.10 and 1.25. The production of NO_x decreases with the increase of NH_3 concentration, which due to the low flame temperature.

Nozari et al. [12] investigated the NO_x emission variation of NH_3/H_2 /air flame dependent to the equivalence ratio at 17 atm and 673 K. According to results; the NO_x concentration increased first and then decreased when the equivalence ratio changed

from 0.5 to 1.2. The maximum NO_x mole fraction occurred under fuel lean conditions, similar to ammonia/air flames.

Valera - Medina et al. [13] numerically and experimentally investigated the NO_x emission of premixed NH_3/H_2 (50:50) mixtures under fuel lean condition in a swirl combustor. It was found that the pollution emission is higher than the fuel rich condition.

Xiao et al. [14] numerically investigated the effect of pressure in NH_3/H_2 flames by using an improved reaction mechanism developed by Mathieu et al. [15]. The NO_x concentration significantly decreases with the rise of pressure.

Rocha et al. [16] numerically investigated the change of NO_x emission dependent to H_2 addition ratio ranged from 0 to 1 by using ten mechanisms for ammonia/hydrogen/air flames at 1 atm and 298 K. Results show that with an increase of the H_2 content, the NO_x emission increased before the mole fraction of H_2 reached 0.8 and then rapidly decreased when the mole fraction of H_2 higher than 0.8 (Figure 1.6).

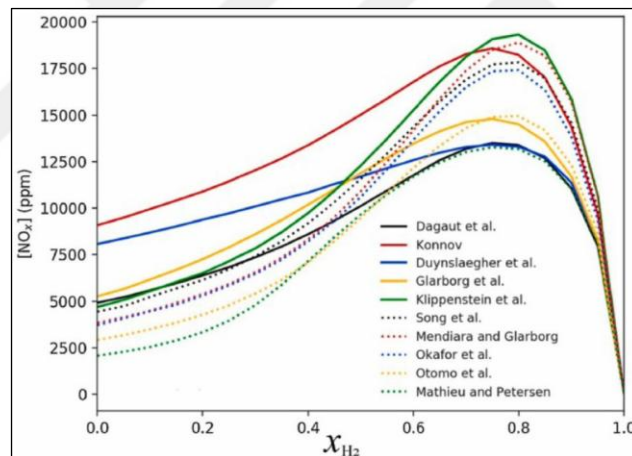


Figure 1.6 : Simulated NO_x concentration versus H_2 mole fraction in NH_3/H_2 blends for stoichiometric mixtures at 1 bar and 298K [2, 16].

According to the study of Franco et al. [9]; NO_x emissions increase with the addition of H_2 for a fixed equivalence ratio. For a constant fuel composition, NO_x increases with equivalence ratio up to 0.9, with a slighter increase between 0.8 and 0.9.

The concentration of CO_2 also influences the formation of NO_x . The high CO_2 content has a positive impact on NO_x production under fuel rich condition, while has a negative effect under stoichiometric and lean conditions [5].

Erdemir and Dincer [4] compared the effects of different ammonia fuel blends on the CO_2 and NO_x emissions in Figure 1.7. Mixing ammonia with common hydrocarbon fuels gives higher flame speeds, heat release rate and radiation intensity than ammonia, and of lower CO_2 emission than hydrocarbons [7].

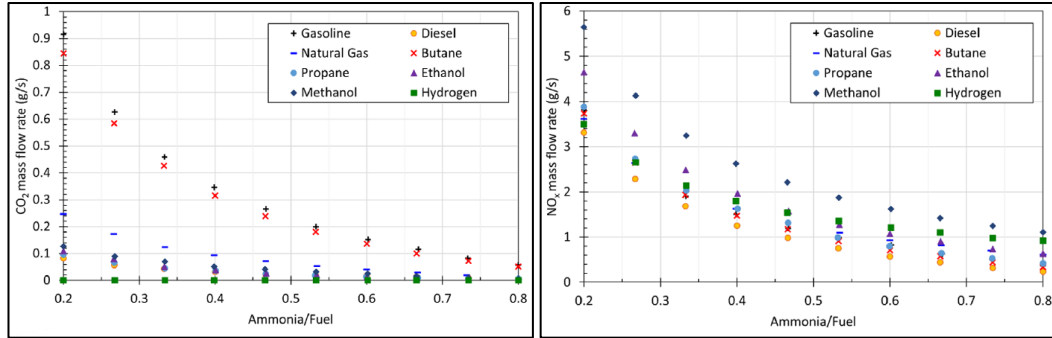


Figure 1.7 : CO_2 and NO_x emissions for different ammonia fuel blends [4].

Li et al. [5] and Herbinet et al. [1] summarized the effects of different parameters on the laminar burning velocity of ammonia flame. At 1 atm and 298 K, the laminar burning velocity increase before the equivalence ratio reaches 1.1, and then decrease when the equivalence ratio is large than 1.1 (Figure 1.8). Although all of the experiments were performed under the same conditions, some authors reported uncertainties up to ± 1 cm/s on their measurements which is significant compared to the absolute values of recorded flame speeds (in the range 2–8 cm/s) [1].

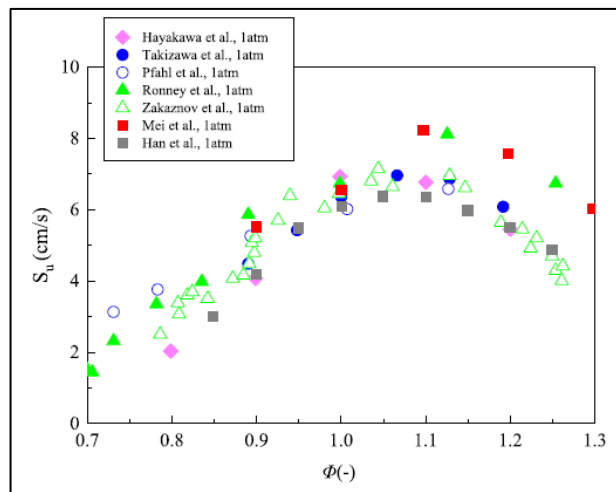


Figure 1.8 : Laminar burning velocity of ammonia flame with a function of equivalence ratio at 298 K and 1 atm [1, 5].

The influence of temperature is also showed in Figure 1.9. According to the results, it can be said that the laminar burning velocity increases with the increase of temperature for a constant equivalence ratio [5].

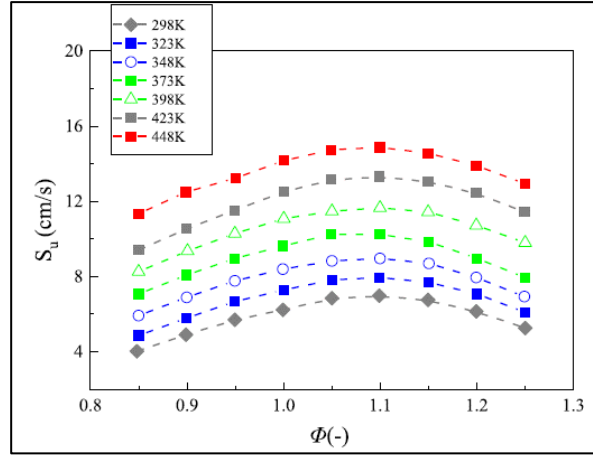


Figure 1.9 : Laminar burning velocity of ammonia flame with a function of equivalence ratio at various temperature [5].

In Figure 1.10, the effects of different reaction mechanisms on the laminar burning velocity of ammonia flame are shown by Li et al. [5]. Although GRI 3.0 mechanism is very close to experimental results, it lacks some ammonia oxidation reactions which are very important for the simulation of NO concentration in ammonia/air flame. Under various pressure conditions, it can be said that the flame velocity decreases with the rise of the initial pressure.

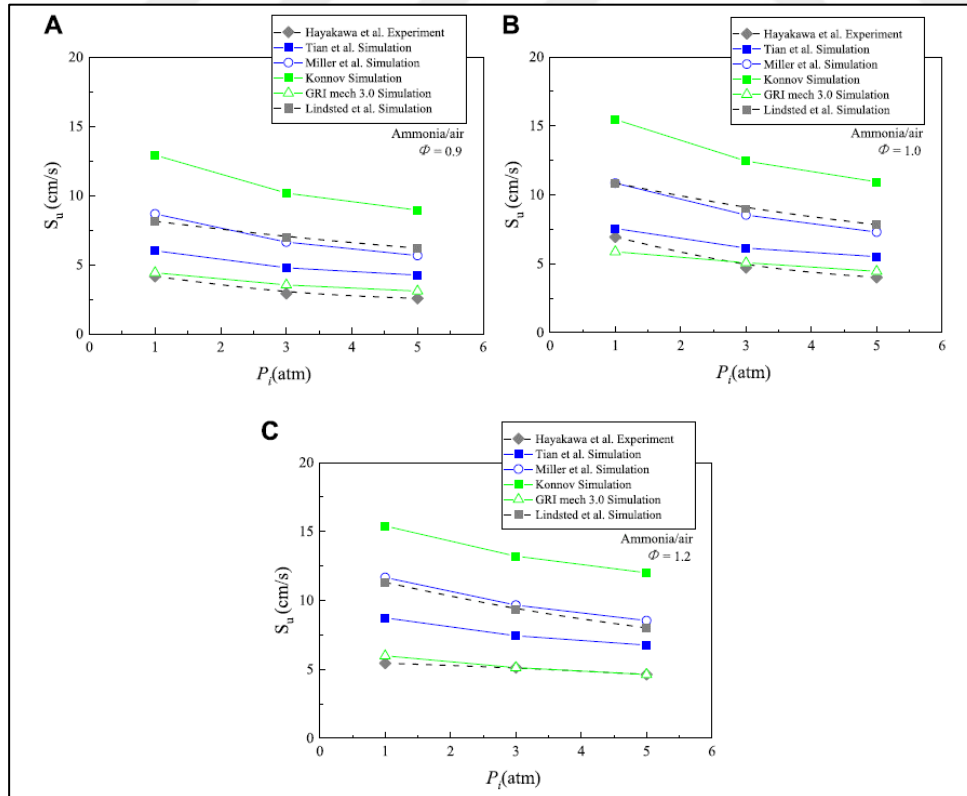


Figure 1.10 : Laminar burning velocity of ammonia flame with a function of initial mixture pressure at $\phi=0.9, 1$ and 1.2 [5].

Under oxygen enrichment conditions, the flame speed of ammonia/air flames increases with an increase of the O_2 concentration (Figure 1.11) [5]. Oxygen enrichment improves the radiation characteristics of ammonia flame also [8].

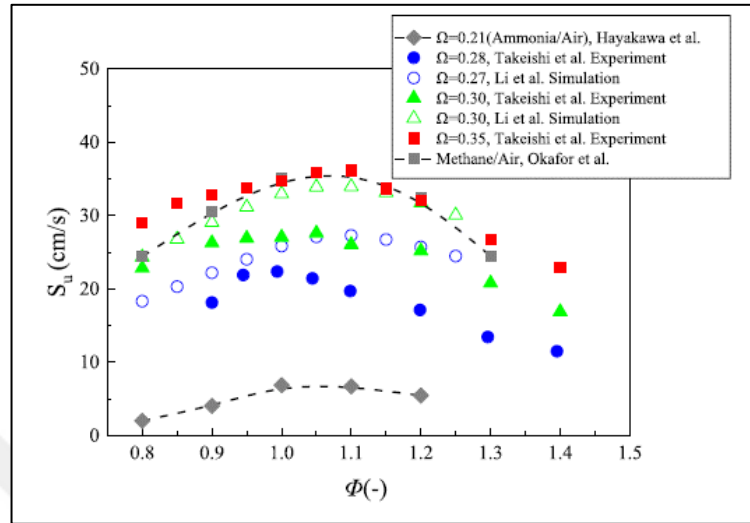


Figure 1.11 : Laminar burning velocity of ammonia flame with a function of equivalence ratio at various oxygen enrichment level [5].

It is difficult to keep stable the NH_3 laminar diffusion flame at atmospheric oxygen level and room temperature. Ishikawa et al. [3] investigated oxygen-enriched combustion to make stable flame. The effects of the fuel and the oxidizer velocities were investigated under 24% and 25% volume fractions of O_2 . According to the results; there were three regions with different extinction mechanisms of the ammonia coaxial jet diffusion flame under the relatively higher fuel velocity.

The low burning velocity of ammonia/air flames makes flame enhancement important for the successful application of ammonia [7]. The addition of H_2 can significantly increase the flame speed. Enhancing ammonia with H_2 is advantageous for simultaneously achieving a carbon-free combustion process in addition to flame stabilization [1, 8]. In their study; Ichikawa et al. [17] shows that the laminar burning velocity increases exponentially as the hydrogen fraction increases and that the laminar burning velocity becomes the same order as that of conventional hydrocarbon flame when the hydrogen fraction in the fuel is 0.4 at stoichiometry (Figure 1.12).

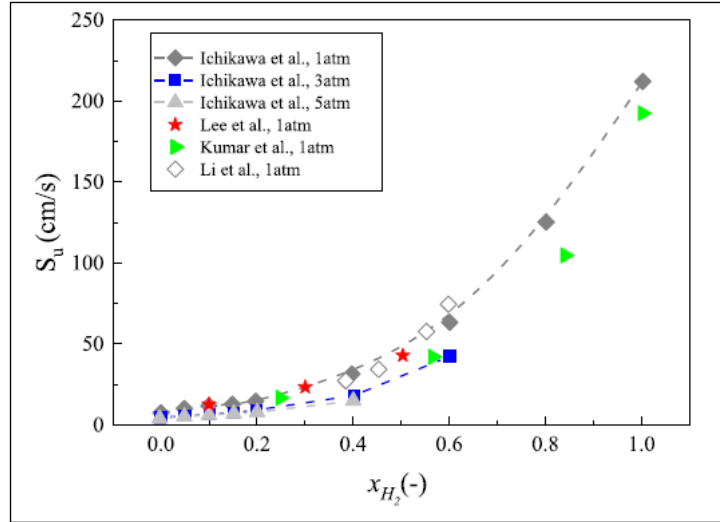


Figure 1.12 : Laminar burning velocity of ammonia flame with a function of volumetric hydrogen fraction at 298K [5].

The unstretched laminar burning velocity of pure ammonia was compared with hydrogen and other hydrocarbon fuels (methane, propane, ethylene) for various equivalence ratios under atmospheric pressure at Figure 1.13. The results clearly indicate that ammonia exhibits a considerably lower laminar burning velocity compared to hydrogen and conventional hydrocarbon fuels. Similar to hydrocarbon combustion behavior, the burning velocity of ammonia increases as the mixture becomes richer, reaching a peak around equivalence ratio 1.1, beyond which it starts to decline with further enrichment. The maximum burning velocity recorded for ammonia under these conditions is approximately 7 cm/s.

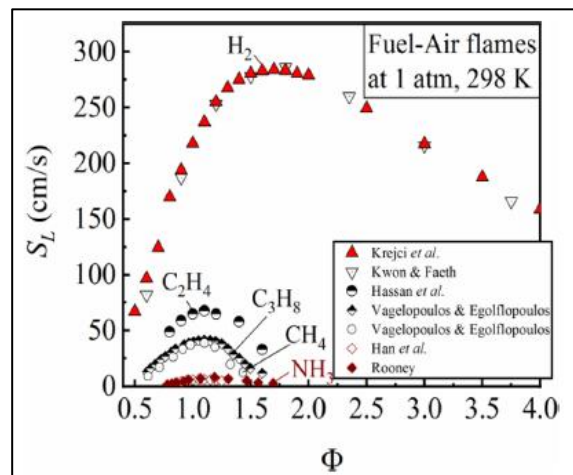


Figure 1.13 : Variation of the unstretched laminar burning velocity of pure ammonia versus hydrogen and other hydrocarbon fuels with mixture equivalence ratio at 0.1 MPa [2].

1.1.5 Experimental studies of ammonia combustion

Literature studies show the potential and the benefit of coupling kinetics and CFD codes for the development of advanced technologies using ammonia through a better understanding of hydrodynamics and kinetics. As an important point; the results are very sensitive to the chemistry used in simulations. Thus, the reliability of the chemistry included in the detailed kinetic model is a key point for chemistry coupled CFD simulations. Even though there are many chemical kinetic models for combustion of ammonia, ammonia/hydrocarbon blends, (Glarborg mechanism, Okafor's mechanism, Mathieu's mechanism, Tian's mechanism, Konnov's mechanism, Lindstedt et al., Miller et al., Li's et al, etc.), reduced kinetic models are required to make computations affordable for CFD modelling. Therefore, several reduced mechanisms have been developed employing different reduction methods over the years. Most of these reduced models use different detailed kinetic mechanism as a starting point, thus giving different results based on their independent development path. This causes to disagreement between users [18]. Thus, an experimental data required to validation of CFD simulations [1].

Even though the challenges of conducting ammonia combustion experiments, obtaining additional experimental data in different reactor types with various sampling methods and analytical tools by different groups under similar conditions is desired [1].

Hayakawa et al. [8] experimentally investigated the fundamental flame characteristics of ammonia in a swirling flame. 2 different swirlers were compared under room temperature and room pressure conditions (Table 1.2).

Table 1.2 : Swirler specifications [8].

Swirler	Vane Angle α_v [°]	Number of vanes [-]	Swirl number S [-]
Type 1	45	12	0.736
Type 2	60	12	1.27

According to the experimental results that examined by Hayakawa et al. [8]; as shown in Figure 1.14, ammonia/air premixed flame could be stabilized in the swirl burner without any additives to enhance the reaction. This proves the realizability of the premixed type ammonia fueled gas turbine.

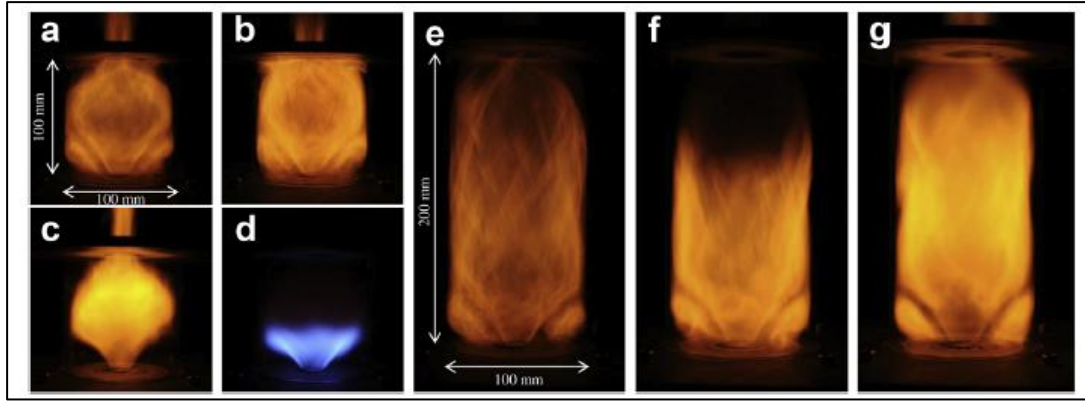


Figure 1.14 : Flames stabilized in the swirl burner with cylindrical liners: (a) ammonia/air flame, $\phi=1$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; (b) ammonia/air flame, $\phi=1.2$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; (c) ammonia/air flame, $\phi=1.2$, $h=100\text{mm}$, $U_{in}=3.35\text{ m/s}$; (d) methane/air flame, $\phi=1$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; (e) ammonia/air flame, $\phi=0.8$, $h=200\text{mm}$, $U_{in}=3.14\text{ m/s}$; (f) ammonia/air flame, $\phi=1$, $h=200\text{mm}$, $U_{in}=3.14\text{ m/s}$; (g) ammonia/air flame, $\phi=1.2$, $h=100\text{mm}$, $U_{in}=3.14\text{ m/s}$; [8].

Figure 1.14 d shows the methane/air flame stabilized in the same burner configuration as Figure 1.14 a-c. Due to the faster laminar burning velocity of methane/air premixed flame in Figure 1.14 d, the flame height is much shorter than ammonia/air flame.

For the stable combustion, the effects of fuel concentration and inlet velocity on the blow-off limits need to be determined. In their experimental study; Hayakawa et al. [8] obtained the stabilization map of the ammonia/air flame in the swirl burner (Figure 1.15). They also investigated the blow-off limits for methane/air and compared the results.

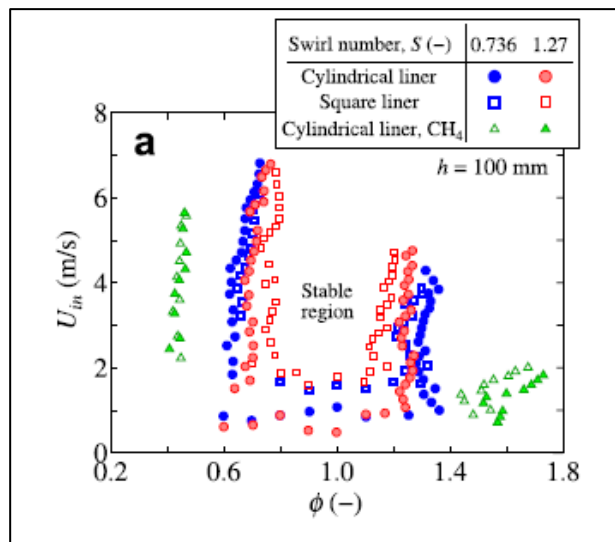


Figure 1.15 : Flame stability map of ammonia/air premixed flame in the swirl burner [8].

Although the stable region of ammonia/air flames is narrower than methane/air flames, ammonia/air flame can be stabilized for various velocity and equivalence ratio conditions by adopting a swirling flow. The flame stability limits narrows down when a higher swirl number was employed.

Franco et al. [9] designed and tested a novel combustor fired by a swirl and bluff-body stabilized burner (Figure 1.16 a). They measured the emissions of NO_x and unburnt NH_3 for a range of equivalence ratios and NH_3 mole fractions (Figure 1.16 b). They used ANSYS® with CHEMKIN PRO® to perform a 3-D transient analysis. The physical reacting flow was assumed to be a partially premixed in combustion case. The burner output rating was kept constant at 1.9 kW. The mass flow inlet boundary condition was selected at the combustor inlet, while the pressure outlet boundary condition was specified at combustor exit. According to the results; the novel laboratory combustor works well in terms of flame stability and both NO_x and NH_3 emissions (Figure 1.17).

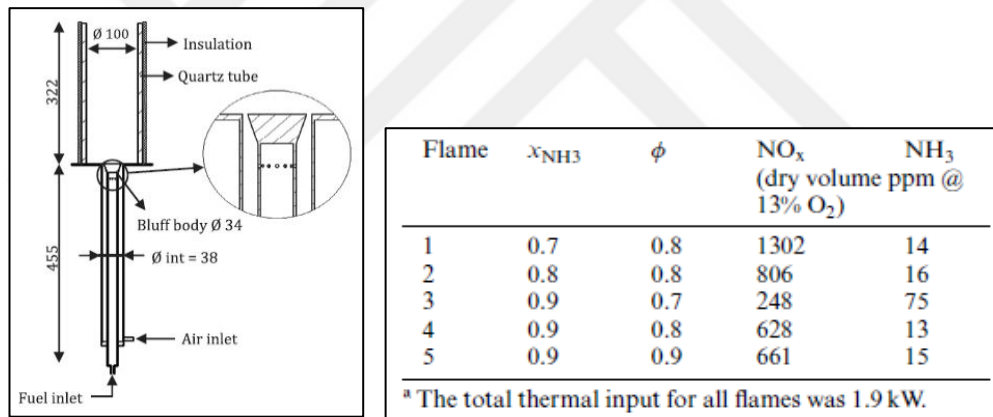


Figure 1.16 : (a) Schematic of the burner and (b) flame conditions [9].

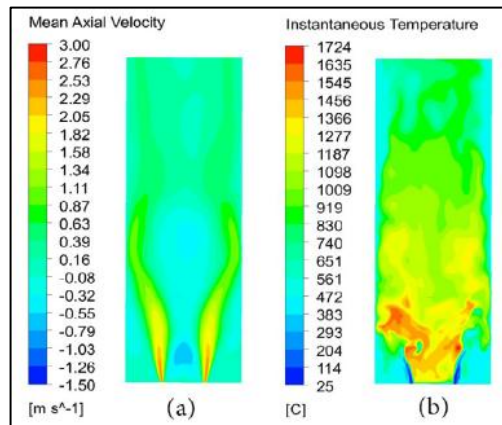


Figure 1.17 : Predicted flow pattern for flame 5. (a) Contours of mean axial velocity; (b) contours of instantaneous gas temperature. [9].

Figure 1.18 presents axial profiles of mean O_2 and NO_x concentrations and gas temperature for various flames, which allows to investigate the effects of NH_3 fraction and equivalence ratio on the combustor performance [9].

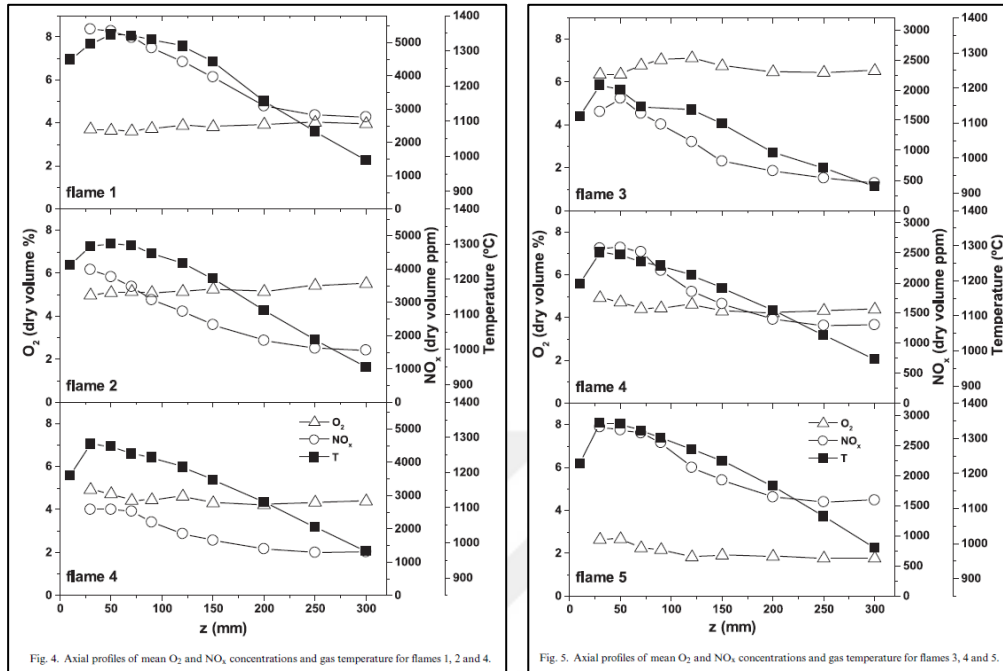


Figure 1.18 : Axial profiles of mean O_2 and NO_x concentrations and gas temperature for flames [9].

Pacheco et al. [19] investigated the combustion of ammonia/air mixtures experimentally and computationally, enriched by H_2 in a swirl and bluff body stabilized burner at stoichiometric to fuel-rich conditions (Figure 1.19).

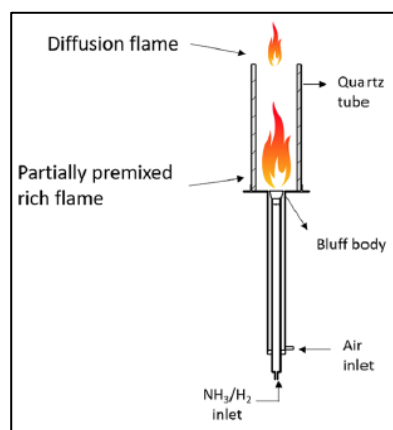


Figure 1.19 : Experimental setup [19].

Stability tests were performed for a fixed thermal input (2.8 kW), and flames of equivalence ratios of 1.0, 1.1, and 1.2, with molar fractions of ammonia in fuel of 0.7 and 0.8, were studied (Figure 1.20). Temperature profiles along the combustor axis

were measured. Measurements for NO_x emissions, unburned NH_3 and H_2 concentrations were performed also. According to the results, it was found that the present laboratory combustor performed well in terms of flame stability. Moreover it generates low levels of NO_x emissions in all fuel-rich conditions. Both H_2 and NH_3 emissions increase with the equivalence ratio.

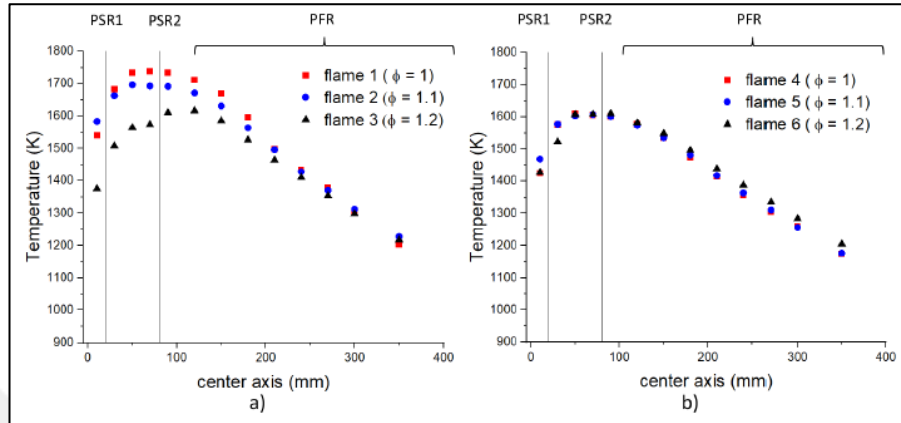


Figure 1.20 : Flame temperature along the centerline of the burner at different distances from the burner exit plane for (a) $x_{\text{NH}_3} = 0.7$ and (b) $x_{\text{NH}_3} = 0.8$ [19].

As a result of experiments, NO_x level above 2500 ppm is measured at the stoichiometric combustion conditions. NO_x production reduces when equivalence ratio increases.

1.1.6 CFD Simulation of ammonia combustion

There are several CFD studies in the literature that investigate the combustion phenomena. Most of them interested with hydrocarbon combustion. In recent years, with the increasing decarbonization trend, ammonia and hydrogen CFD studies accelerated. Both hydrocarbon and carbon-free fuel CFD studies summarized in this section.

Munteanu and Amzaini [20] investigated the pollutant emissions of bluff-body stabilized non-premixed flames by using Siemens Star-cm⁺[®]. They examined RANS with $k-\epsilon$ turbulence model to validate Sandia B4F3A flame (50:50 CH_4 / H_2 fuel). GRI-MECH (325 reactions / 53 species) mechanism was used to investigate the emissions. Although some underpredictions are observed mainly for NO and CO at downstream locations in the flame, these results are consistent with earlier reported studies using more complex combustion models.

Mauro et al. [21] performed CFD validation for both cold and reactive flows of Sydney bluff body burner (HM1 flame). Converge CFD[®] was used as a CFD solver with AMR strategy in the steady state RANS simulations. RSM-SSG and k- ϵ turbulence models were compared by using full burner geometry in cold flow validation study. k- ϵ turbulence model gave the best validation with experiments. By using slice geometry, they investigated 2 different combustion models (FGM model and SAGE detailed solver) coupled with 2 different reaction mechanisms (CRECK and GRI-MECH 3.0). Also, standart and enhanced near wall approaches were compared to validate reactive flow.

To investigate the cold flow characteristics of a partially premixed bluff body burner; Meraner et al. [22] performed CFD simulations with 5 turbulence models and 2 different lance heights. They used ANSYS Fluent[®] with incompressible ideal gas approach and validated their CFD results by comparing with PIV experiments. Although the CH₄/H₂ fuel was used in the study, reactive flow simulations were not performed.

In the study by Sudarma et al. [23], lean premixed combustion in a bluff-body stabilized burner was numerically investigated using RANS-based CFD methods. The performance of two turbulence models, k- ϵ and RSM, was compared and validated against experimental data. While the k- ϵ model provided better global flame predictions, RSM was more accurate for local flow details. These findings highlight the importance of selecting appropriate turbulence models for the simulations under premixed conditions.

Muppala et al. [24] performed a comparative analysis of various turbulent reaction models applied to hydrogen-enriched methane-air flames. The study showed that conventional models often struggle to predict combustion behaviour at high hydrogen concentrations, mainly due to diffusion-related effects.

In the work of Rajak et al. [25], CFD models were used to simulate combustion and NO_x emissions for different gaseous fuels, including hydrogen-air mixtures. The study demonstrated that fuel type, flame temperature, and thermal radiation effects play a critical role in NO formation. The model was validated with experimental results, especially in terms of NO concentration profiles.

Okafor et al. [26] combined the numerical and experimental studies to investigate the effects of ammonia injection angle, equivalence ratio, pressure and inlet temperature in laboratory. They also investigated the dependence of NO emission to equivalence ratio numerically.

Cai et al. [27] numerically investigated the effect of bluff body on the NO_x emissions in a micro-planar combustor by using ammonia/oxygen as a fuel. They showed that proper design of bluff body increases combustor performance and reduces NO_x emissions.

Rocha et al. [28] conducted ammonia combustion simulations for three different stationary gas turbine concepts. They used detailed chemical mechanism from Mendiara and Glarborg [29] that consisting of 97 species and 779 reactions.

Zhang et al. [30] explored ammonia/air and ammonia/ methane/air flames in a swirl stabilized combustor by performing both experiments and LES simulation with Okafor mechanism [31]. Results show that 50% methane addition into the ammonia can significantly extend blow off limit and increasing the swirl number only affects mixture stability, unlike pure ammonia flame.

Honzawa et al. [32] were simulated the NH₃/CH₄/air combustion in a swirl burner by employing LES with a non-adiabatic FGM approach. They underlined the importance of heat losses for their significant impact on NO and CO emission.

Valera-Medina et al. [18] performed CFD simulations with Siemens Star-cm+[®] by using Okafor's reduced reaction mechanism. They compared the performance and accuracy of the results against the experiments to explore the impact of ammonia/hydrogen blends on species such as NH₂ and NO. They employed RANS k- ω SST modelling for CFD model, that is known to provide good average results for tangential swirling flows. By using the advantage of symmetry, only one-third of the burner was meshed with 3.4 million cells. Periodicity was applied in all the side boundaries of the mesh in order to simulate the entire domain (Figure 1.21). The mesh was refined locally in the downstream zone of the burner, just passed the nozzle. Residual values ranged from 10⁻⁴ to 10⁻⁹. Initial analyses were performed to validate the hydrodynamics within the system by focusing on velocity profiles, coherent structures and flame features (i.e. angle, diameter, etc.). For the comparison and

calibration of combustion, they used previous experiments performed by Valera-Medina et al. [33].

Once the isothermal profiles were validated, Figure 1.22 (a), the combustion patterns were compared with the previous experiments (Figure 1.22 (b)). After validating the CFD model under atmospheric pressure, they expanded results to various inlet pressure and temperature conditions, hence explored the contribution of these parameters to the behavior of NH_2 and NO .

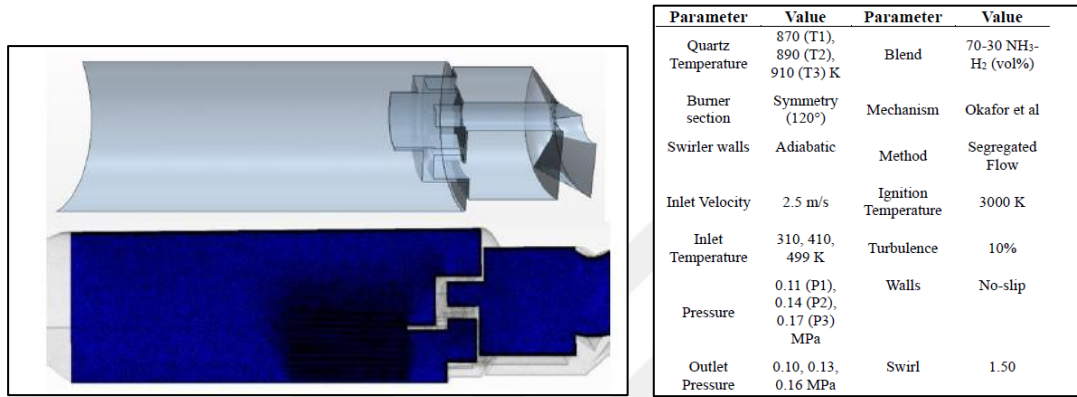


Figure 1.21 : Burner geometry and mesh, boundary conditions [18].

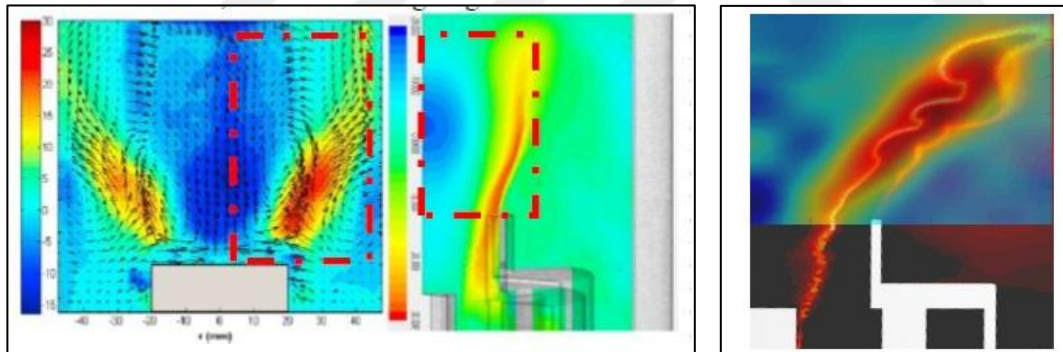


Figure 1.22 : (a) Isothermal validation, (b) Comparison with previous experiments [18].

Vigueras-Zuniga et al. [34] aimed to characterize various ammonia/methane blends and describe the effects of flame, radical formation and stability on the swirling burners. A tangential swirl burner was employed at 8 kW power and 1.05 swirl (Table 1.3). RANS simulation with k- ω SST turbulence model was conducted by using Siemens Star-cm+[®]. Okafor's reduced reaction mechanism (42 species and 130 reactions) was applied and validated by laminar burning velocity of ammonia/methane mixtures. Simulations were only performed on the stoichiometric ($\phi = 1$) cases. CFD simulation results were validated by using experimental emission measurements. One-

third of the burner section was used to represent the entire geometry with periodic interface boundaries (Figure 1.23). A computational grid consisting of 4.1 million cells and it was locally refined. Residuals were maintained below 10^{-4} for the solved simulation.

Table 1.3 : Experimental and numerical boundary conditions [34].

Parameter	Value	Parameter	Value
Blends CH ₄ /NH ₃ (vol%)	20/80, 40/60, 60/40	Quartz Temperature	1185, 1177, 1190 K
Mixing	Fully pre-mixed	Burner Section	Symmetry (120°)
Equivalence Ratio (ϕ)	0.8, 1.0*, 1.2	Swirler walls	Adiabatic
Power	8 kW	Ignition Temperature	3000 K
Inlet Temperature	300 K	Turbulence	10%
Inlet Pressure	0.11 MPa	Walls	No-slip
Outlet Pressure	0.10 MPa	Method	Segregated Flow
Swirl	1.05	Mechanisms	Okafor

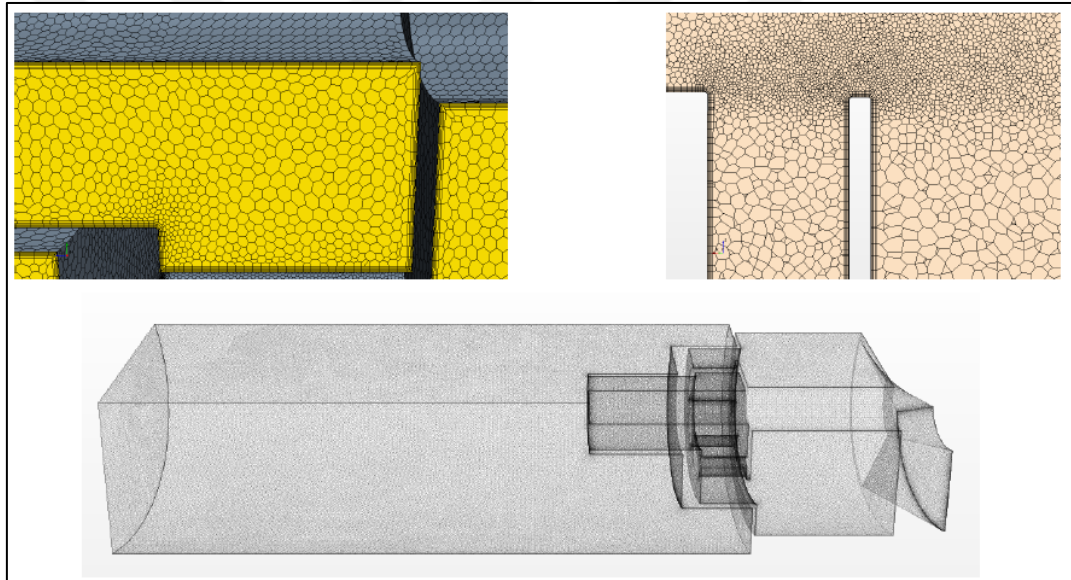


Figure 1.23 : Meshed geometry [34].

Initial numerical calculations were compared with isothermal experiments in order to determine the hydrodynamic validation of the system. As shown in Figure 1.24; the CFD model and experiments have a good accuracy with the same trends, peak values, and shearing flow location [34].

According to the results in Figure 1.25; correlation between species (CO, CO₂, and NH₃) is adequate. It should be noted that CO and CO₂ are higher in the CFD simulations for the cases 40/60 and 60/40 (methane/ammonia). Ammonia is well predicted, whilst CO and CO₂ are calculated at similar orders of magnitude.

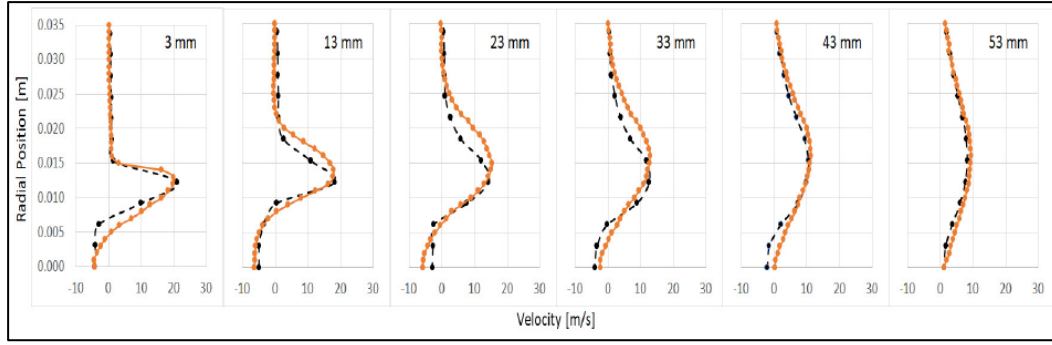


Figure 1.24 : Isothermal results at different axial positions. Experiments (solid, orange line) and numerical (dashed, black line) [34].

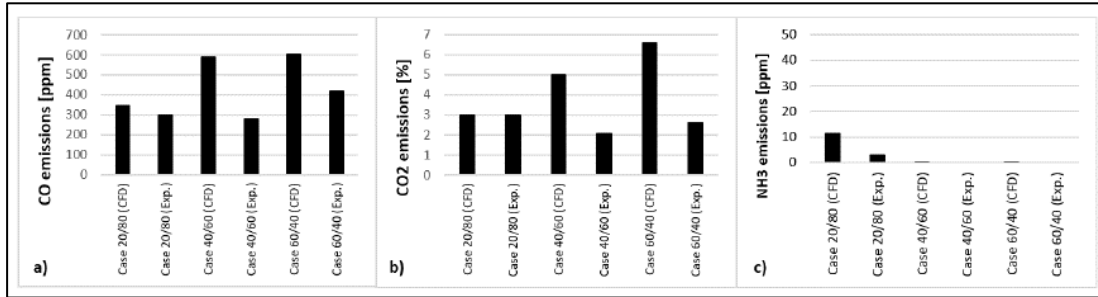


Figure 1.25 : Emission results. (a) CO (ppm); (b) CO₂ (%); (c) NH₃ (ppm) [34].

Vigueras-Zuniga et al. [35] examined a numerical study to characterize ammonia combustion systems by using novel reaction models. RANS simulations via Siemens Star-cm+[®] were performed with complex chemistry of a 70%–30% (mol) ammonia/hydrogen blend. A fixed 1.2 equivalence ratio, 0.8 swirl ratio and confined conditions are applied to determine the flame and species propagation at different working pressures and temperature inlet values. The analyses were conducted using k- ω SST turbulence model. Complex chemistry was employed by using a reduced kinetics mechanism developed by Okafor et al. [36] for the resolution of combustion. To investigate the non-adiabatic operating conditions of the system (higher NO_x and lower NH₃ case), tests were performed in a high-pressure optical combustor and validated with previous results. 1450 K wall temperature was applied and a numerical mesh consisting of ~1.5 million cells was used for the calculations (Figure 1.26). The mesh was improved locally in the inner flame region downstream of the nozzle. One-third of the burner section was used to represent the entire geometry with periodic interface boundaries. Residual values ranged from 10⁻⁴ to 10⁻⁶. In Table 1.4, the boundary conditions for the initial validation are specified [35].

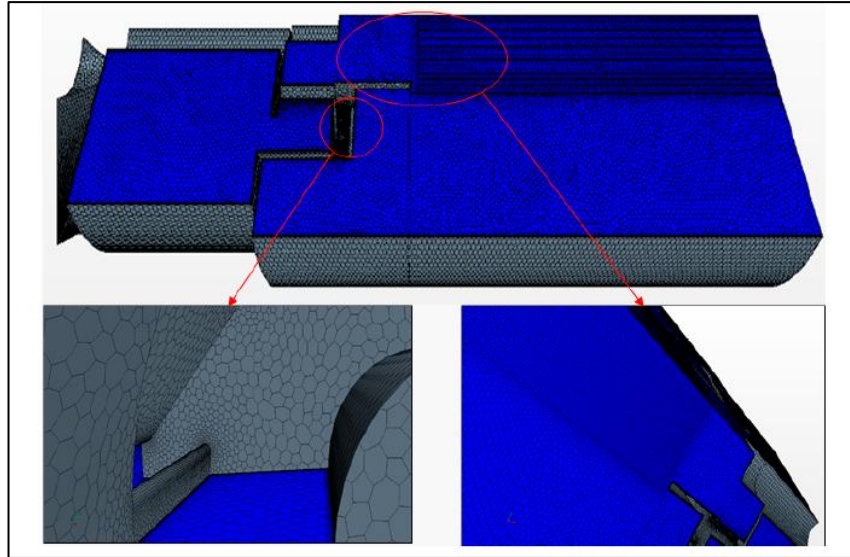


Figure 1.26 : Mesh used for modelling. (Top) Full mesh; (Bottom left) Details of the swirl vanes; (Bottom right) Close-up local mesh refinement [35].

Table 1.4 : Boundary conditions; atmospheric conditions [35].

Parameter	Value	Parameter	Value
Quartz Temperature	1450 K	Okafor Mechanism	130 Reactions
Inlet Velocity	3 m/s	Method	Segregated Flow
Inlet Temperature	304 K	Ignition Temperature	300K
Pressure	101300 Pa	Turbulence	10%
Outlet Pressure	99274 Pa	Burner Section	Symmetry (120°)
Walls	No-slip	Swirler walls	Adiabatic

CFD models were validated by using the results from Valera-Medina et al. [33], Pugh et al. [37] and Runyon et al. [38]. Then, the study was expanded to high inlet temperatures, high pressures, and high flowrates at different boundary conditions (Table 1.5). Thermal power of the system was set at 196 kW and the ammonia-hydrogen blend's specific energy was 48.6 MJ/kg.

Table 1.5 : Boundary conditions; high pressure, high inlet temperature conditions [35].

Parameter	Value	Parameter	Value
Quartz Temperature	1450, 1800, 2150 K	Okafor Mechanism	130 Reactions
Inlet Velocity	20 m/s	Method	Segregated Flow
Inlet Temperature	500 K	Ignition Temperature	300K
Inlet Pressure	0.90 MPa	Turbulence	10%
Outlet Pressure	0.88 MPa	Burner Section	Symmetry (120°)
Walls	No-slip	Swirler walls	Adiabatic

In Figure 1.27, ammonia emissions are in good agreement with previous experimental campaigns. However, predicted hydrogen is higher than measurements.

Simultaneously, NO emissions are over-predicted. Even though the ammonia has been well predicted, the consumption of hydrogen and its reaction close to the flame need to be further assessed by reaction mechanism developers. Since there is no experimental characterization of the hydrodynamics of ammonia/hydrogen flames yet; both simulations and PIV experiments were performed under isothermal conditions. In Figure 1.28; the comparison between experiments and simulations show the same trends, velocity profiles, and magnitude of coherent structures.

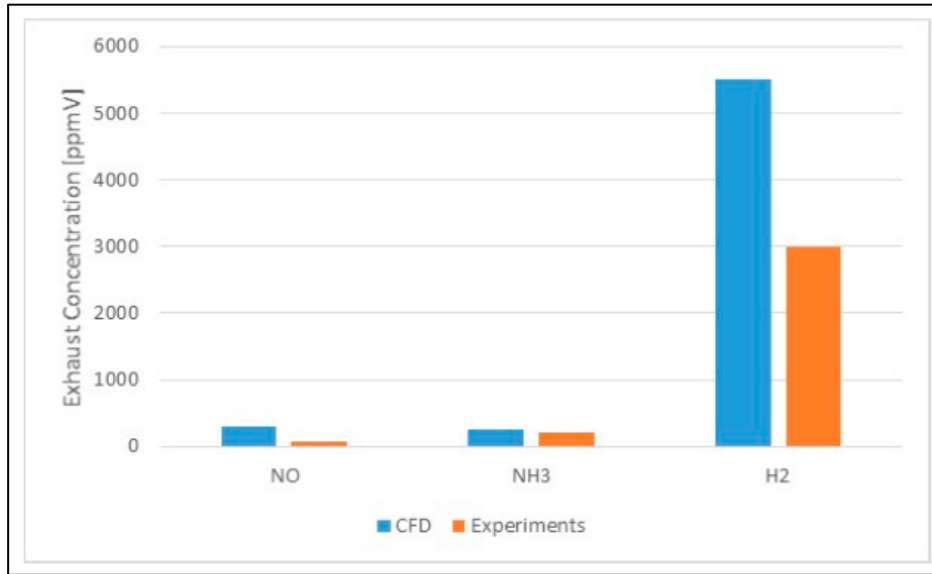


Figure 1.27 : Validation using exhaust emissions profiles. Experiments as in [33, 37].

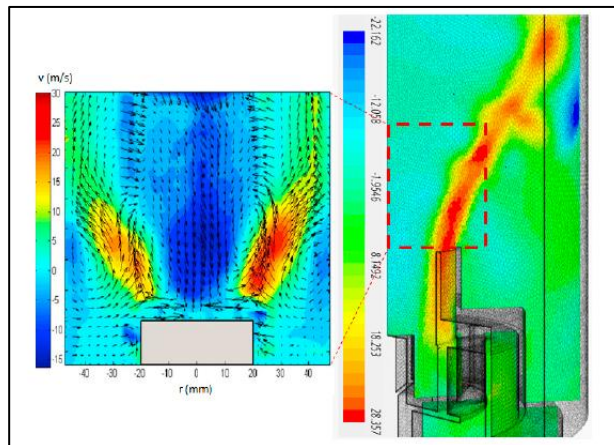


Figure 1.28 : Isothermal results. (Left) Experiments from [38]; (Right) numerical analysis (zone of interest is highlighted).

In Figure 1.29, the results are in the same order of magnitude to those obtained experimentally, thus enabling the analysis to move forward to semi-industrial conditions.

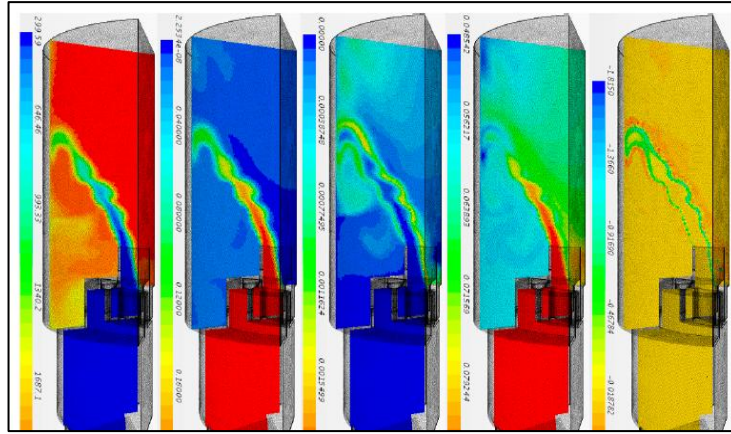


Figure 1.29 : (A) Temperature (K); (B) ammonia concentration (mol%); (C) NO concentration (mol%); (D) hydrogen concentration (mol%); (E) hydrogen rate of production ($\text{kg/m}^3\text{s}$). Operating conditions: 101 kPa, 304K [35].

Figure 1.30 shows the emission profiles of this burner at high pressure and high inlet temperature with greater power output. Other high pressure and high inlet temperature results can be found in the paper.

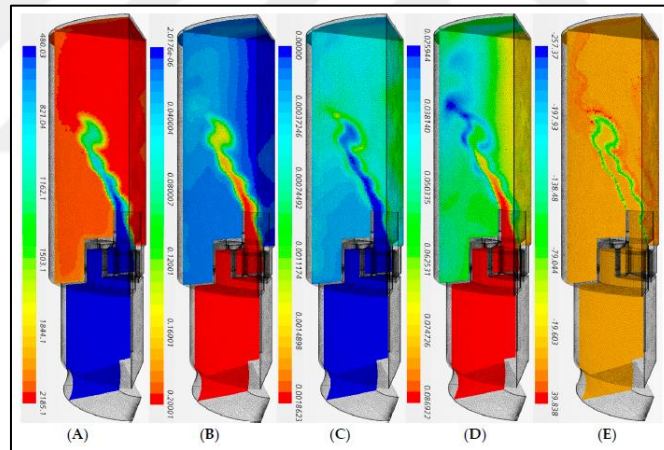


Figure 1.30 : (A) Temperature (K); (B) ammonia concentration (mol%); (C) NO concentration (mol%); (D) hydrogen concentration (mol%); (E) hydrogen rate of production ($\text{kg/m}^3\text{s}$). Operating conditions: 900 kPa, 500K inlet temperature, 1800K quartz tube [35].

Mikulcic et al. [39] performed RANS simulations for methane/ammonia combustion under conditions approaching industrial ones. Three chosen mechanisms (Table 1.6) were compared using commercial CFD software AVL Fire[®] and their predictions on the experimental premixed swirl burner was investigated. Required experimental data and burner CAD geometry was taken from Valera-Medina et al. [40]. The burner is a part of the experimental rig situated at the Gas Turbine Research Centre of Cardiff University (Figure 1.31) and it has 1.05 geometric swirl number. In simulations; a

constant (1500 K) temperature was imposed to wall and the outlet boundary conditions was set to 1 bar (Figure 1.32). k- ϵ turbulence model was applied and solution was considered converged when residuals in transport equations reach to below four orders of magnitude.

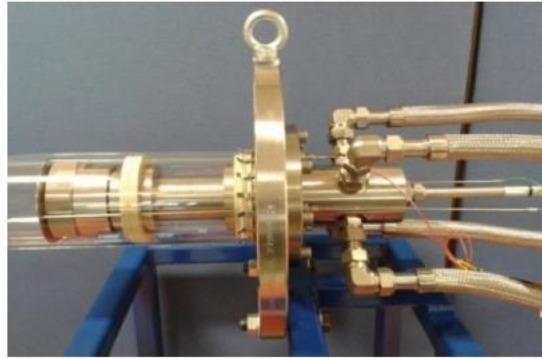


Figure 1.31 : Generic swirl burner at the Gas Turbine Research Centre [40].

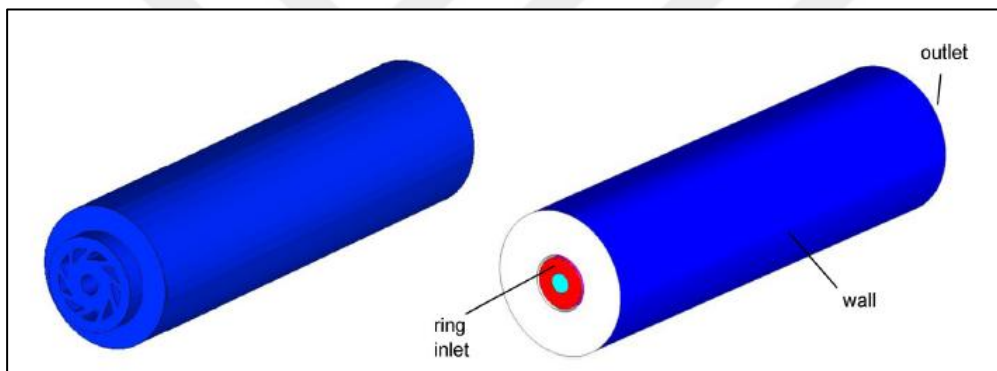


Figure 1.32 : Computational domain: with swirler (left) and simplifies (right) [39].

Table 1.6 : Chemical kinetics model used in the Mikulcic et al. [39].

Mechanism	Number of reactions	Number of species
Okafor	42	130
Konnov	51	420
San Diego	68	330

As it can be seen from the Table 1.7; equivalence ratio ranges from 0.81 to 1.24 while constant burner power is 44kW. Although equivalence ratio and oxidizing air vary, flow rates of fuels were kept constant.

Results in central cross section were compared in Figure 1.33. Concentration of various species (CO, CO₂, H₂, NO and OH radical) at the outlet were reported in Figure 1.34 [40]. According to the comparison between experiment and simulation results;

the most accurate NO concentration is predicted with San Diego mechanism, while the worst prediction is obtained with Konnov mechanism. However, San Diego mechanism is the most expensive simulation in terms of computational time since nitrogen chemistry is added into the main mechanism. Other species are not so well predicted. None of the models was able to accurately reproduce CO emission after equivalence ratio exceeds 0.81 also.

Table 1.7 : Simulated cases [39].

Case No.	Air mass flow [g/s]	Methane mass flow [g/s]	Ammonia mass flow [g/s]	Equivalence ratio [-]
1	16.66	0.47	0.8	0.81
2	13.25	0.47	0.82	1.02
3	11.88	0.47	0.82	1.14
4	10.86	0.47	0.82	1.24

Mutual comparison of the mechanisms presented that San Diego mechanism is fairly distinct compared to other two in all aspects, even velocity field. It is the most encouraging mechanism, especially in terms of NO emissions.

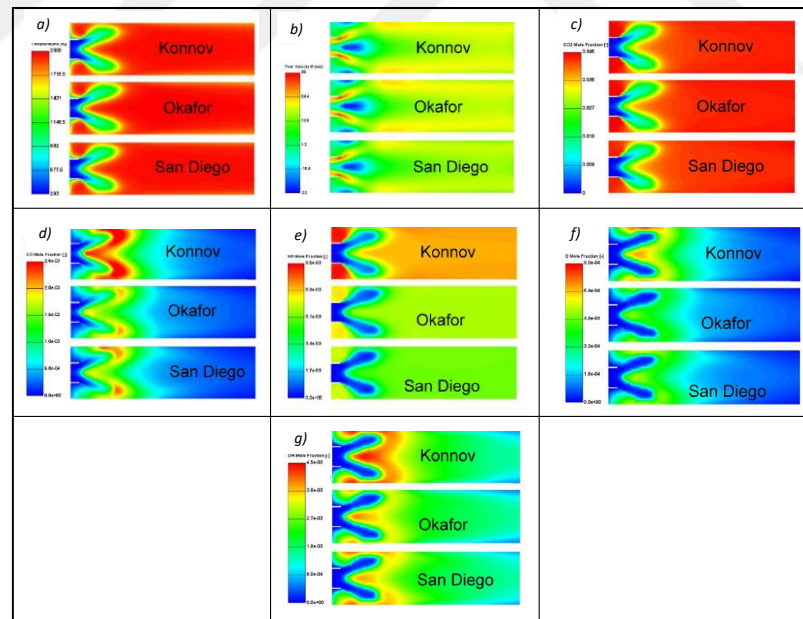


Figure 1.33 : Comparison of the results in central cross section for $\phi=0.81$: a) temperature field, b) axial velocity field, c) CO_2 concentration, d) CO molar concentration, e) NO molar concentration, f) O radical concentration, g) OH radical concentration [39].

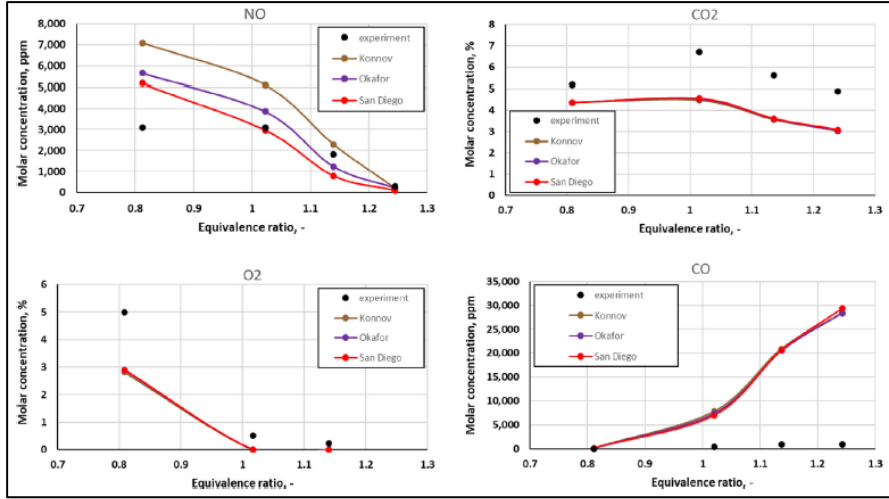


Figure 1.34 : Emission comparison for various equivalence ratios: a) NO, b) CO₂, c) O₂, d) CO [39].

Wiseman et al. [41] performed DNS simulations in Converge CFD[®] by using CH₄ and NH₃/H₂/N₂ (40%/45%/15% by volume) fuels. They investigated the blow-out limits of bluff-body stabilized burner that are measured experimentally also (Figure 1.35). Short Smooke and Giovangigli mechanism was used for CH₄ fuel and San Diego nitrogen sub-mechanism (21 species / 40 reactions) was used for NH₃/H₂/N₂ fuel. Simulation results compared with OH PLIF and OH chemiluminescence images (Figure 1.36 and Figure 1.37). They used fixed fuel flow rate and increased air flow rate to measure the blow-out curves.

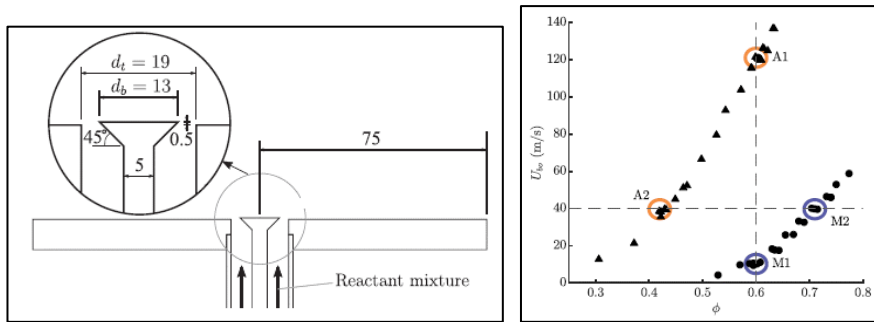


Figure 1.35 : a) Sketch of burner geometry with dimensions in mm; b) Measured blow-out curves for the NH₃/H₂/N₂ blend [41].

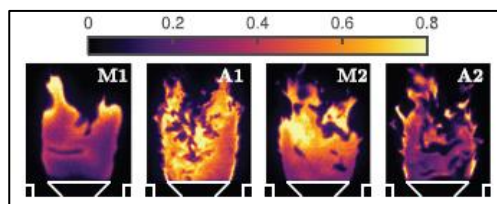


Figure 1.36 : OH PLIF images of flames 1 s before blow-out. The intensity is normalized by the peak value [41].

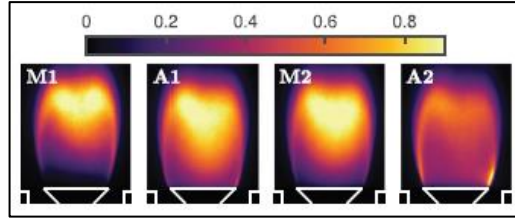


Figure 1.37 : Time-averaged OH chemiluminescence images of flames from 1.1 s to 0.9 s before blow-out. The intensity is normalized by the peak value [41].

Somarathne et al. [42] numerically investigated emissions of premixed swirl combustor by using LES and Miller mechanism. In the subsequent work Somarathne et al. [43] investigated non-premixed ammonia/air combustion and similar results were reached, with exception of obtaining heterogeneous NO distribution compared to premixed flames. Although the NO emission decreases with an increase of the global equivalence ratio, Φ_{global} , similar to premixed flames, the distribution of NO concentration is non-uniform, unlike in the premixed flame case Figure 1.38.

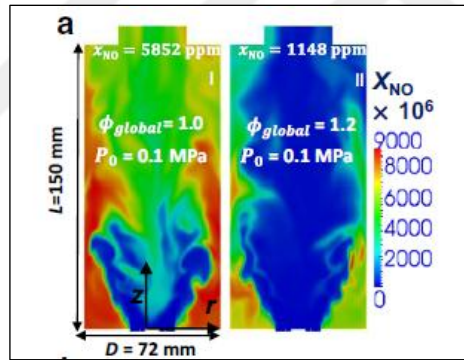


Figure 1.38 : NO distribution in turbulent non-premixed NH_3/air flames in terms of equivalence ratio, ϕ (the fuel and air stream inlet temperatures are 500K and the swirl numbers are 0.69 and 0.68, respectively. Combustor walls are adiabatic) [43].

In their another work, Somarathne et al. [44] conducted LES simulation of high pressure NH_3/air flames by using reduced reaction mechanism from Okafor et al. [31] to explore the influence of various wall thermal boundary conditions.

According to the 3D-CFD results [42, 45] those performed by using LES; generation of fuel NO can be dramatically decreased under rich flame conditions at high pressure (Figure 1.39(a)). The significant reduction in OH radicals causes to this result (Figure 1.39(b)). Miller's mechanism [46] was used in these numerical studies [7].

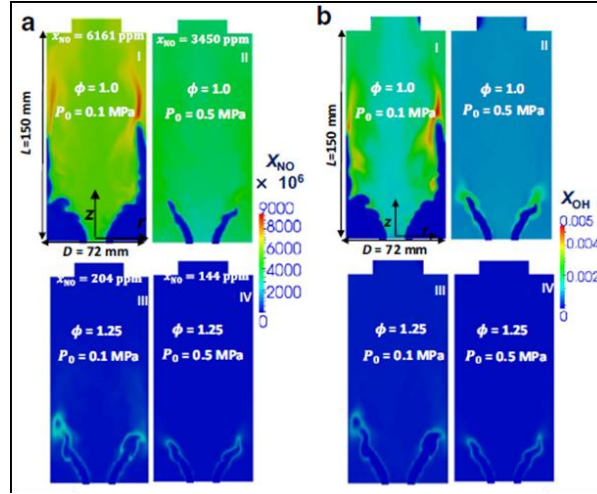


Figure 1.39 : (a) NO; (b) OH; concentration distributions in turbulent premixed NH₃/air flames in terms of equivalence ratio and pressure [7].

Numerical studies [42, 45] and experimental studies [8, 26] confirmed that there is a specific equivalence ratio under rich flame conditions at which NO and unburnt NH₃ emissions are minimum and that the emissions follow the same order as shown in Figure 1.40. According to the results of [42] and [45]; the specific equivalence ratio is 1.2 when the mixture inlet temperature is 500 K and an adiabatic wall condition is used. Further, Hayakawa et al. [8] found that the value is 1.05 as a result of experiments for a mixture temperature of 300 K and an isothermal combustor wall condition. Thus, it was validated that a slightly rich condition presents minimum NO and NH₃ emissions independent from the flame configuration.

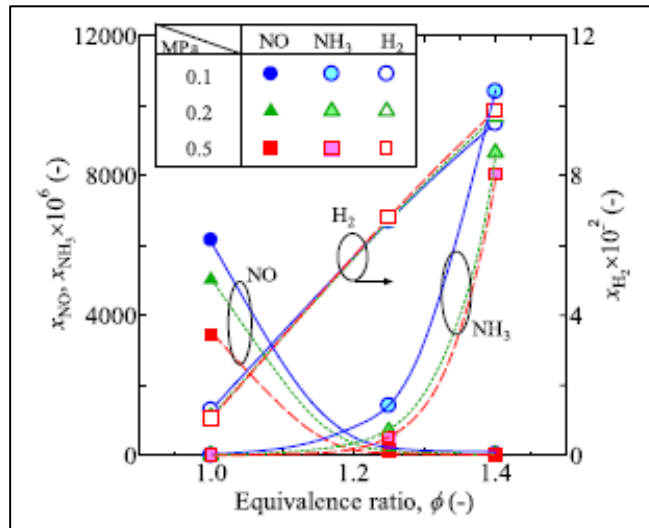


Figure 1.40 : Space and time averaged emissions of NO, x_{NO} , NH₃, x_{NH_3} , and H₂, x_{H_2} in turbulent premixed NH₃/air flames in terms of equivalence ratio and pressure [7].

1.1.7 Kinetic mechanism studies

It is essential to establish a standardized methodology for comparing and verifying the reaction mechanisms. Therefore, generalized approaches should be created for determining the 'best' mechanisms for the various combustion parameters [47]. Experimental data is critical for comparison with numerical data. In this way, the accuracy of the kinetic mechanisms can be assessed [47].

Alnasif et al. [47] reviewed the latest trends in the chemical kinetics of ammonia extensively. Various experimental results are considered to verify the evaluation of the kinetic reaction mechanisms. The main findings show that most of the reaction mechanisms perform poorly in estimating ammonia flame combustion characteristics such as ignition delay, laminar flame speed and NO_x emissions. The predictive performance of the mechanisms varies with the equivalence ratio, mixing ratio and operating conditions. Many mechanisms dealing with mixed ammonia combinations give reliable predictions at low hydrogen concentration conditions but deteriorate gradually due to the shift in reactions at high hydrogen concentration conditions. This is one of the issues that requires further study in the literature. It is a challenging task to develop a reliable kinetic model that is consistent with experimental results. The behavior of ammonia and hydrogen mixtures can be different from pure ammonia combustion and chemical kinetic models need to capture these differences precisely. A lot of work has been done to establish a kinetic mechanism that precisely predicts NO_x emissions from ammonia flames under many different conditions. In the last 10 years; a great improvement has been made in the prediction of combustion characteristics by improving kinetic mechanisms and reducing the inconsistency between measurements.

Alnasif et al. [48] elucidated the differences between the mechanisms for predicting NO mole fractions by studying the effects caused by the combustion of ammonia mixtures. They considered a range of operational conditions to successfully predict the experimental results of NH_3/H_2 flames. Despite many efforts to improve the performance of kinetic mechanisms, they showed poor prediction quality at all equivalence ratios for the NO mole fraction.

A reduced kinetic mechanism of $\text{NH}_3/\text{H}_2/\text{Air}$ combustion was developed by Duynslaegher et al. [49] to optimize NO_x formation and laminar flame speed. The

mechanism has 80 reactions and 19 species for a temperature of 400°C, a pressure of 1.4 Bar and an equivalence ratio of 0.5. It was identified that the Duynslaegher et al. [49] mechanism reproduces the experimental measurements correctly under lean conditions, but under rich conditions the results deteriorate. In these conditions, the Nakamura et al. [50] mechanism was used for a good prediction of the flame speed. According to the evaluation, the Duynslaegher et al. [49] mechanism shows poor performance when the hydrogen content exceeds 40% and has a tendency to overestimate the response of fuels with low hydrogen content. According to Alnasif et al. [51] studies, the kinetic model formulated by Duynslaegher et al. [49] showed the greatest precision in estimating laminar flame speed measurements under atmospheric conditions for 70/30 vol% NH_3/H_2 mixture. A different chemical pathway was identified through sensitivity analysis in NH_3/H_2 mixtures compared to pure NH_3 fuel. Duynslaegher et al. [49] underpredicted at high hydrogen content and overpredicted at low hydrogen content.

Nakamura et al. [50] developed a model for high temperature and highly diluted $\text{NH}_3/\text{O}_2/\text{Ar}$ mixtures to improve the prediction of ignition delay times. According to the results, the model reported a better prediction of species as NH_3 , O_2 , and H_2O . They also noted that NO and N_2O profiles were well predicted in the post-flame region, but overestimated at the reaction region.

Stagni et al. [52] intended to develop a kinetic mechanism for NH_3 oxidation in their study. They covered a wide range of studies under lean conditions using both flow reactors and jet stirred reactors. Thus, the study covered a wide range of operating temperature from 500 K to 2000 K. Importantly, they determined critical pathways leading to NO formation in two representative scenarios.

In a separate study, Alnasif et al. [48] aimed to determine the most accurate kinetic model to estimate experimental measurements of NO mole fractions in NH_3/H_2 (70/30 vol%) binary flames. This study evaluated 67 different kinetic reaction mechanisms. Alnasif's study results showed that the kinetic model suggested by Nakamura et al. [50] has suitable predictive capabilities and precisely match experimental measurements within the specified uncertainty limits.

1.1.8 Burner optimization studies

In the literature, there are many studies about the burner optimization. These studies investigate different parameters such as burner geometry, fuel mixture, wall temperature, pressure, inlet velocity, mass flow rate, equivalence ratio etc. Although the number of ammonia studies are increasing today, there are few studies about the ammonia focused burner optimization.

Kurata et al. [53] modified the micro gas turbine injector for operating with ammonia/kerosene, ammonia/methane, and pure ammonia. This combustor was originally designed to be operated on kerosene, then it was modified to operate with ammonia blends.

Thompson et al. [54] performed multi-objective optimization of an industrial pre-mixer by using ANSYS Fluent® and ANSYS Design Exploration®. They tried 4 different turbulence models to validate their cold flow CFD model and selected the standard k- ϵ model after the comparison of the results. 4 geometric dimensions were optimized to achieve the correct AFR (air-fuel ratio), complete the mixing of the air and fuel prior to entry into the combustion chamber and lower NO_x emissions. NSGA-II and Nelder Mead optimization algorithms were compared by using natural gas as a fuel. Both multi-objective optimization algorithms achieved 30% improvement in the extent of mixing with design modification.

Khelladi et al. [55] investigated the effect of bluff body shape on flame stability in a non-premixed methane/hydrogen/air mixture combustion. They validated their ANSYS CFX® model with the experimental data of Sydney HM1 flame. They compared 3 different bluff body shapes: cylindrical, semi-spherical and conical. According to the results; only the cylindrical form satisfies the stability criteria, which necessitates a high temperature zone in conjunction with a slow speed zone in order to provide a continuous thermal source capable of maintaining combustion.

Kashir et al. [56] used OpenFoam® to investigate the impact of hydrogen enrichment and bluff body lip thickness on the characteristics of blended C₃H₈/H₂ bluff body stabilized turbulent diffusion flames. Before starting the parametric studies, they validated their steady RANS model by using Sydney HM1 flame. After validation; they performed parametric unsteady RANS simulations for 2 different bluff-body geometries (lip thickness and diameter) and 4 different fuel mixture compositions.

They used PolimiC1C3 reaction mechanism (82 species / 1485 reactions) with flamelet and radiation approaches.

In his thesis, Deger [57] shows that by doing parametric studies on selected 3 synthesis gasses, it is possible to decrease CO and CO₂ emissions without making any concessions about the power via using optimization methods. In the beginning of his study, he used experimental data of non-premixed Sandia swirl burner with pure CH₄ fuel (HM1 flame) to validate the steady state ANSYS Fluent® 2D-CFD model. Then, he used the non-commercial optimization software Optikor to perform optimizations with genetic algorithm. 3 different optimizations were performed for each bio synthesis gas separately. Inlet boundary conditions and operating pressure were optimized to reduce emissions with constant burner geometry.

Baej et al. [58] was conducted CFD simulations by using the premixed swirl burner that is part of the experimental rig situated at the Gas Turbine Research Centre of Cardiff University (Figure 1.41). Experiments were performed with 100kW power under atmospheric conditions (1Bar, 300K) and results were used to investigate flame stability limits. ANSYS Fluent® was used with SST k- ω turbulence model. Burner geometry was meshed with 150k elements using ICEM Meshing®.

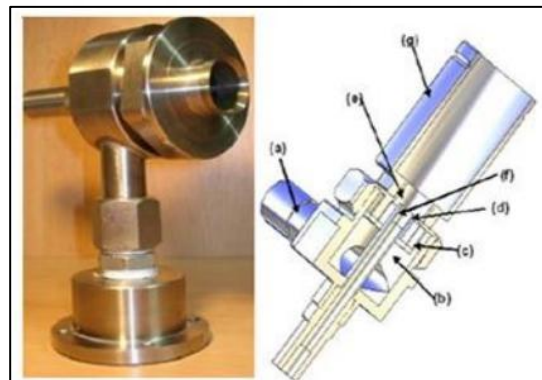


Figure 1.41 : Swirl burner and schematic diagram, respectively [58].

Two swirlers (1.05 with four tangential inlets; 1.5 with nine tangential inlets) and various divergent angles (30°, 45°, 60°, 90°) were investigated in simulations by applying two different inlet conditions (Table 1.8 and Figure 1.42). CH₄ and CO₂ fuel blends were used with various equivalence ratios. Laminar flame speeds were calculated by using CHEMKIN-PRO/PREMIX and imported to CFD model. Axial velocities were compared for different angles (Figure 1.43).

Table 1.8 : Inlet boundary conditions [58].

Test	Inlet T	Inlet P	CH ₄ [g/s]	AIR [g/s]	CO ₂ [g/s]	Total [g/s]
T1	300K	1 Bar	0.27	5.5	None	5.85
T2	300K	1 Bar	0.27	4.94	0.27	5.48

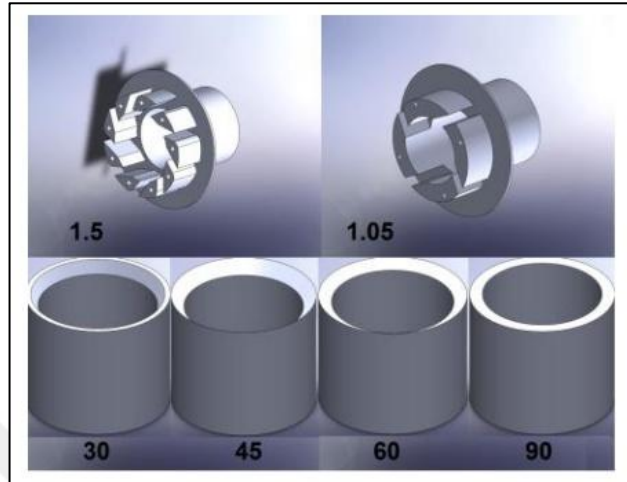


Figure 1.42 : Geometrical swirl number 1.5, 1.05 and various divergent angles nozzles, respectively [58].

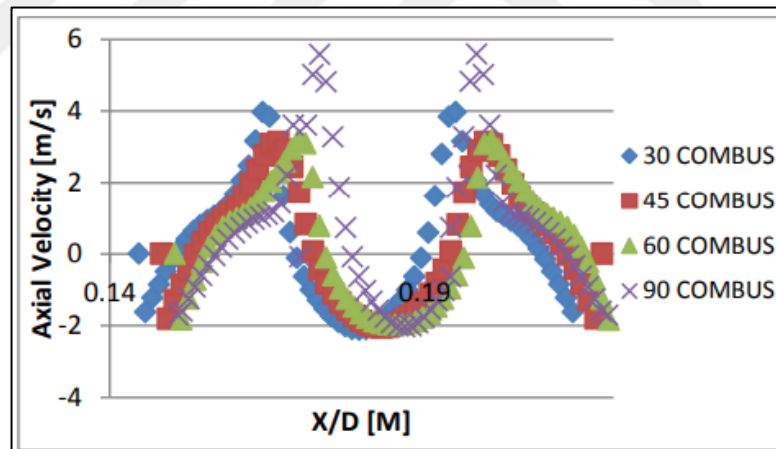


Figure 1.43 : Comparison of the axial velocity of different angles [58].

1.2 Purpose and Scope of the Thesis

The purpose of this thesis is the optimization of the existing burner to obtain efficient NH₃/H₂/N₂/O₂ fuel burner. Also, the mass fractions of fuel species were optimized to reduce the total fuel consumption and H₂ usage while increasing the efficiency of the modified burner. 4 steps were followed to achieve these targets respectively;

- CFD validation of selected burner both for cold flow and reacting flow regimes

- b. Burner geometry optimization to minimize the fuel consumption for the same heat release rate by keeping the flame stability (efficiency improvement phase)
- c. Secondary fuel blend optimization to reduce the H_2 use with minimum NO_x emissions (emissions optimization phase)
- d. Investigation of the effects of various inlet boundary conditions (temperature and pressure) for $NH_3/H_2/N_2/O_2$ flame and final burner improvements

1.3 Unique Aspect

Extensive experimental and numerical studies in the literature have investigated burner optimization and NH_3/H_2 combustion. However, the majority of existing work remains limited to parametric analyses or focuses on isolated aspects such as fuel blending, operating conditions, or simplified geometrical configurations. In particular, studies that integrate a validated CFD framework with multi-objective optimization techniques for NH_3 combustion systems are still scarce. Moreover, no previous study has been identified in which coupled CFD software and optimization tool to perform a multi-objective optimization of an NH_3 fueled swirl burner.

The present thesis addresses these gaps by establishing an integrated optimization framework that combines validated reacting flow CFD simulations with NSGA-II based multi-objective optimization. Unlike most existing studies, which investigate NH_3 or NH_3/H_2 combustion using predefined hydrocarbon burner geometries, this work aims to improve combustion performance while simultaneously reducing fuel consumption and NO_x emissions through geometry modification. In this respect, the study moves beyond conventional design approaches and targets the development of an efficient and environmentally friendly burner configuration.

A further distinctive aspect of this study is the use of the adaptive mesh refinement capability of Converge CFD[®] which significantly reduces computational cost compared to similar studies relying on fixed mesh structures. This advantage enables a more efficient exploration of the design space and facilitates faster convergence of the optimization process. Additionally, the application of NSGA-II optimization eliminates the need for exhaustive full-factorial DOE studies, providing an effective alternative to the predominantly parametric approaches reported in the literature.

Finally, unlike most existing optimization studies that focus on a limited number of design variables, the present thesis systematically investigates the combined influence of vane angle, number of vanes, confinement ratio, and NH_3/H_2 fuel blend within a unified multi-objective optimization framework. By simultaneously varying both geometrical parameters and fuel composition, the study enables a comprehensive exploration of the coupled effects of burner design and fuel reactivity on combustion performance and emissions. This integrated treatment of geometry–fuel interactions represents a distinct contribution beyond conventional single parameter or sequential optimization approaches commonly reported in the literature.

1.4 Impact

This thesis provides a practical and systematic guideline for the efficient optimization of NH_3/H_2 swirl burners using a coupled CFD and multi-objective optimization framework. The integration of optimization with validated CFD simulations represents a valuable methodological contribution to the NH_3 combustion literature and offers a transferable approach that can be readily applied to the optimization of other burner configurations.

By combining NSGA-II optimization with the AMR strategy, the proposed methodology enables the development of eco-friendly and high performance NH_3/H_2 burners with significantly reduced computational effort compared to conventional parametric or full-factorial approaches. This efficiency facilitates faster design iterations and supports the practical adoption of optimization driven burner development.

Moreover, the robust and validated numerical framework presented in this thesis contributes to the transition toward zero-carbon energy systems by reducing both fuel consumption and simulation time. The resulting decrease in burner modification costs and fuel demand has the potential to positively impact overall energy efficiency and operating expenses. Applying this optimization strategy to existing burner designs further provides a cost effective pathway for emission reduction, thereby enhancing the industrial relevance and societal impact of NH_3 based combustion technologies.



2. COLD FLOW

Cold flow validation is one of the most crucial steps in the numerical combustion studies. Reaction mechanisms are directly driven by velocity distribution and they cannot be solved correctly without the valid cold flow model. Furthermore, it will not be possible to accurately estimate the emissions, which have been the hot topic of the last couple of decades. Owing to the relatively cheap and safe test equipment requirements, there are several experimental studies on the cold flow characteristics of burners. In this thesis progress report; the LDA data of the unconfined low swirl burner in Cardiff University was validated with CFD model [59]. Six different turbulence models were applied for the numerical validation by using Converge CFD[®]. The first and the second order solutions of each turbulence model were compared with experimental results to find the most proper numerical model. According to the results; the second order k- ω SST turbulence model is the most appropriate model compared to others. The selected turbulence model and mesh settings are applied to the reacting flow model in the next step of the thesis.

In this chapter; the cold flow validation was performed for the selected swirl burner as a first step of the study. The numerical results of unconfined low swirl burner were compared with experimental results under cold flow conditions. Burner geometry and LDA data were taken from Gas Turbine Research Centre of Cardiff University. Converge CFD[®] was used to simulate the burner geometry with various turbulence models and axial velocity profiles were compared with experiments. The results of cold flow validation were used as an input for the next chapter; reacting flow validation.

2.1 Experimental Setup

The burner geometry and experimental data used in this study were taken from Gas Turbine Research Centre at Port Talbot, Wales, UK, which is a research facility of Cardiff University. The burner setup was shown in Figure 2.1 and detailed elsewhere [59-62].

The diagram illustrates the experimental setup for the CH₄-NH₃ system. A central vertical quartz tube reactor is the core component. At the top, a CH₄ inlet leads to a heated pipe and a pilot flame. A laser sheet from a Nd:YAG and Sirah dye laser system is directed at the reactor. The reactor has four pressure transducers (1-4), a swirler, and a flashback protector. Inlets for NH₃/air and H₂ are at the bottom. Various sensors (thermocouples, spectrometers, cameras) are connected to a central controller and data storage.

Technical drawing of a fuel injector assembly. The main view shows a cross-section of the injector with labels 'a' through 'e' and 'd'. A dimension of 0.3 is indicated for the upper section. Two orange arrows point towards the central nozzle, labeled 'Fuel + Air'. A detailed view of the nozzle tip is shown in the upper right, with dimensions 0.0212, 0.0115, and 0.0116. A circular view of the nozzle tip is shown in the lower right, with dimensions 0.0121, 0.0046, 0.0089, and 0.0015.

40

2.2 Numerical Model

Simulation of unconfined swirl burner was performed by using Converge CFD[®]. The slice that contains the 1/3 of the burner geometry was simulated to reduce the computational cost by using the advantage of symmetry. Transient solver was used with adaptive mesh refinement that applied to solve critical zones, especially close to swirler.

In Figure 2.3 surface meshed model was shown. In order to accurately simulate the unconfined test and prevent numerical errors that may arise from boundary conditions, the radial boundary of the burner was extended to double. Since the maximum axial-length of LDA data is 120mm, CFD model was cut from 200mm axial-length to reduce the computational time while keeping results independent from the boundary conditions. Constant mass flow rate was applied to inlet surface and all the outlet surfaces are assumed equal to atmospheric conditions.

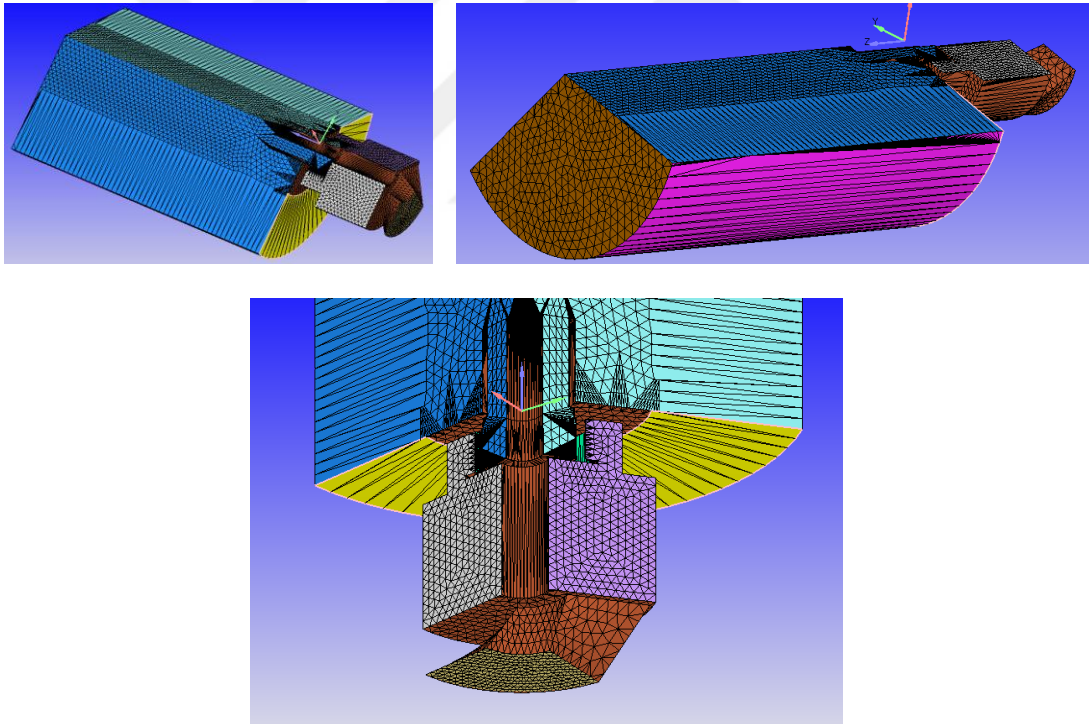


Figure 2.3 : Surface meshed burner model.

Volume mesh of second order k-W SST turbulence model that has 1.17 million cells is presented in Figure 2.4 to show the AMR controlled mesh structure in Converge CFD[®]. 6 different turbulence models were compared with both first and second order solvers (Table 2.1). Cell size of base grid is used as 4mm, with 0.2 m/s sub-grid criteria and 4 maximum embedding level.

Table 2.1 : Turbulence models used in CFD simulations.

No	Turbulence Model
1	RNG k- ϵ
2	Realizable k- ϵ
3	k- ω SST
4	Spalart-Allmaras
5	RSM-SSG
6	RSM-LRR

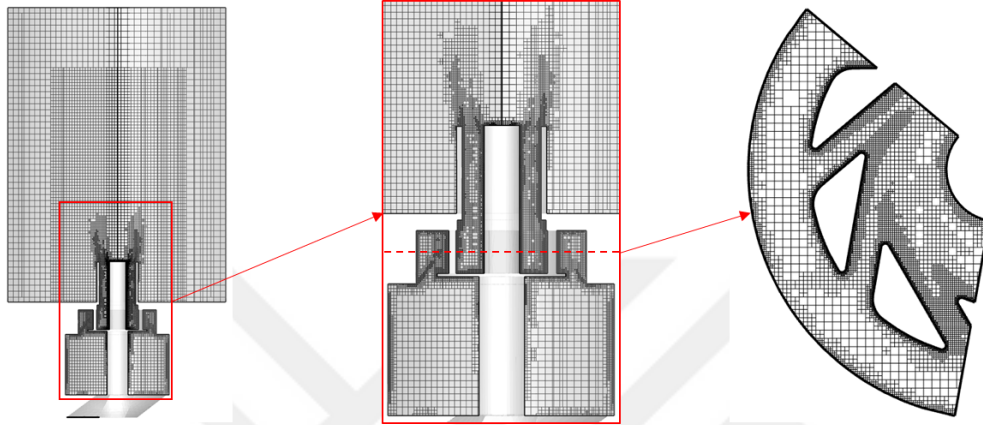


Figure 2.4 : Volume mesh of second order k- ω SST model.

A wall resolved mesh strategy was adopted using a target y^+ value of 2 within the model framework to ensure accurate near wall resolution while maintaining reasonable computational cost. The use of adaptive near wall mesh refinement provides a consistent numerical framework that satisfies the near wall resolution requirements of all turbulence models considered. Models with less restrictive y^+ requirements are therefore naturally covered within the same mesh configuration.

To overcome the complexity of CFD results, axial velocity profiles were obtained by using 2.5D method. In this method; equal spaced 2D planes were defined along the azimuthal direction of the volume meshed geometry. 3D data was converted to 2D plane by combining these planes with linear interpolation. The methodology of 2.5D method is described in Figure 2.5 below. Tecplot[®] was used to investigate the 2.5D results of CFD study.

The governing equations solved in the cold flow simulations are identical to those employed in the reacting flow cases; therefore they are not repeated in this chapter. A detailed description of the governing equations is provided in the following chapter. For the cold flow simulations, chemical source terms and thermal effects were deactivated, and the flow was defined as non-reacting.

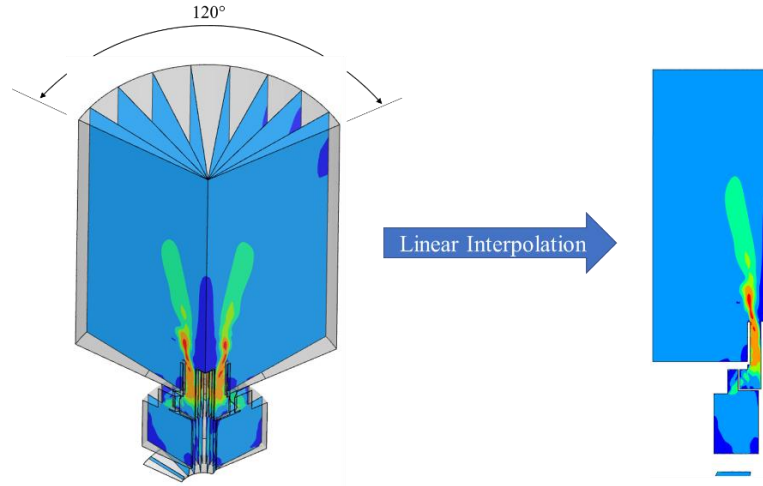


Figure 2.5 : Converting 3D data to 2D plane by using 2.5D method.

2.3 Governing Equations

The cold flow simulations were performed using Converge CFD[®], which solves the unsteady, compressible Navier–Stokes equations. Turbulence models simulated within the RANS framework [63].

The governing equations were discretized using the finite volume method and solved with the Converge CFD[®] solver. Details of the numerical schemes, pressure-velocity coupling and solution algorithms follow the standard implementation described in the Converge CFD[®] theory manual [63]. An ideal-gas equation of state was assumed for the gas mixture and density was evaluated as a function of local temperature, pressure, and composition.

2.3.1 Conservation of mass

The conservation of mass for a compressible flow is expressed as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (2.1)$$

Density variations due to the temperature changes and chemical reactions are fully accounted for in reacting flow simulations.

2.3.2 Conservation of momentum

The conservation of momentum is governed by the RANS equations:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[(\mu + \mu_t) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \right] \quad (2.2)$$

2.3.3 Turbulence models

2.3.3.1 RNG k-ε turbulence model

The RNG k-ε model solves transport equations for the turbulent kinetic energy k and its dissipation rate ε where R_ε is the additional RNG correction term:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \rho \varepsilon \quad (2.3)$$

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho u_j \varepsilon)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} - R_\varepsilon \quad (2.4)$$

2.3.3.2 Realizable k-ε turbulence model

The realizable k-ε model solves the following transport equations:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \rho \varepsilon \quad (2.5)$$

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho u_j \varepsilon)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 S \varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} \quad (2.6)$$

2.3.3.3 k-ω SST turbulence model

The k-ω SST model solves transport equations for k and the specific dissipation rate ω :

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \sigma_k \mu_t \right) \frac{\partial k}{\partial x_j} \right] + P_k - \beta^* \rho k \omega \quad (2.7)$$

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \sigma_\omega \mu_t \right) \frac{\partial \omega}{\partial x_j} \right] + \alpha_{sst} \frac{\omega}{k} P_k - \beta \rho \omega^2 + 2(1 - F_{sst}) \rho \sigma_\omega \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad (2.8)$$

2.3.3.4 Spalart-Allmaras turbulence model

The Spalart-Allmaras model solves a transport equation for the modified eddy viscosity variable $\tilde{\nu}$:

$$\frac{\partial(\rho \tilde{\nu})}{\partial t} + \frac{\partial(\rho u_j \tilde{\nu})}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \rho \tilde{\nu} \right) \frac{\partial \tilde{\nu}}{\partial x_j} \right] + C_{b1} \rho \tilde{S} \tilde{\nu} - C_{w1} \rho \left(\frac{\tilde{\nu}}{d} \right)^2 \quad (2.9)$$

2.3.3.5 RSM-SSG turbulence model

The RSM–SSG model solves transport equations for the Reynolds stresses R_{ij} where Φ_{ij}^{SSG} denotes the SSG pressure–strain model:

$$\frac{\partial(\rho R_{ij})}{\partial t} + \frac{\partial(\rho u_k R_{ij})}{\partial x_k} = P_{ij} + \Phi_{ij}^{SSG} - \varepsilon_{ij} + D_{ij} \quad (2.10)$$

2.3.3.6 RSM-LRR turbulence model

The RSM–LRR model also solves transport equations for the Reynolds stresses where Φ_{ij}^{LRR} represents the Launder–Reece–Rodi pressure–strain formulation:

$$\frac{\partial(\rho R_{ij})}{\partial t} + \frac{\partial(\rho u_k R_{ij})}{\partial x_k} = P_{ij} + \Phi_{ij}^{LRR} - \varepsilon_{ij} + D_{ij} \quad (2.11)$$

2.4 Results

Axial velocity contours those were obtained from LDA measurements are shown in Figure 2.6. The maximum velocity is 20 m/s on the swirler exit. Measurements were conducted from swirler exit to 120mm distance on the axial-direction with 36mm radius. According to the results; the flow slows down after the 120mm away from the burner. Although the left and right halves are looks symmetrical, they are not exactly same due to the swirling flow. Therefore, it is meaningful to compare the CFD results both with left and right halves of the LDA data.

Axial velocity profiles at various z-positions were extracted from CFD simulations. Velocity profiles, plotted from first and second order CFD solutions, were compared with LDA results in Figure 2.7 and Figure 2.8 respectively.

According to the results in Figure 2.7; there is not any turbulent model that compatible with the LDA measurement until the z-axis height reaches to 30 mm from the burner exit. This incompatibility shows the weakness of the first order solvers against the swirling flows as independent from the turbulence models. Also, the CFD results between (a) and (d) are offset compared to LDA at radial axis due to same reason. The maximum CFD axial velocities are lower than experiments until the swirl effect decrease above the 30 mm z-height (d). The axial velocities those are not dominated by swirl flow (below 6 mm and above 24mm radii) are more reliable to validate with

experiments. Above the 30 mm z-height; (e) and (f) plots are good enough to compare turbulence models with the first order solver.

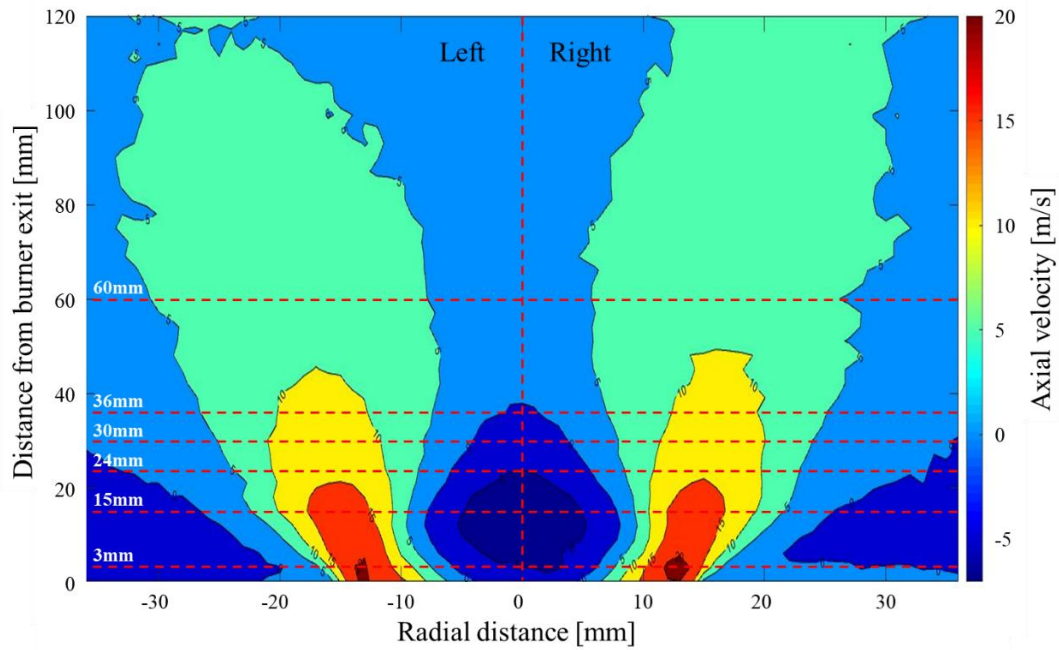


Figure 2.6 : Isothermal air flow velocity vector maps with axial velocity contours for the unconfined swirl burner [59].

The axial velocity profiles of (e) and (f) plots are compatible with experimental results, including maximum velocities. Although the results are very close to experiments at lower and higher radii, the first order Spalart-Allmaras model mismatches the velocity profiles at any z-position. The first order RSM-SSG and RSM-LRR models capture the maximum axial velocity above the 30 mm z-height, but they can not cover the lower axial velocity regions. The first order Realizable k- ϵ gets better to match with LDA as the z-height increases. However it distinctively leaves from the experimental results between the center of burner and the radial position of maximum axial velocity. The most capable first order turbulence models are RNG k- ϵ and k- ω SST. Both turbulence models give reliable results with experiments, but RNG k- ϵ is slightly better at lower radial positions. Also; RNG k- ϵ model is computationally cheaper than the k- ω SST model.

Similar to first order solutions; all of the chosen turbulence models give very similar results at 3mm above from the burner exit by using second order solver in Figure 2.8(a). However, they are much closer to experimental results compared to Figure 2.7(a). There is an offset between 15mm and 18mm radii at Figure 2.8(a) and there are small differences at lower radii also.

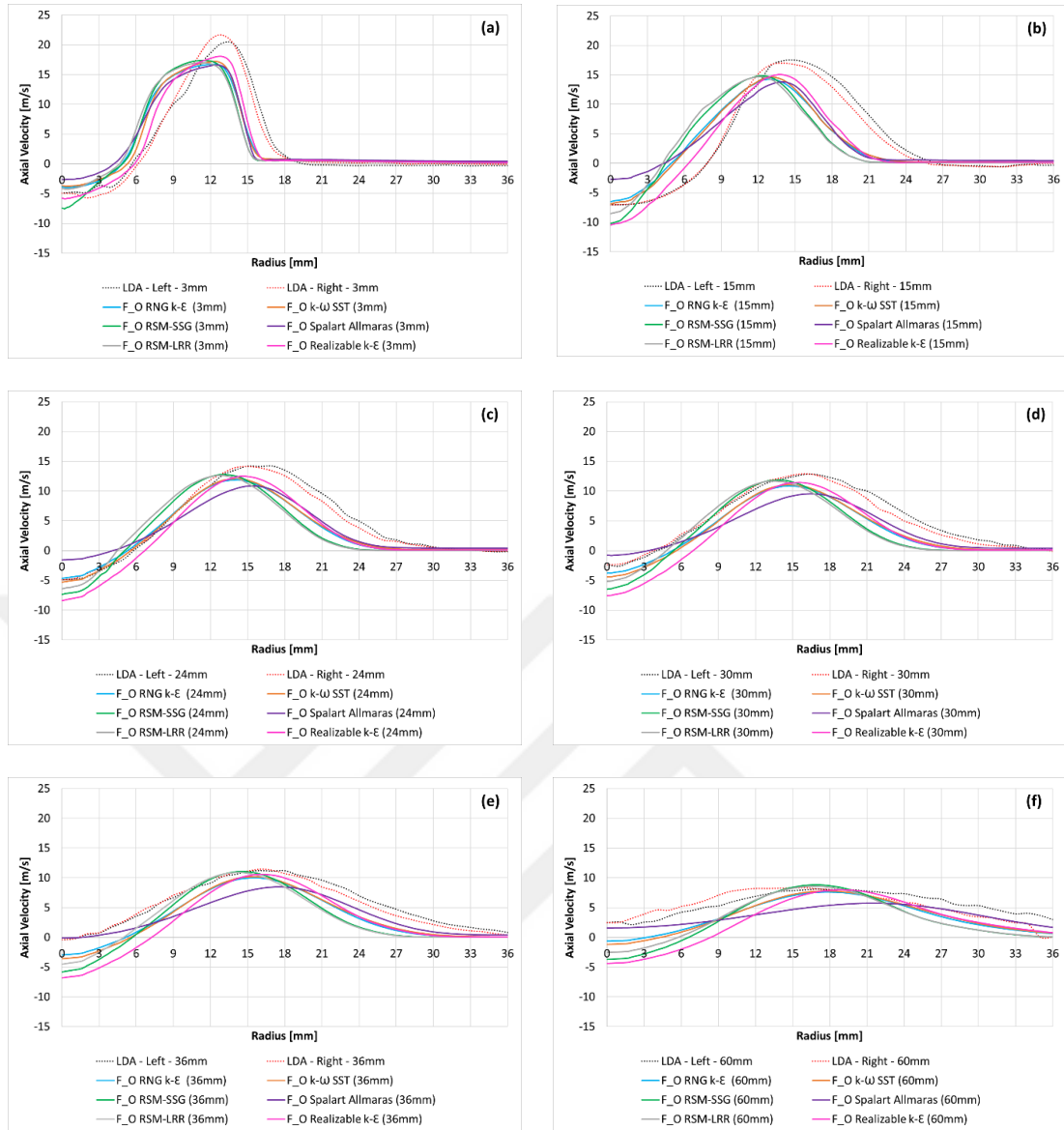


Figure 2.7 : Comparison of LDA and first order CFD results: (a) 3mm, (b) 15 mm, (c) 24mm, (d) 30mm, (e) 36mm, (f) 60mm.

Although the CFD results are perfectly matching with LDA below the 15mm at axial-direction; the differences of turbulence models increase above this axial position. The second order Spalart-Allmaras model does not capture neither the maximum velocity value not the characteristics of the plot likewise the first order one. The second order Realizable k- ϵ represents the lower radii velocity profile and the maximum velocity value at lower than 24mm axial-length, but it becomes to be different completely at higher axial-lengths unlike first order solution. Even tough the first order RNG k- ϵ gives the best results among the first order solutions; its second order version does not match with the experimental results. There are both offset with LDA results and axial velocity differences on the lower radii. The second order RSM-SSG and RSM-LRR

plots are very analogous except (c), (d) and (f) in Figure 2.8. RSM-SSG is better at lower radii while RSM-LRR gives maximum velocity more accurately. Both turbulence models are much preferable compared to their first order solutions. However, they do not fit to experimental results as much as the second order $k-\omega$ SST model. According to the results; the second order $k-\omega$ SST calculates the maximum velocity truly along the axial-direction. Although there are some insignificant differences, the axial velocity profiles and the characteristics of these profiles are proper to experimental results.

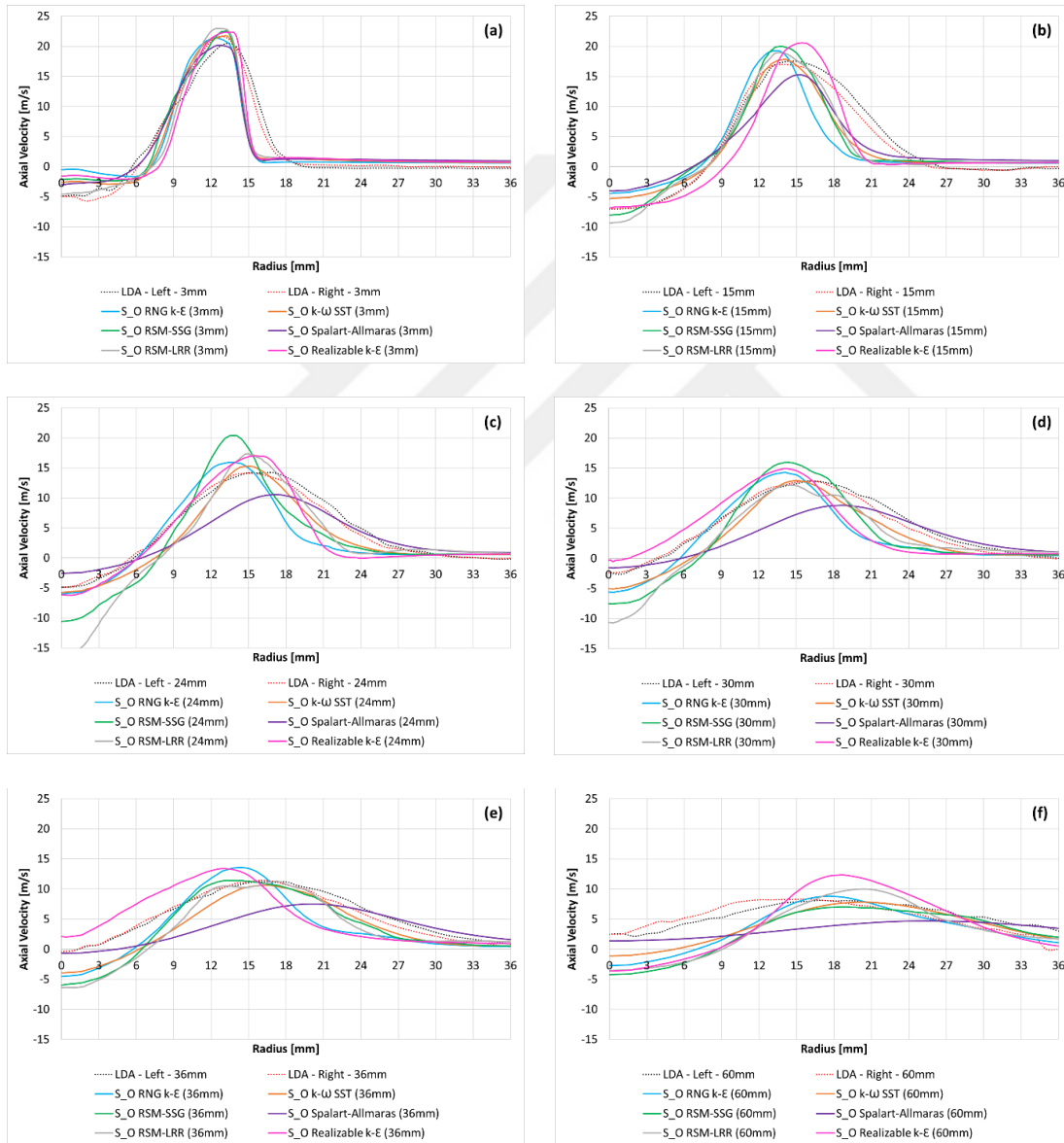


Figure 2.8 : Comparison of LDA and second order CFD results: (a) 3mm, (b) 15 mm, (c) 24mm, (d) 30mm, (e) 36mm, (f) 60mm.

To make a clear decision about the order of solution and the turbulence model; the winners of first and second order solutions were compared in Figure 2.9. According to

the results; the second order k- ω SST turbulence model was determined the most suitable model to LDA experiments.

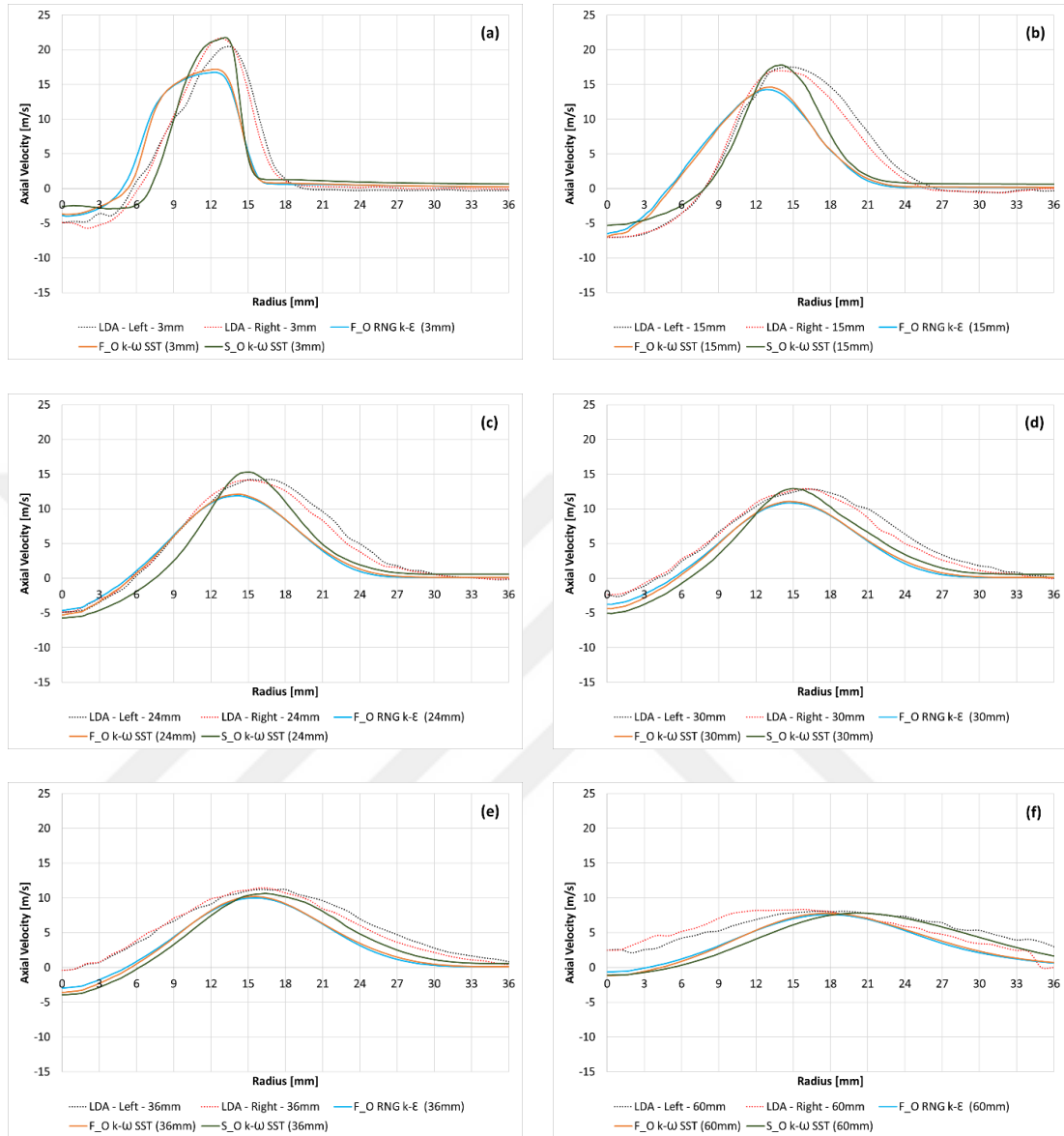


Figure 2.9 : Comparison of the first and second order solver results: (a) 3mm, (b) 15 mm, (c) 24mm, (d) 30mm, (e) 36mm, (f) 60mm.

To investigate the mesh dependency of numerical model; the results of 2mm (fine), 4mm (medium) and 6mm (coarse) base grid sizes were compared. The models have 0.53 million (coarse), 1.17 million (medium) and 4.2 million (fine) cells respectively. Velocity profiles of 15 mm axial length were investigated in Figure 2.10. Although there is not any significant difference between medium and fine results; coarse meshed velocity profile is separated from them. Therefore; 4mm base grid size is accepted as the proper mesh size for the numerical model.

In the present study, AMR strategy was employed to efficiently resolve the fluid flow while avoiding unnecessary mesh increase. Instead of relying on a uniformly fine static mesh, the computational grid was dynamically refined based on local solution gradients and complemented by fixed embedding in critical regions such as the swirler vanes and injector zones. This approach allows mesh to automatically concentrate resolution only where it is physically required, which is a defining advantage of the Converge CFD[®] framework. As a result; grid independent and experimentally consistent results were obtained with approximately 1.17 million cells in a 1/3 periodic domain. In contrast, studies based on static or locally refined meshes often require significantly higher cell counts to achieve comparable accuracy, highlighting the efficiency of the AMR methodology adopted in this work.

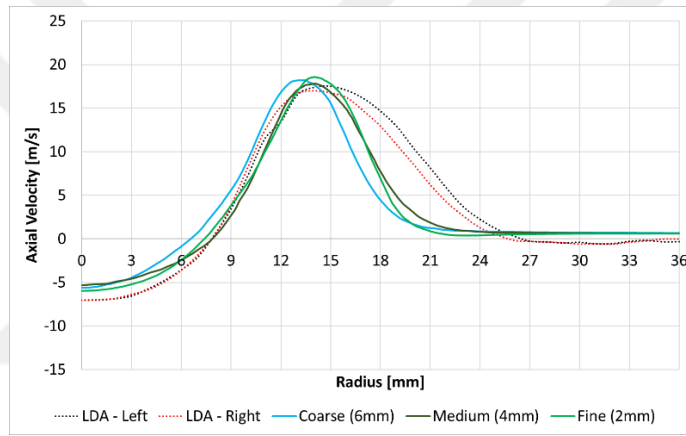


Figure 2.10 : Mesh dependency study at 15mm axial length.

In addition to local velocity profiles in Figure 2.10, integral quantities including pressure drop and outlet-averaged mass flow rate and velocity were compared on Table 2.2. The medium grid (4 mm) was selected for subsequent simulations as it provided similar integral trends while reducing the computational cost significantly compared to the fine grid.

Table 2.2 : Mesh dependency metrics.

Grid Size [mm]	Number of Cells [million]	Simulation Time [day] (6 cores CPU)	Pressure Drop [Pa]	Outlet Avg Mass Flow Rate [g/s]
6 (coarse)	0.53	3	665.1 (-4.8%)	13.10 (-0.6%)
4 (medium)	1.17	7	696.9	13.19
2 (fine)	4.20	20	674.5 (-3.3%)	12.85 (+2.6%)

The simulations were carried out using Converge CFD[®] with fully adaptive temporal and spatial discretization [63]. An adaptive time step strategy was employed, in which

the time step is dynamically adjusted based on CFL constraints and local flow conditions, ensuring numerical stability throughout the transient simulation. The simulation was initialized with 1.0e-7 seconds, while the allowable time-step range was defined by minimum 1.0e-8 seconds and maximum 0.001 seconds. The maximum CFL_u number based on velocity was set to unity together with $CFL_v=2$ for viscous effects. During the solution process, the adaptive algorithm selected an effective time-step magnitude that stabilized around 2.7e-6 seconds. According to the results; it is observed that the time step value is primarily limited by the CFL_u , with consistently approaching its prescribed upper bound. This behavior indicates that the temporal resolution is governed by the local flow dynamics rather than by user imposed time step limits and ensuring adequate resolution of the transient flow field.

2.5 Conclusions

The numerical validation of unconfined low swirl burner was performed by using Converge CFD[®]. The axial flow characteristics of the burner was obtained with LDA experiment. 6 different turbulence models were compared with experimental results both for the first and the second order numerical solutions. On the numerical models; the AMR was applied to accurately capturing the velocity profile without increasing the number of cells. Boundaries of numerical model were extended axially and radially to keep the results independent from boundary conditions. The numerical results were converted from 3D slice to 2D plane by applying 2.5D method. Calculated axial velocity profiles were compared with experimental results at various axial lengths. According to the results; the second order k- ω SST turbulence model is the most appropriate model compared to others.



3. REACTING FLOW

In this study, a tangential swirl burner at an industrial scale was numerically simulated. 50-50 (vol%) $\text{NH}_3\text{-H}_2$ fuel blend was employed for three power levels under rich (equivalence ratio 1.2) and lean (equivalence ratio 0.7) conditions across three power levels (10, 15, and 20 kW). The numerical modelling of the burner was explained in detail and simulations were performed using three different reaction mechanisms. Experimental temperature and exhaust emission data were used for model validation.

3.1 Experimental Setup

In this study, the burner geometry and related experimental data available at the Gas Turbine Research Centre (Port Talbot, Wales, England), a research facility of Cardiff University, were used. Figure 3.1 illustrates the burner setup. Further details can be found in other sources [59-62].

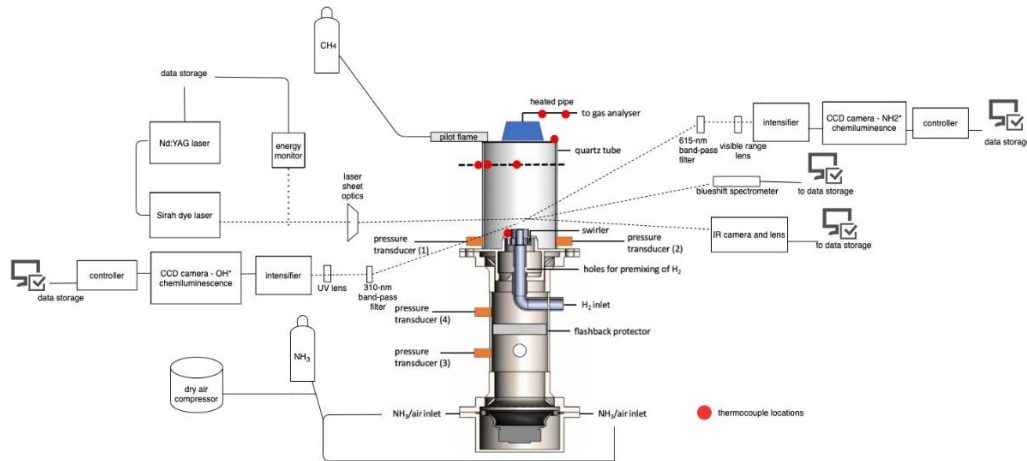


Figure 3.1 : Tangential combustor with measuring techniques and control systems [59].

A tangential swirl burner at an industrial scale, characterized by a geometric swirl number of $S_g=1.05$, was examined. A detailed geometric view of the burner is given in Figure 3.2. Fuels and air exit the burner's nozzle ($r = 28$ mm) from the premix chamber (label a) via a single radial-tangential swirler (label b), with the central

injection lance (label c) serving as a bluff body ($r = 16$ mm). The flame was contained within a cylindrical quartz enclosure (label d) featuring an expansion ratio of 3 in relation to the burner's exit nozzle. A honeycomb (label e) was implemented to reduce the risks linked to flashback and to homogenize the flow [62].

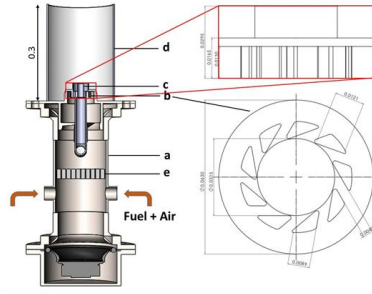


Figure 3.2 : Detailed geometrical view of the burner. Dimensions in meter (m) [62].

The burner was provided with Bronkhorst controllers for mass flow ($\pm 0.5\%$ within a range of 15–95% mass flow). Air and NH_3 are injected at the mixing chamber, while the H_2 is injected from the 6 equispaced holes those have 1.5mm diameter. They are located 4 cm below the burner exit, angled at 45° , give H_2 into the swirler directly for premixing with ammonia and air [40,59-61]. GE214 quartz material was used at the burner walls for the optical access [61].

Time-averaged flame images were obtained with two simultaneously operating intensified cameras (LaVision Imager intense) [59]. 500 frames were collected at each case with LaVision Davis v10. Abel Deconvolution was applied to the time-averaged data, following a 3x3 pixel median filter. Chemiluminescence images were normalized to their peak intensity in the colourmaps to showcase the variations in species distributions for each flame. The results of measured species are given in the section 3.3 (Figure 3.9-3.11-3.13). Temperature profiles were measured using K and R type thermocouples linked to a data logger with a sampling frequency of 1 Hz. Thermocouple data were collected at each point for 120 s and averaged. The thermocouples were calibrated with an average error of 3%. The collected temperature data were corrected according to [64] to account for conductive heat transfer between the thermocouple bead and the connecting thermocouple wires, and radiative and convective heat transfer between the thermocouples and their surroundings. A custom quantum cascade laser analyzer (Emerson CT5100) with a sampling frequency of 1 Hz ($\pm 1\%$, 0.999 linearity) and operating at 463 K was used to measure exhaust emissions consisting of NO , NO_2 , N_2O , NH_3 , H_2O and O_2 . An isokinetic funnel with

an inlet diameter of 30 mm was positioned 50 mm above the outlet of the quartz restriction to obtain homogeneous samples from the exhaust under the specified operating conditions. A heated line at 160 °C was used to obtain exhaust samples and prevent condensation [61]. All emission data were collected for 120 s and averaged. The emission data provided here are normalized to a reference of 15% O₂ [65].

The dilution methodology was presented by adding N₂ to the sample [61]. Bronkhorst EL-FLOW Prestige MFC with the high sensitivity was used in this process. Before mixing with the exhaust samples, N₂ is heated by the system to 160 °C. The flow meter in the analyzer, calibrated by the manufacturer, is sufficient for its standard purpose. equation (3.1) is used for the calculation of the flow rate of the exhaust process sample in the system during the dilution methodology. The repeatability in this dilution methodology is ±10%. This methodology is applied when wet readings are above the detection range of the analyser.

$$F_s = F_{t,in} - F_{d,N_2} \quad (3.1)$$

Temperature values at various locations and exhaust emissions were measured for 6 different cases. Three power levels were investigated both for the rich (equivalence ratio 1.2) and lean (equivalence ratio 0.7) conditions. Equivalence ratio changed by adjusting the air flow for the constant fuel flow rate. The cases and test parameters are given at Table 3.1.

Table 3.1 : Simulated cases.

Case number	NH ₃ /H ₂ (vol.%)	NH ₃		H ₂		Air		Equivalence ratio (Φ)	Power (kW)
		Vol. flow rate (L/min)	Mass flow rate (g/s)	Vol. flow rate (L/min)	Mass flow rate (g/s)	Vol. flow rate (L/min)	Mass flow rate (g/s)		
1	50/50	51	0.613	51	0.073	254	5.168	1.2	20
2	50/50	51	0.613	51	0.073	435.4	8.86	0.7	20
3	50/50	38.3	0.46	38.3	0.0545	190.7	3.881	1.2	15
4	50/50	38.3	0.46	38.3	0.0545	327	6.653	0.7	15
5	50/50	25.5	0.306	25.5	0.0363	127	2.584	1.2	10
6	50/50	25.5	0.306	25.5	0.0363	217.7	4.43	0.7	10

3.2 Numerical Model

Converge CFD[®] [63] was used for the numerical simulation of the swirl burner. In Figure 3.3; the surface meshed 3D model is shown. In order to minimize the computational cost, the burner geometry was modeled as a 1/3 slice by taking advantage of periodic boundaries. The axial length of burner was extended 30 mm

from the outlet surface to accurately simulate the experiments and prevent numerical errors that may arise from boundary conditions. Also, the extended outlet volume represents the exhaust gas sample that is used for emission analysis in experiments. Therefore, it used to calculate numerical emissions from the simulation results. The inlet surfaces were defined with a constant mass flow rate (Table 3.1) with 288 K gas temperature, and outlet surface was assumed to be at atmospheric conditions. All of the burner and swirler walls are defined as adiabatic with no-slip boundary conditions. A transient RANS model was employed with adaptive mesh refinement to address critical regions, particularly near the swirler.

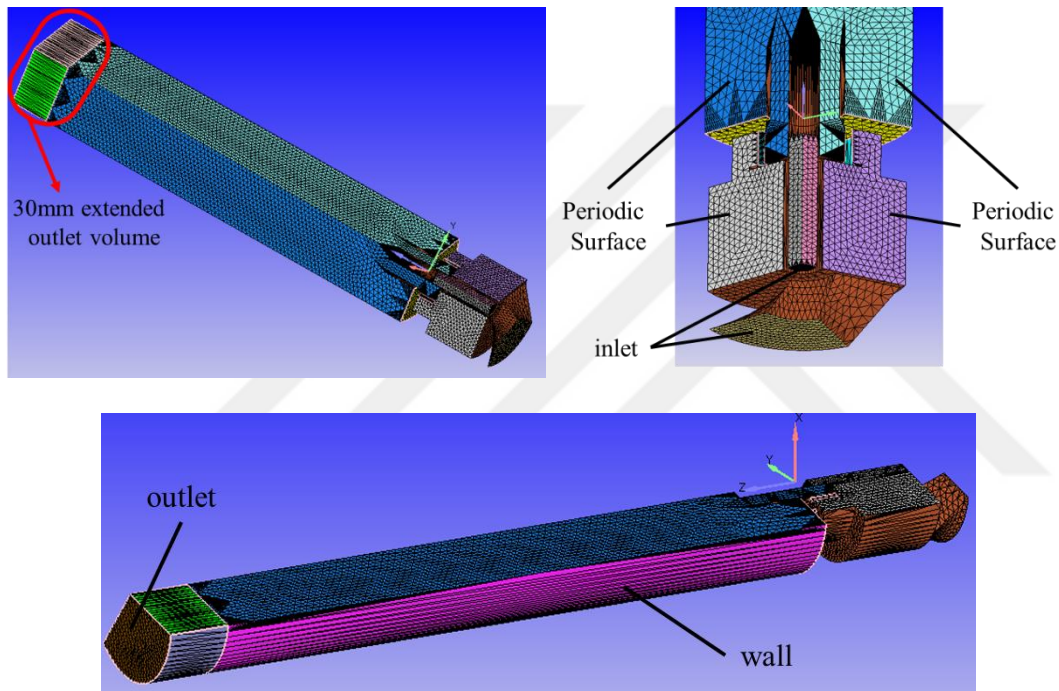


Figure 3.3 : Surface meshed burner model.

Figure 3.4 represents the AMR controlled volume mesh structure of the model with 1.2 million cells generated in Converge CFD®. The base grid size of the cell is selected as 4 mm with 3 maximum embedding levels for temperature AMR and a 3K sub-grid criterion. 0.05 m/s velocity sub-grid criteria applied to inlet and swirler region while the other regions have 0.2 m/s velocity sub-grid criteria. All of the domains have 4 maximum embedding level for the velocity AMR. Surface of the swirler vanes improved with 2 embed layer with 5 scale fixed embedding. 2 embed layers were added to inner surface of the nozzle holes with 4 scale fixed embedding also. As a final mesh improvement; the lower axial half of the domain refined with 1 scale fixed embedding. With this meshing strategy; all critical zones are captured accurately while

avoiding over-meshing, which reduces total computational time. Readers interested in the adaptive meshing technique and its definitions are referred to [63] for further details.

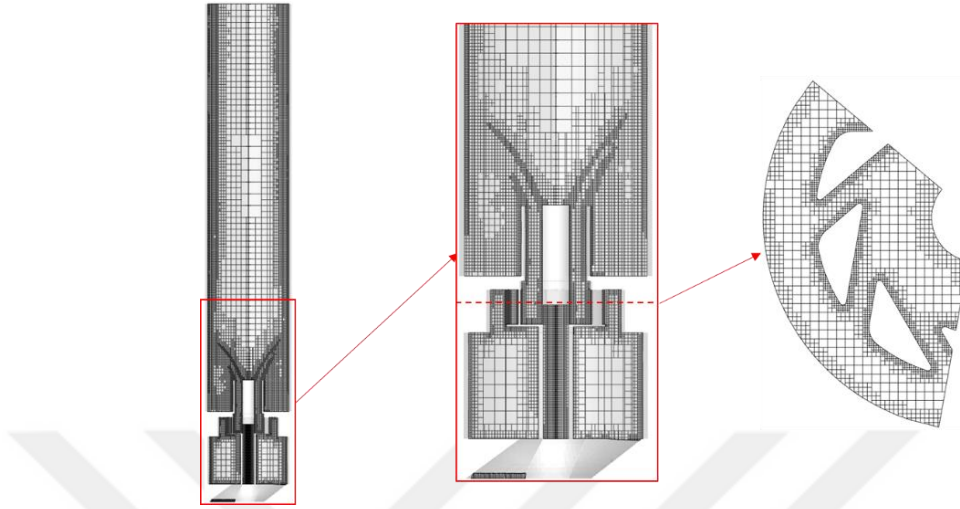


Figure 3.4 : Adaptive volume mesh of the model.

The cold flow validation of this burner is performed at previous study [66]. Gulsan and Boke [66] compared six different turbulence models both for the first and second order solvers to obtain the most proper model with the LDA experiments. As a result of the comparison of axial velocity profiles at various axial positions; the second order k-w SST turbulence model was selected the most suitable model with experiments (Figure 3.5). It is consistent with previous studies [18, 34-35, 58, 67] that have used k-w SST turbulence model in similar burner simulations. Also, the one of them [67] has an additional turbulence model comparison that chooses k-w SST for the tangential swirling flows. Once the isothermal profiles were validated; the numerical model was modified for the investigation of reacting flow in this study.

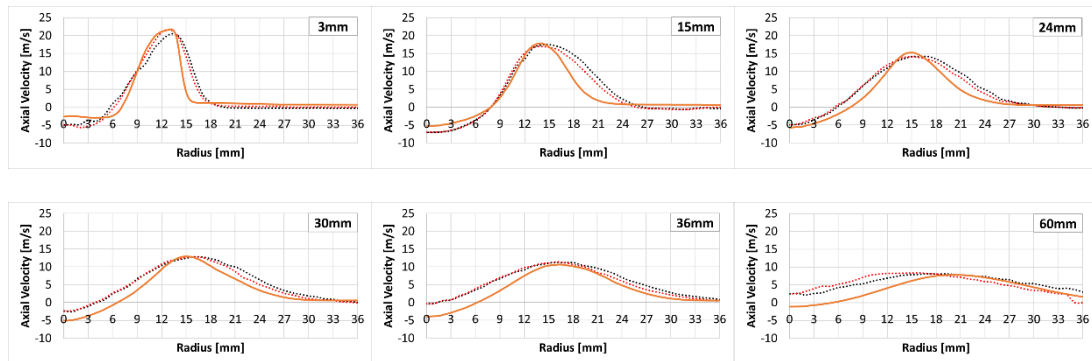


Figure 3.5 : Comparison of velocity profiles at various axial positions. LDA experiments (dashed red line-right side, dashed black line-left side) and numerical (solid orange line) [66].

The selection of kinetic mechanisms in this study was guided by the comprehensive comparative framework proposed by Alnasif et al. [51], who evaluated a wide range of NH_3 and NH_3/H_2 reaction mechanisms over different Φ , NH_3/H_2 blends and combustion regimes. Their analysis clearly demonstrates that the predictive capability of a kinetic mechanism is strongly dependent on the target application and operating conditions, and that no single mechanism can simultaneously provide optimal accuracy, robustness, and computational efficiency across all regimes relevant to NH_3 based combustion systems.

Within this framework, the reduced mechanism developed by Duynslaegher et al. [49] represents an approach primarily driven by computational efficiency. By limiting the number of species and elementary reactions, this mechanism enables large scale parametric investigations and optimization studies within feasible computational time. However, such simplification inevitably restricts the representation of detailed nitrogen chemistry, particularly the formation and consumption of intermediate species such as NH , NH_2 , and N_2H , which play a critical role in NH_3 oxidation and NO_x formation. As a result, while this mechanism may reproduce global combustion trends under certain conditions, its ability to accurately capture NO_x sensitivity to fuel blending and Φ variations remains limited.

The mechanism proposed by Nakamura et al. [50] places specific emphasis on reproducing flame reactivity and laminar flame speed with high fidelity. These characteristics are directly linked to flame stabilization, reaction zone location, and heat release rate distribution where geometric parameters and NH_3/H_2 blending ratios are systematically varied. Although the treatment of NO_x chemistry in the Nakamura mechanism is less detailed than in more comprehensive nitrogen chemistry mechanisms, it has been shown to provide numerically stable and consistent trends in combustion behavior over a wide operating range. From an optimization perspective, this robustness in predicting relative performance changes between different designs is more critical than achieving absolute accuracy in emission levels.

In contrast, the detailed mechanism developed by Stagni et al. [52] offers an extended and more rigorous description of nitrogen chemistry, including multiple NO_x formation and interconversion pathways. This level of chemical detail allows a more in-depth interpretation of emission mechanisms and species evolution, particularly under conditions where fuel bound and thermal NO_x pathways interact. Nevertheless,

the increased complexity of the mechanism leads to a substantially higher computational cost and may introduce numerical sensitivity when applied to complex flow configurations characterized by strong swirl and intense flame and flow interaction. Previous comparative studies [51] have also reported that such detailed mechanisms can exhibit increased sensitivity to operating conditions, which may reduce their suitability for optimization driven design exploration.

Based on the categorization and performance trends reported in [51], these three mechanisms (Table 3.2) were selected to represent distinct levels of chemical fidelity and modeling priorities, ranging from reduced formulations to detailed nitrogen chemistry. This approach enables a systematic evaluation of the trade offs between computational cost, combustion dynamics and NO_x prediction capability within the simulations. Rather than assuming a priori superiority of a single mechanism, the performance of each mechanism under identical geometric and fuel blending conditions were assessed in this chapter. The comparative reacting flow results are therefore used as the basis for interpreting the strengths and limitations of each mechanism and for identifying the most suitable modeling strategy for the targeted operating range. The summary of the boundary conditions and parameters of the study is provided in Table 3.3.

Table 3.2 : Compared reaction mechanisms.

No	Reaction Mechanism	Number of Reactions	Number of Species
1	Duynslaegher [49]	80	19
2	Nakamura [50]	232	33
3	Stagni [52]	210	31

Simulations were performed with SAGE detailed chemistry solver by using 50-50 (vol%) NH₃-H₂ blend. Six different experimental cases (Table 3.1) were simulated with Duynslaeger et al. [49], Nakamura et al. [50] and Stagni et al. [52] mechanisms to obtain the most appropriate model.

Table 3.3 : Boundary conditions and parameters.

Parameter	Value
Quartz Wall Temp	Adiabatic
Burner Section	Symmetry (120°)
Swirler Walls	Adiabatic
Inlet Boundary Condition	Table 3.1
Inlet Temperature	288K
Inlet Pressure	1.1 Bar
Outlet Pressure	Atmospheric P
Blend	50-50 NH ₃ -H ₂ (vol%)
Mixing	Fully Pre-Mixed
Equivalence Ratios	0.7 and 1.2
Power	10/15/20 kW
Turbulence Model	k- ω SST
Walls	No-Slip
Swirl	1.05

3.3 Governing Equations

The reacting flow simulations were performed using Converge CFD[®], which solves the unsteady, compressible Navier–Stokes equations coupled with energy and species transport equations. Turbulence–chemistry interaction effects were modeled within the RANS framework using the k– ω SST turbulence model [63]. The governing equations and turbulence formulation are identical to those described in Section 2.3.

In addition to the governing equations presented for the cold flow simulations, the reacting flow cases include the solution of the energy equation and species transport equations in order to account for heat release and chemical source terms under reacting conditions.

3.3.1 Conservation of energy

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial(\rho u_j e)}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left[(K + K_t) \left(\frac{\partial T}{\partial x_j} \right) \right] + S_e \quad (3.2)$$

The energy source term S_e includes the heat release due to chemical reactions.

3.3.2 Species transport

For each chemical species, the transport equation is written as:

$$\frac{\partial(\rho Y_m)}{\partial t} + \frac{\partial(\rho u_i Y_m)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\rho (D_m + D_{t,m}) \left(\frac{\partial Y_m}{\partial x_i} \right) \right] + \dot{\omega}_m \quad (3.3)$$

3.4 Results

The results of numerical model were compared with experimental measurements for the reacting flow validation. Temperature values and exhaust species were investigated with simulations to choose the most proper reaction mechanism with experiments. The thermocouple locations are shown in Figure 3.1. Temperature data taken from four different thermocouple locations (Figure 3.6) was compared with CFD results in Figure 3.7.

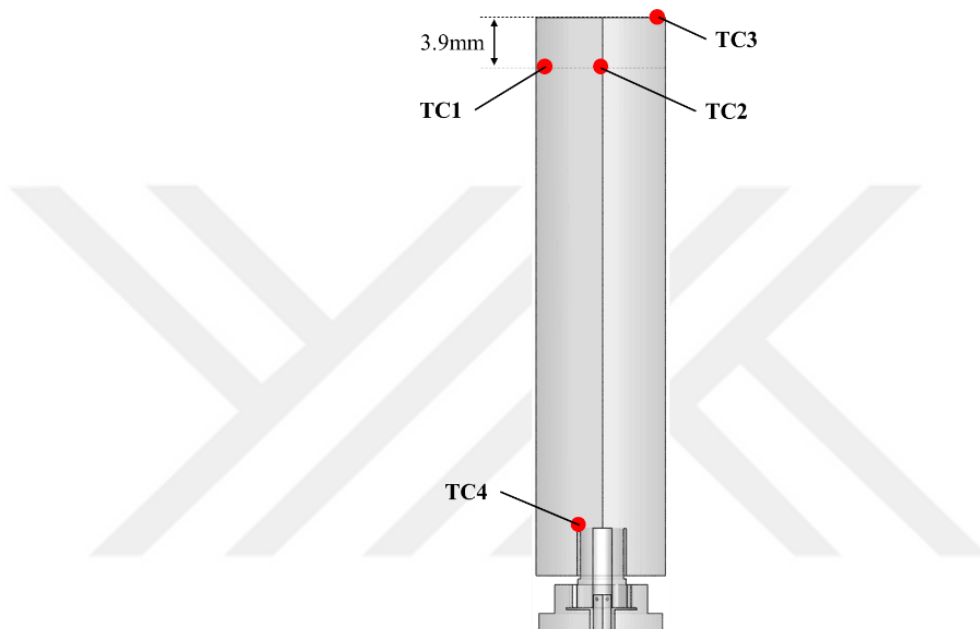


Figure 3.6 : Thermocouple names and locations.

For the thermocouple TC1 that located on the 3.9 mm inside of the burner exit; the temperature values of the rich cases (1-3-5) are lower than the lean cases (2-4-6) in experiments. Dependent to the fuel flow; the temperature of TC1 is decreases from case 1 to 6. At the case 2 and 4; the numerical errors are below the measurement error and all of the mechanisms match perfectly with experimental data. Stagni et al. [52] overpredicts at the case 3 and Nakamura et al. [50] underpredicts at the case 6; although the Duynslaeger et al. [49] have valid results for both cases. The numerical errors are at significant level only for the rich cases 1 and 5. Although the percentage of errors are close to each other; Nakamura et al. [50] gives the best results with experiments at case1 and case5. Compared to rich cases (1-3-5); the CFD results are much closer to experimental measurements at lean cases (2-4-6) independent from the mechanism. While the errors of numerical models are lower (4%) at lean cases, they increase to nearly 9% under rich conditions.

For the thermocouple TC2 which at the center of the burner exit; all of the CFD results give lower errors ($\leq 5\%$) with the experiments. Rich cases (1-3-5) have a good accuracy with all mechanisms, all of the errors are below the thermocouple reading error. At the lean cases (2-4-6); Nakamura et al. [50] and Stagni et al. [52] have better results compared to Duynslaegher et al. [49]. The lean experiments have higher temperature values than simulations.

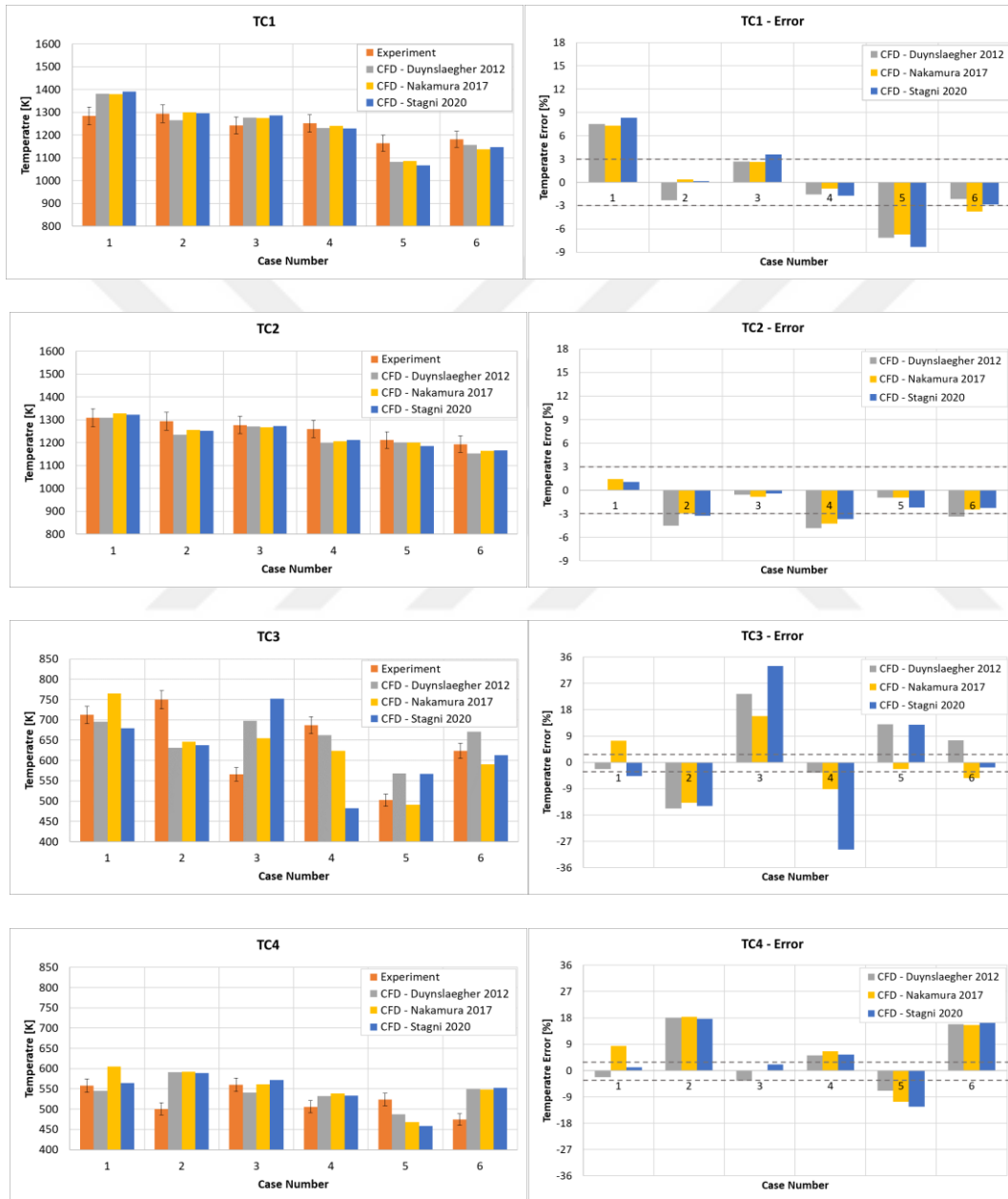


Figure 3.7 : Comparison of temperature data at various burner locations.

For the TC3; the thermocouple temperature increases at lean conditions compared to rich ones. Stagni et al. [52] mismatches with experiments both for the rich and lean conditions especially at cases 2, 3 and 4. Although the Duynslaegher et al. [49] gives

better results than Stagni et al. [52]; it gives higher variances with experiments. Compared to these two mechanisms, Nakamura et al. [50] represents the TC3 temperature better.

Similar to TC2; the temperature decreases at lean conditions on the TC4. The errors nearly 18% for the cases 2 and 6. Nakamura et al. [50] has the highest overprediction at the cases 1 and 4. Although it has very high errors at case 2 and 5; Stagni et al. [52] has the good results for other cases. Although the results of each mechanism are challenging; there is not any physical correlation between the temperature values and combustion parameters.

In Figure 3.8; the temperature distribution of simulations is presented for each case. Independent from the reaction mechanism, it can be said that the average temperature of burner is lower for the rich cases (1-3-5) except Duynslaegher Case1 and Case2. With the increase of air flow; the maximum temperature locations getting smaller and the higher temperature zones shrink. Compared to other two mechanisms; Duynslaegher et al. [49] have lower mixing zone temperature especially for the first three cases. It also has higher local temperature values for the last three cases. Nakamura et al. [50] and Stagni et al. [52] mechanisms have similar trends at all of the cases.

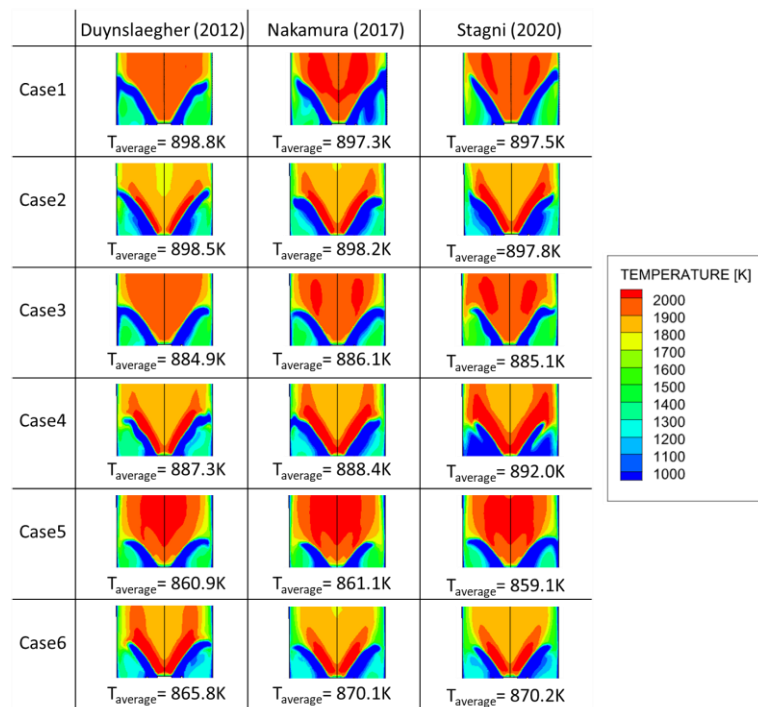


Figure 3.8 : Temperature distributions of simulated cases.

These temperature differences reflect how each mechanism handles ammonia-hydrogen combustion under different conditions. Duynslaegher [49], which was originally developed for low-temperature environments, tends to predict lower flame temperatures, especially in lean mixtures, likely due to slower NH_3 oxidation rates [47]. Nakamura [50] provides better results in rich conditions, where fuel-N conversion is more dominant and oxygen availability is limited [48]. Furthermore, the overall lower flame temperatures observed in rich cases are consistent with earlier studies, which associate fuel-rich combustion with incomplete oxidation and reduced adiabatic flame temperature [7].

On the experimental studies; the OH, NH and NH_2 species were measured with chemiluminescence. Images were normalized to the maximum value of each image to show the differences of species for each case.

In Figure 3.9; OH distribution of experiments are presented. The maximum OH generation occurs at the stagnation points around the recirculation zone. Dependent to the stagnation point of the recirculation zone; OH generation region relocates from liner walls to the center of the burner while the flow rate decreases at rich cases (1-3-5). In contrast to the rich cases; the max OH is seen on the center of the burner under lean conditions (2-4-6). There is not any region close to the liner walls that has higher OH value. Due to the higher flow rates at lean conditions; stagnation points, those generate higher OH, disappear from the recirculation zone.

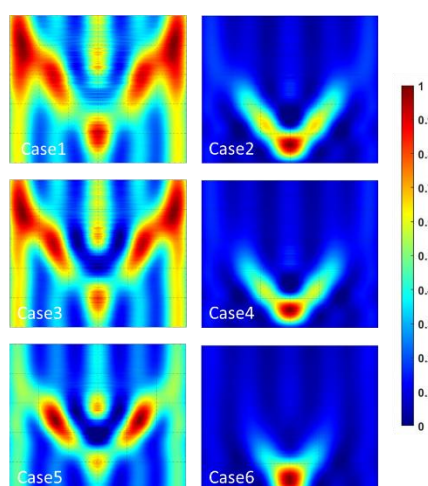


Figure 3.9 : OH distribution of experiments.

In Figure 3.10; the OH distributions of simulations were given also. The models successfully show the OH distribution for the rich cases (1-3-5). All of the three

mechanisms give similar results. The lean conditions (2-4-6) generate higher OH and the maximum OH is seen at case 4. Duynslaegher et al. [49] follows a different pattern at lean cases while other mechanisms are similar. Since the tendency of lower OH at Case 2; Nakamura et al. [50] one step closer to the experimental measurement.

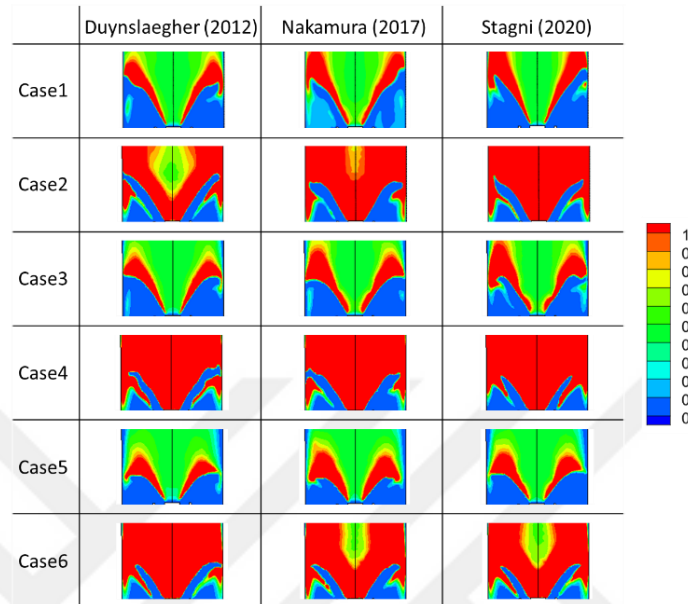


Figure 3.10 : OH distributions of simulated cases (*normalized with max $5.0e-4$ mole fraction*).

The observed OH distributions are closely linked to the flow structure, particularly the central recirculation zone generated by the swirl flow. Under lean conditions, the excess oxygen supports higher OH radical formation along the centerline, consistent with previous studies that highlight the oxidizing nature of fuel-lean flames [7]. In contrast, rich conditions result in more laterally distributed OH zones, likely due to fuel stratification and limited oxidizer availability near the core. While all three mechanisms qualitatively capture these trends, Nakamura [50] provides the closest match to the experimental OH profiles, particularly in terms of intensity and spatial alignment.

In Figure 3.11; the NH distribution of chemiluminescence measurements were given. The trend of NH distribution is very similar to OH for the lean conditions (2-4-6). The maximum NH is seen at the center of burner. For the rich cases (1-3-5); there are critical zones those same with the OH distribution. However; the liner walls getting higher NH values while the power of burner decreases in constast to OH distribution. When compared with simulations (Figure 3.12); only the Stagni et al. [52] gives similar distribution with experiments under rich conditions. The NH distribution of

Nakamura et al. [50] is different from the measurements and Duynslaegher et al. [49] has more NH than other mechanisms. For the lean conditions; Nakamura et al. [50] and Stagni et al. [52] have similar trends.

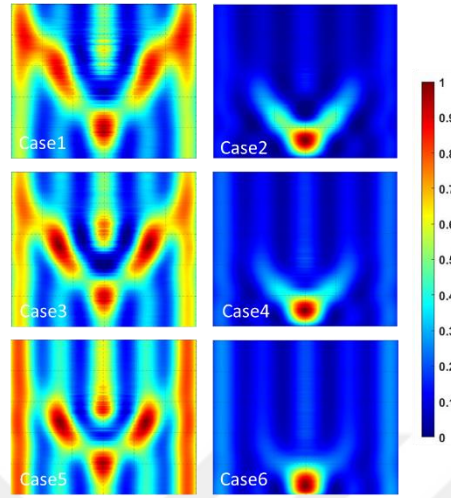


Figure 3.11 : NH distribution of experiments.

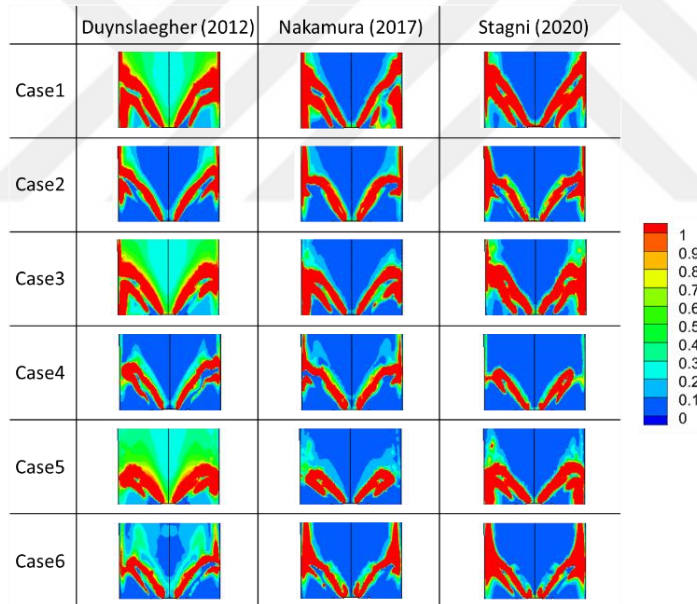


Figure 3.12 : NH distributions of simulated cases (*normalized with max $3.0e-7$ mole fraction*).

NH₂ distributions are not same for the experiments and simulations (Figure 3.13 and Figure 3.14). The max NH₂ is seen around the recirculation zone under rich conditions. It spreads to center of the burner when the power level decrease. This trend is seen on the rich case simulations also. Under lean conditions; the maximum NH₂ is seen at the center of the burner. Although it diffuses towards the walls, it moves to center while power decreases. This phenomenon is seen from the lean simulations also.

Duynslaegher et al. [49] generates higher NH_2 for all the cases when compared with other two mechanisms. At the rich cases (1-3-5); Stagni et al. [52] generates more NH_2 than Nakamura et al. [50]. In contrast to it; Nakamura et al. [50] gives higher values than Stagni et al. [52] at lean conditions (2-4-6). Although there is not a powerful correlation between the experiments and simulations; Nakamura et al. [50] and Stagni et al. [52] are more appropriate candidates for the validation.

The formation of NH and NH_2 radicals is significantly influenced by the equivalence ratio. Under rich conditions, where oxygen is limited, the simulations show elevated concentrations of NH_x species, in agreement with previous studies that highlight the persistence of fuel-derived intermediates under incomplete combustion regimes [11]. Among the mechanisms evaluated, Stagni [52] provides the closest match to the experimental NH profiles in these cases, likely due to its relatively slower oxidation pathways for nitrogen-containing radicals. Conversely, in lean mixtures, both Nakamura [50] and Stagni [52] predict centrally located NH_x peaks, which can be attributed to more efficient post-flame oxidation promoted by the higher availability of oxygen. This behavior is consistent with the expected chemical shift from intermediate nitrogen species toward final products such as NO or N_2 in fuel-lean flames.

NO , NO_2 and NH_3 measurements were performed with gas analyzer. For the quantitative comparison, error was defined as the percentage difference between numerical results and experimental measurements for each operating condition. In Figure 3.15; the NO emissions increase at rich cases (1-3-5) while the power level decreases. At lean cases (2-4-6); NO was measured up to 1000ppmV, but further measurements could not be taken due to the analyzer limit. The trend of rich cases may be seen at lean cases when they measured with appropriate tools also. Up to that time; it can be only said that the NO level of lean cases is higher than the rich cases (1-3-5). According to the CFD simulations; all of the compared mechanisms show the same trend with experiments. Except the case 1; Duynslaegher et al. [49] have the worst approximation with NO measurements. Stagni et al. [52] is better than Duynslaegher et al. [49], but Nakamura et al. [50] gives the best matching especially at the rich cases.

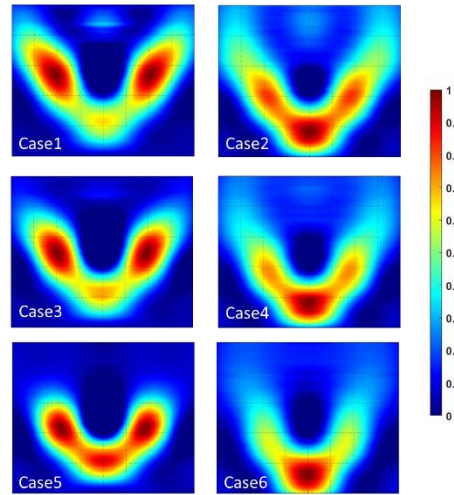


Figure 3.13 : NH_2 distribution of experiments.

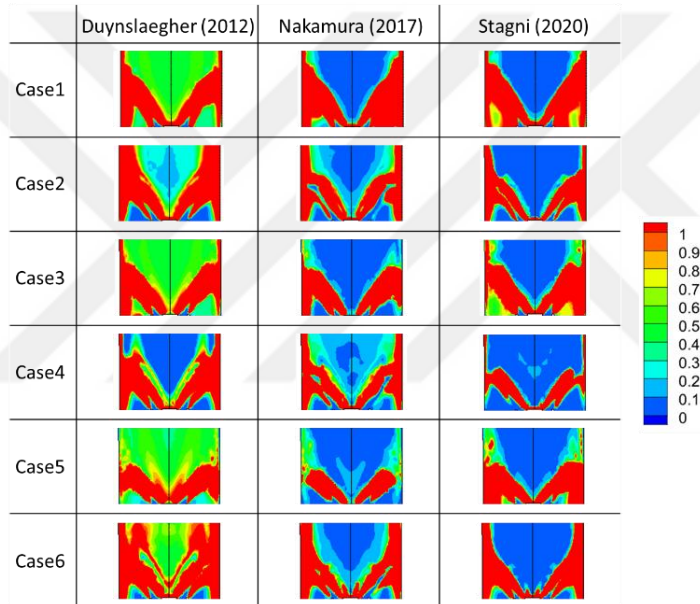


Figure 3.14 : NH_2 distributions of simulated cases (*normalized with max $1.0e-6$ mole fraction*).

NO_2 production is excessive at lean cases (2-4-6) and they were measured with the dilution as explained in the experimental setup section. In contrast; it could not be measured at rich cases (1-3-5) since the low production level. Therefore, there is not any experimental data for these cases. The evidence of low NO_2 production is CFD results also (Figure 3.16). All of the rich cases have very low NO_2 levels compared to lean cases. All of the reaction mechanisms have a good approach at case 4. Duynslaegher et al. [49] and Stagni et al. [52] have higher errors compared to Nakamura et al. [50] both for the case 2 and 6.

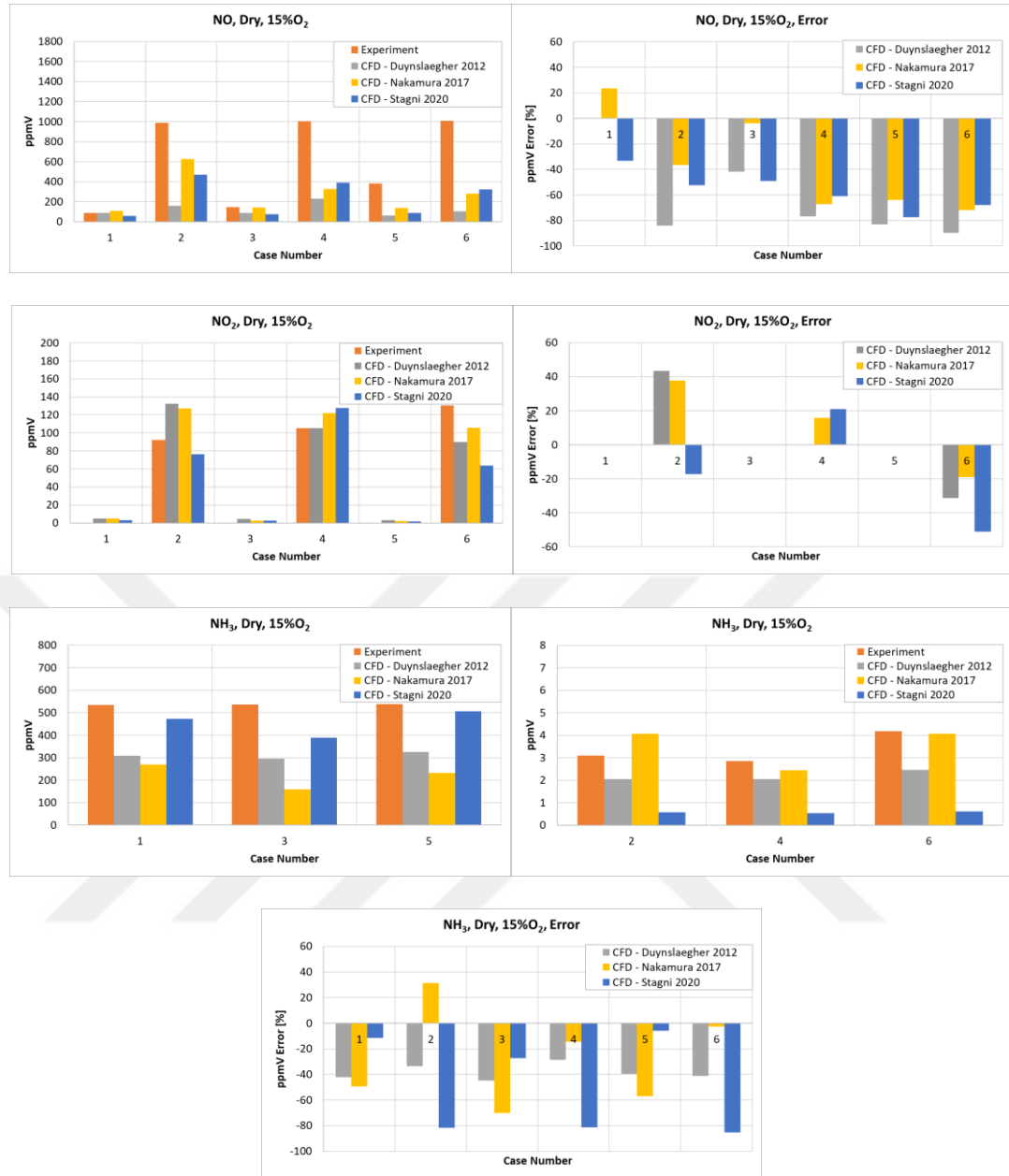


Figure 3.15 : The comparison of reaction mechanisms with experiments for the exhaust emissions.

Since the degree is different between the rich and lean cases; NH₃ measurements are presented with two graphs at Figure 3.15. The rich cases (1-3-5) are beyond the analyzer measurement ability, therefore their NH₃ values are limited around the 530 ppmV. Stagni et al. [52] gives the nearest results at rich cases with max 25% error at case 3. With the 70% maximum error at case 3; Nakamura et al. [50] has the highest error values at all of the rich cases. Duynslaegher et al. [49] has around 40% error independent from the power level of rich cases. Although it is the best choice for the rich conditions; Stagni et al. [52] is the worst option for the lean conditions (2-4-6)

when compared with experimental results. Similar to this contraction; Nakamura et al. [50] gives the most accurate NH_3 expectation under lean conditions. Duynslaegher et al. [49] is an unresponsive reaction mechanism that gives the same error level independent from the power level of burner. These mechanism dependent differences and trends are consistent with the comparative observations reported by Alnasif et al. [51] for $\text{NH}_3\text{-H}_2$ combustion under varying equivalence ratios.

Similar to Figure 3.15; Duynslaegher et al. [49] have the lowest NO contour compared to other two mechanisms at Figure 3.17. Nakamura et al. [50] and Stagni et al. [52] give very similar results under lean conditions (2-4-6). However, Nakamura et al. [50] closes to experiments for the rich cases (1-3-5).

In Figure 3.16; there is not any significant difference between mechanisms for the rich conditions. Also, the experimental data is not available. Therefore, it cannot be compared with the rich test conditions. Duynslaegher et al. [49] has different results under lean conditions. Although the Stagni et al. [52] and Nakamura et al. [50] have close distributions; Nakamura et al. [50] gives the better validation with measurements.

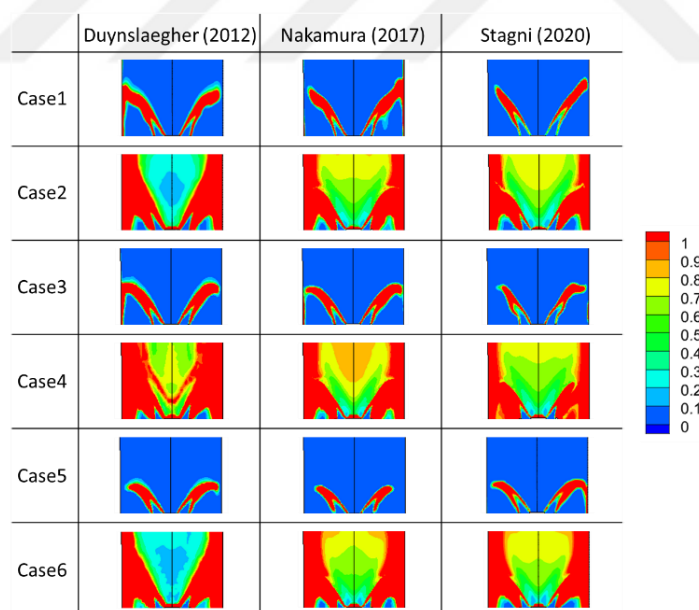


Figure 3.16 : NO_2 distributions of simulated cases (*normalized with max $1.0\text{e-}5$ mole fraction*).

NO formation is observed to be higher under lean conditions, which is consistent with elevated flame temperatures and increased concentrations of OH radicals—key drivers in the oxidation of fuel-bound nitrogen [48]. This trend aligns with established

knowledge that thermal and prompt NO mechanisms are enhanced in oxygen-rich, high-temperature environments. Among the evaluated models, Nakamura [50] provides the best agreement with experimental NO levels in rich flames, possibly due to its more detailed representation of intermediate species and fuel-N to NO conversion pathways. As for NO₂, which forms primarily through the post-flame oxidation of NO, its levels are considerably higher in lean conditions, where excess oxygen is available. Nakamura [50] again predicts this behavior more accurately, particularly at moderate thermal loads, likely due to its inclusion of extended NO_x sub-mechanisms and post-flame chemistry.

Similar to experimental results; there is a major difference between the rich and lean cases in Figure 3.18. Although it is not the best at any cases; Duynslaegher et al. [49] represents the NH₃ with about 40% error for any case. Stagni et al. [52] perfectly matches with rich cases (1-3-5), but it significantly underpredicts the lean cases (2-4-6). In contrast to it; Nakamura et al. [50] is the best mechanism for the lean cases (2-4-6) but it overpredicts the rich cases (1-3-5).

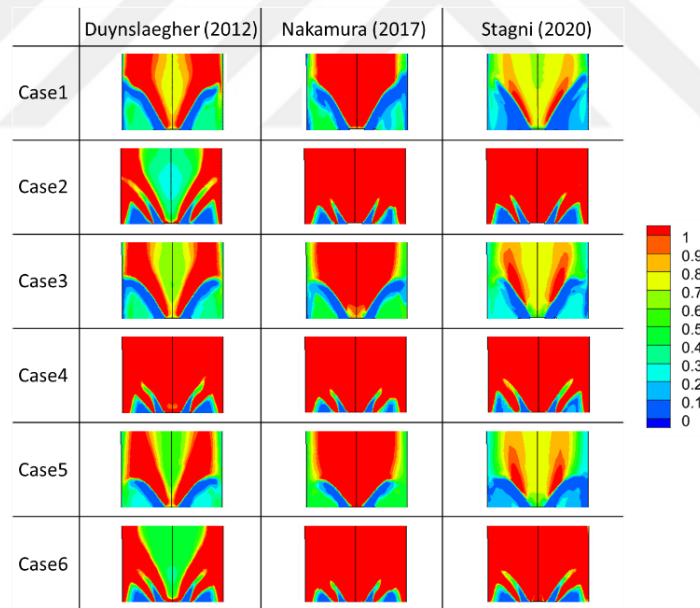


Figure 3.17 : NO distributions of simulated cases (*normalized with max 3.0e-3 mole fraction*).

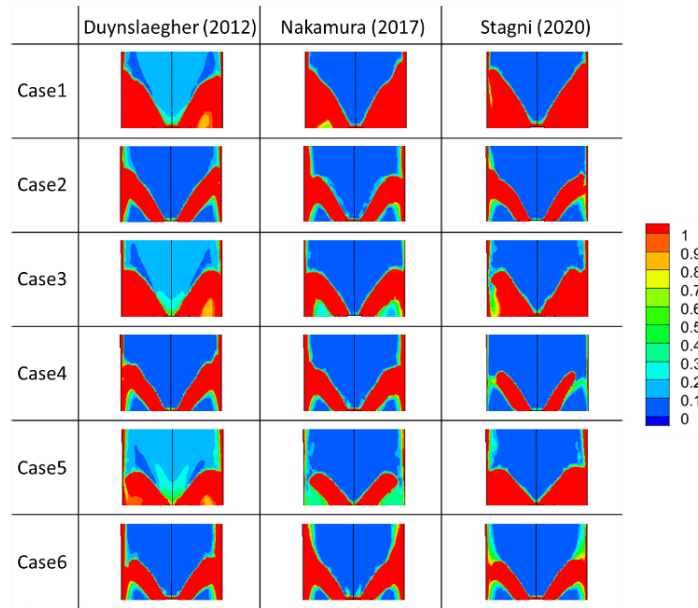


Figure 3.18 : NH_3 distributions of simulated cases (*normalized with max $1.0\text{e-}3$ mole fraction*).

NH_3 emissions are notably higher under rich conditions, which is expected due to incomplete oxidation caused by limited oxygen availability. The persistence of unreacted ammonia in these cases is consistent with earlier studies on NH_3/H_2 combustion, where fuel-rich operation often results in elevated ammonia slip [48]. Among the mechanisms, Stagni [52] offers the best prediction of NH_3 levels in rich flames, likely owing to its more conservative treatment of NH_3 conversion rates. In contrast, Nakamura [50] tends to overpredict NH_3 under rich conditions but aligns better with experimental trends under lean operation. These differences underscore the importance of reaction mechanism selection, particularly in capturing the balance between radical propagation and complete fuel conversion, which directly affects pollutant emissions.

3.5 Conclusions

Ammonia has the potential to be a key solution for reducing carbon emissions by transitioning hydrocarbon combustion systems to hydrogen-based alternatives. Although pure hydrogen is the desired fuel for achieving zero emissions, several technical challenges inhibit its widespread application. Utilizing ammonia as a fuel directly, partially decomposed, or blended with other fuels offers significant advantages in decarbonizing the energy sector and promoting the adoption of

hydrogen. At this point; ammonia emerges as a promising energy vector with its carbon-free molecular structure and several advantages over hydrogen.

Extensive research has been conducted to optimize the combustion characteristics of ammonia, either as a pure fuel or blended with other fuels. However, implementing a kinetic mechanism that accurately models all combustion parameters across different equivalence and fuel mixture ratios, and for a wide range of operating conditions remains a challenge. Existing reaction mechanisms exhibit variable predictions under different operating conditions, indicating that each mechanism is tailored to specific scenarios. Therefore, comparative studies of various reaction mechanisms are essential to validate numerical models against experimental data.

In this study; an industrial scale swirl burner operating with a 50-50 ammonia-hydrogen fuel blend by volume was numerically investigated. Three reaction mechanisms (Duynslaegher, Nakamura and Stagni) were compared at three power levels (10, 15 and 20 kW) and two equivalence ratios (1.2 and 0.7). Experimental temperature and exhaust emissions data were used to determine the most appropriate mechanism for these conditions. The temperature results (Figure 3.7-3.8) indicate that the Nakamura et al. [50] mechanism provides the most comprehensive predictions. To further validate this conclusion, exhaust emission measurements and spatially resolved OH, NH, and NH₂ chemiluminescence distributions were investigated. Nakamura et al. [50] exhibited the closest match to experimental distributions, with Stagni et al. [52] as the second-best alternative. As a last indicator; Nakamura et al. [50] aligned most accurately with gas analyzer results (Figure 3.15), compared to Stagni et al. [52] and Duynslaegher et al. [49].

Although experimental species distributions were unavailable, simulated NO, NO₂, and NH₃ distributions presented to show the differences between mechanisms. These prediction discrepancies, particularly for NO and NO₂, are largely attributed to differences in the representation of nitrogen chemistry in the evaluated mechanisms, such as variations in fuel-bound nitrogen conversion and post-flame oxidation pathways. Nevertheless, inconsistencies between numerical models and experimental data continue, particularly for NO₂ and NH₃ predictions.

Based on the comparative assessment, the Nakamura et al. [50] mechanism was selected as the primary kinetic model for the subsequent CFD analyses and

optimization studies. Although both the Nakamura et al. [50] and Stagni et al. [52] mechanisms show similar predictive capability for several combustion characteristics under the investigated conditions, the selection was based on application specific considerations rather than overall accuracy alone. In particular, the Nakamura et al. [50] mechanism provides a more reliable representation of flame reactivity and stabilization behavior, which directly affect the feasibility and direction of the optimization process. Since the present study focuses on geometry, flow and chemistry interactions and involves repeated CFD simulations within a multi-objective optimization framework, accurate prediction of flame response and stability was prioritized over a more detailed description of NO_x formation pathways.

While Nakamura et al. [50] appears to be the most suitable mechanism for this study, more detailed and refined mechanisms will be necessary for future numerical investigations. Future work should focus on refining the nitrogen sub-mechanisms through validation against broader experimental datasets and improving pressure and temperature dependent pathway modeling to enhance the accuracy of NO and NO_x predictions.

4. OPTIMIZATION

In this study, a multi-objective optimization of a selected swirl burner was conducted to improve combustion efficiency and reduce emissions. Initially, sensitivity analyses were performed to evaluate the influence of different design parameters on combustion performance. Based on these analyses, a set of parametric solutions was generated and used as the initial input for the optimization model. The upper and lower bounds for each parameter, along with the specific optimization objectives, were clearly defined to guide the process. The selection of an appropriate optimization method was made by considering the complexity of the objective functions, the nature of the parameters, and the overall sensitivity of the combustion model. As stated in previous chapters; the objectives of this study are given in Table 4.1.

Table 4.1 : Optimization parameters and objectives.

Objective	Main Target
Decrease the Fuel Consumption	Efficiency Improvement
Increase the Heat Release Rate	
Minimize NO _x Emissions	Emission Reduction
Minimize H ₂ Usage	

4.1 Mathematical Definition of the Optimization Problem

The design of a premixed NH₃/H₂ swirl burner is formulated as a multi-objective optimization problem, in which both geometric parameters and fuel blend ratio are varied to improve combustion performance while reducing emissions and hydrogen consumption. The optimization problem is mathematically defined in terms of design variables, objective functions, and physical constraints, as described below.

The vector of design variables x is defined as:

$$x = [CR, N_v, \alpha_v, X_{NH_3/H_2}] \quad (4.1)$$

Each design variable is bounded within lower and upper limits to ensure geometric feasibility, flame stability, and numerical robustness of the CFD simulations:

$$P_i^{min} \leq P_i \leq P_i^{max} \quad i = 1, 2, 3, 4 \quad (4.2)$$

4.1.1 Objective functions

Based on the physical findings obtained in the previous sections, the optimization problem is defined in equation 4.3. Objectives of efficiency improvement target (Table 4.1) were combined and represented by a single performance metric, namely the “specific heat release” that is the ratio of the heat release rate to total fuel flow.

The multi-objective optimization problem is defined as:

$$\text{Maximize } O1(x)$$

$$\text{Minimize } O2(x)$$

$$\text{Minimize } O3(x)$$

where $O1(x)$ is the specific heat release, $O2(x)$ is the NO_2 emission level and $O3(x)$ is the H_2 mass flow rate.

The problem can be expressed in vector form as:

$$\min \mathbf{F}(x) = [-O1(x), O2(x), O3(x)] \quad (4.3)$$

subject to the constraints defined in the design space.

To facilitate comparison among Pareto-optimal solutions and to select a representative design for detailed investigation, additional decision-making approaches may be employed after completion of the multi-objective optimization. In practice, Pareto solutions can be ranked using normalized weighted scores, distance based criteria, or other established design selection methods depending on the engineering priorities of the problem.

4.1.2 Constraints

To ensure a fair comparison among different designs and operating conditions, the following constraints are imposed:

$$\phi = \text{constant} \quad (4.4)$$

$$\dot{Q}_{total} = \text{constant} \quad (4.5)$$

where the ϕ and $\dot{Q}_{total}$ are kept constant throughout the optimization process, and the design parameters are bounded within predefined physical limits.

4.2 Optimization Methods

The selection of optimization method depends on the complexity of the objectives, the nature of the parameters and the sensitivity of the model. Considering the current thesis scenario; some prominent optimization methods are evaluated with their advantages and disadvantages.

4.2.1 Genetic algorithm (GA)

Genetic algorithm is ideal for multi-objective optimization studies and gives good results when there are complex interactions between parameters. It is effective in non-linear and multi-modal (multiple peak) functions. Genetic algorithm is commonly used in cases where the objectives conflict with each other (for example, controlling NO_x production while reducing H₂ fuel consumption). If the running time of the models is not too long and sufficient computational resources are available; GA is a good choice.

Advantages:

- Since it is population-based, it performs a comprehensive search and has a high probability of reaching a global optimum.
- It provides Pareto optimal solutions for multiple objective functions and shows trade-off points.
- It works effectively with complex and high-dimensional parameters.

Disadvantages:

- The computational cost is high, especially when there are many parameters and large search areas. Therefore; parameter limits must be well determined.

4.2.2 Multi-objective particle swarm optimization (MOPSO)

It is preferred in studies where there are continuous and discontinuous changes between parameters, fast optimization and low computational cost are required. If computational time is an important factor and the results are desired to be optimized quickly, MOPSO may be a good option.

Advantages:

- It is generally faster and requires less computation.
- It works well with continuous and discrete parameters.

- Since it is a population-based, there is a chance to find the global optimum.
- It is easy to implement and adjust.

Disadvantages:

- If the parameter space is wide, it can sometimes get stuck in local optimum.
- Solution diversity may be less compared to genetic algorithms.

4.2.3 Multi-objective simulated annealing (MOSA)

MOSA is preferred in cases where the initial estimation of the parameters is difficult and a slow and systematic search is required to reach the global optimum. If the optimization has a very complex and nonlinear structure and the search for the global optimum is important, MOSA is a good alternative.

Advantages:

- It is less likely to get stuck in local optima.
- It uses a comprehensive search strategy and finds better solutions over time.
- The convergence process can be controlled thanks to the cooling parameter.

Disadvantages:

- It converges slowly, so the computation time can be long.
- It works well in complex parameter fields but requires fine tuning.

4.2.4 Non-dominated sorting genetic algorithm (NSGA-II)

NSGA-II is used in areas where genetic algorithms are strong. However, it is designed more specifically to find Pareto optimal solutions in multi-objective problems. It is preferred in cases where diversity and a balanced distribution are expected between solutions.

Advantages:

- It finds Pareto optimal solutions and provides solution diversity.
- It is a well-known method and is widely used in the literature.
- It provides a balanced distribution between solutions with non-dominated sorting.

Disadvantages:

- Like other genetic algorithms, it has high computational cost.

- Parameter adjustments (e.g. crossover and mutation rates) may take time.

4.2.5 Differential evolution (DE)

It is used in cases where the parameters are continuous and complex, initial value estimation is difficult, but optimization speed is important. It is preferred in cases where the model works faster and many trials can be made.

Advantages:

- It has fast and easy implementation.
- It has a comprehensive parameter space search capacity.
- It requires less parameter adjustment than the genetic algorithm.

Disadvantages:

- Sometimes the solution diversity may not be sufficient.
- There is a risk of getting stuck in local optimum.

The advantages and disadvantages of different optimization algorithms are compiled and presented in Table 4.2. According to the optimization objectives given in the thesis study; Genetic Algorithm (GA) or NSGA-II stand out as two options. There are multiple objectives and there are trade-offs between these objectives also.

Table 4.2 : Comparison of various optimization algorithms.

No	Criteria	Genetic Algorithm (GA)	Multi-Objective Particle Swarm Optimization (MOPSO)	Multi-Objective Simulated Annealing (MOSA)	Non-Dominated Sorting Genetic Algorithm (NSGA-II)	Differential Evolution (DE)
1	Ability to Reach Global Optimum	Advantageous	Moderate	Advantageous	Advantageous	Moderate
2	Solution Diversity	Advantageous	Limiting	Moderate	Advantageous	Limiting
3	Convergence Speed	Moderate	Advantageous	Limiting	Moderate	Advantageous
4	Computational Cost	Limiting	Advantageous	Limiting	Limiting	Advantageous
5	Ease of Use & Tuning	Moderate	Advantageous	Moderate	Moderate	Advantageous
6	Usage Prevalence in CFD	Advantageous	Moderate	Limiting	Advantageous	Moderate
7	Pareto Front Success	Advantageous	Moderate	Moderate	Advantageous	Moderate

Population-based Pareto optimization methods (GA or NSGA-II) are more effective for the optimization of such parameters. Although MOPSO provides a simpler implementation and a faster optimization, it is not preferred due to its disadvantages. As a result of the comparison of the optimization algorithms discussed above; despite the computational time and cost, the NSGA-II algorithm was used in this thesis due to its powerful optimization properties (Table 4.3).

Table 4.3 : Comparison of GA and NSGA-II algorithms.

Criteria	Winning
Ability to Reach Global Optimum	GA / NSGA-II
Solution Diversity	NSGA-II
Usage Prevalence in CFD	GA / NSGA-II
Pareto Front Success	NSGA-II

4.3 Normalization

Normalization is very important to bring objective functions of different sizes or scales to the same level when performing multi- objective optimization. Objective functions can be in different units (e.g. fuel consumption in g/s, NO_x emissions in ppm). In this case, large value functions can dominate small value functions. Normalization makes the optimization algorithm work more stable and the results more meaningful (Figure 4.1). Maintaining a balance between targets of different sizes helps to create a better Pareto front. In this study, it is aimed to increase the effectiveness of the optimization process by normalizing the objective functions.

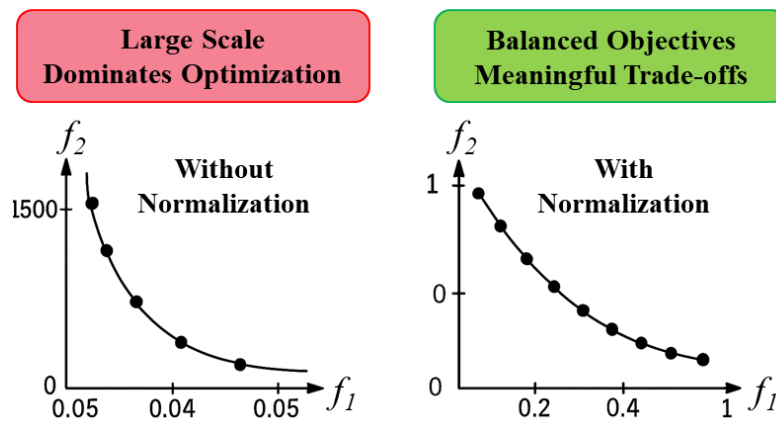


Figure 4.1 : Effect of normalization on the Pareto front.

4.4 Optimization Tool and Coupled Optimization Model

4.4.1 Dakota optimization tool

Dakota (Design and Analysis Kit for Optimization and Terascale Applications) is an open source optimization and analysis tool developed by Sandia National Laboratories [68]. It provides a wide range of solutions for engineering and scientific problems, including parametric analysis, uncertainty analysis, and multi-objective optimization. It supports various optimization algorithms, including genetic algorithms (GA), differential evolution, and derivative-based methods. User-defined objective functions and constraints can be easily integrated with Dakota. It is compatible with many simulation software, allowing users to automate complex simulation-based design work. It offers a flexible input file format and detailed output reporting. When integrated with CFD software, it facilitates the creation of automatic model update and analysis cycles.

4.4.2 Non-dominated sorting genetic algorithm (NSGA-II)

NSGA-II is a variant of the genetic algorithms that developed by Deb et al. [69] to provide Pareto optimal solution set to multi objective optimization problems. NSGA-II has a lower computational cost than the first version NSGA. Also, using the elitism mechanism, it transfers good solutions to future populations, thus ensuring the stable progress of optimization.

Optimization process starts with the random initial population and the solutions are arranged according to the Pareto-optimal order [69-73]. The diversity is preserved by calculating the crowding distance. Then, the elitism mechanism is performed by merging the parent and child populations. The application of elitism mechanism usually done by tournament. A random individuals are compared in a small tournament and the winners are passed on to the next generation. Individuals with better performance have a higher chance of winning the tournament. However, occasionally selecting weaker individuals increases the chance of both preserving diversity in the population and reaching a global optimum. In this way, the probability of selecting stronger individuals increases while diversity is preserved. Crossover and mutation genetic operators are applied to selected new population to create new individuals. In the crossover phase, the genetic information of the selected individuals is exchanged at certain rates and new individuals are created. Crossover gives the chance to generate

better solutions by combining existing solutions and allows the exploration of a larger solution space. In the mutation phase, random small changes are applied to increase the diversity of solutions. Changes made to a single gene or several genes help the algorithm to explore new regions in the solution space. The mutation process is performed to avoid getting stuck in local minima, preserve genetic variation, ensure the continuity of the evolutionary process and obtain broader optimization results. The process is repeated again until the end of optimization (Figure 4.2).

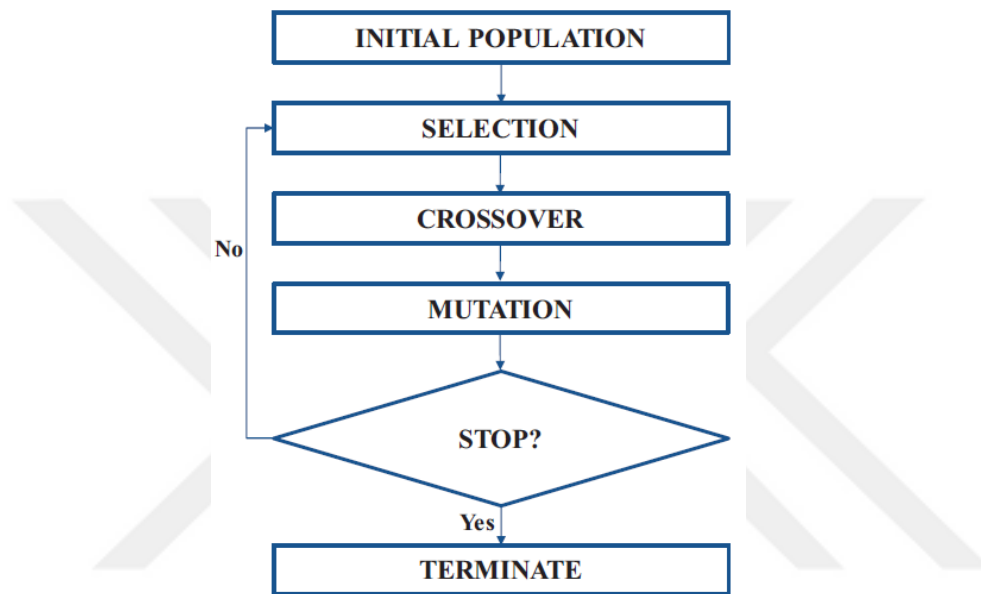


Figure 4.2 : Flow chart of the general genetic algorithms [70].

4.4.3 Coupled optimization model

Optimization tools are coupled with various data analysis software to find optimal solutions to complex problems. The combination of CFD and NSGA-II model is widely used to provide optimal solutions in engineering studies [70, 74-75].

The CFD coupled NSGA-II optimization starts from the CFD model. The parameters are obtained and the initial population is generated by performing CFD simulations. The parameters and the results of CFD simulations are transferred to optimization model. Then, the optimization model generates Pareto-optimal solutions by using NSGA-II algorithm. The new generations of optimization model are sent to CFD model again. This cycle continues until the desired optimum is achieved. In Figure 4.3; the example of coupled Dakota software and simulation model is presented [76]. According to the preferred softwares, the scripts can be required to create communication between CFD model and optimization tool.

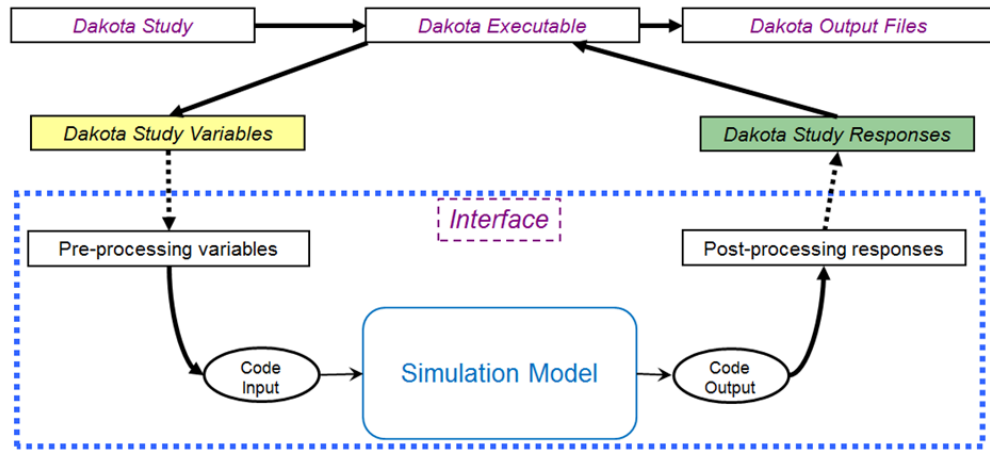


Figure 4.3 : The loosely-coupled or “black-box” interface between Dakota and a user-supplied simulation code [76].

4.5 Parametric CFD Model and Initial Population

According to the current knowledge, validation studies at previous chapters and optimization targets; 4 parameters were selected prior to perform optimization (Table 4.4). The confinement ratio is a dimensionless parameter to quantify the degree to which a flame is geometrically constrained within a combustion chamber. It is defined as the ratio of the confinement diameter to that of the baseline case. This ratio affects several key flow characteristics, including flame shape, recirculation zone strength, and stability limits. A higher confinement ratio generally enhances flame stabilization due to stronger internal recirculation, but it may also increase the risk of flashback. Conversely, a lower confinement ratio allows more freedom for flame propagation but may lead to reduced flame stability. In swirl-stabilized combustors, confinement ratio plays a crucial role on the combustion behavior. Figure 4.4 illustrates typical examples of the burner geometries corresponding to different confinement ratios.

The number of vanes refers to the total count of blades positioned inside the swirler to give an angular momentum to the incoming flow. This parameter influences not only the swirl intensity and flame stabilization but also has a noticeable effect on emission characteristics. Although the impact may vary depending on the operating conditions, changes in vane count can alter the mixing quality and flow structure, thereby affecting the overall combustion behavior. In Figure 4.5, different swirler configurations with varying numbers of vanes are illustrated to represent the geometrical variations considered in this study.

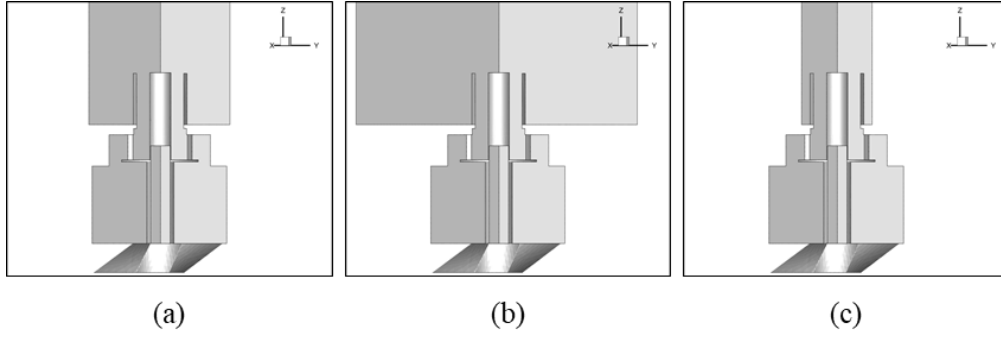


Figure 4.4 : Confinement ratio. (a) base model, (b) x2 confinement ratio, (c) x0.5 confinement ratio.

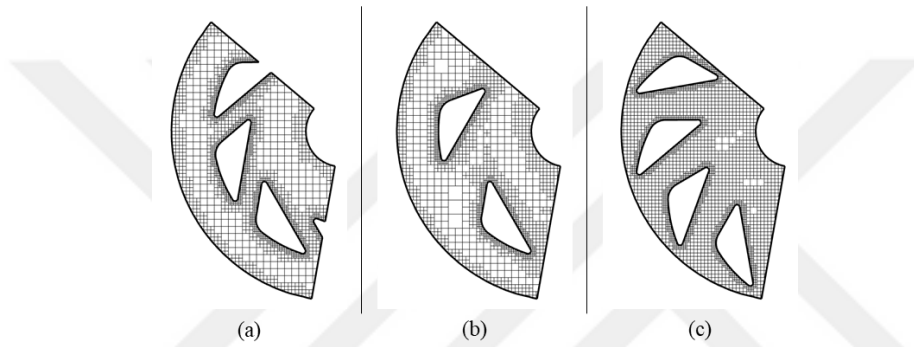


Figure 4.5 : Number of vanes. (a) 9 vanes, (b) 6 vanes, (c) 12 vanes.

The vane angle directly influences the swirl number by controlling the amount of angular momentum given to the air stream. Consequently, it affects flame stabilization, recirculation zone formation, and the mixing process. Variations in vane angle can also impact combustion efficiency and emission levels due to changes in residence time and local turbulence intensity. In Figure 4.6, swirler geometries with different vane angles are illustrated to demonstrate the range of configurations considered in this study.

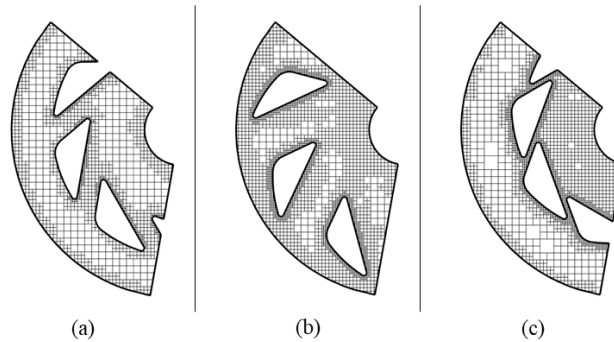


Figure 4.6 : Vane angle. (a) base model, (b) +30° rotated vanes, (c) -15° rotated vanes.

Table 4.4 : Parameters and initial population (parameters in red denote variables).

	PARAMETERS			
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]
Min Limit	0.5	6	-15	50/50
Max Limit	2	12	40	100/0
No	P1	P2	P3	P4
D000	1	9	Base	50/50
D001	2	9	Base	50/50
D002	0.5	9	Base	50/50
D003	1	6	Base	50/50
D004	1	9	+30	50/50
D005	1	9	-10	50/50
D006	1	9	-15	50/50
D007	1	6	-15	50/50
D008	1	12	+40	50/50
D009	0.5	12	+40	70/30
D010	1	9	Base	80/20
D011	1.5	6	-15	60/40
D012	2	12	+10	50/50
D013	1.25	6	-5	75/25

In addition to geometric parameters, the volumetric ratio of NH₃ and H₂ was also considered as a key parameter. Fuel blend directly affects flame characteristics such as burning velocity, ignition delay, and emission formation. By varying the NH₃/H₂ volumetric ratio while maintaining a constant equivalence ratio, the influence of fuel reactivity and hydrogen enrichment on combustion performance was systematically investigated. In order to ensure a consistent combustion regime across varying NH₃/H₂ mixing ratios, particular attention was given to maintaining a constant equivalence ratio ($\Phi = 0.7$) throughout the fuel variation range. For all subsequent fuel ratios, the total air mass flow was recalculated to preserve $\Phi = 0.7$ based on the composite stoichiometric air requirement derived from the weighted contribution of each fuel component. In parallel, the total chemical energy input was carefully kept constant by adjusting the individual fuel mass flow rates according to their respective lower heating values, thereby ensuring a fixed thermal power input across all operating points. This approach ensures that the thermal input, flame temperature, and residence time are governed by fuel chemistry rather than unintended shifts in mixture strength or heating value. It also facilitates a consistent basis for comparing combustion stability, emission trends, and heat release characteristics across different fuel blends.

Based on the defined parameters, an initial population was generated for the optimization process. A total of 14 individuals were created in this initial population, each representing a unique combination of the selected input variables. These individuals serve as the starting point for the evolutionary search, allowing the algorithm to explore a wide range of design solutions within the defined parameter space.



5. RESULTS AND DISCUSSION

This chapter presents the optimization results obtained using the analysis model developed and validated in the previous chapters. Starting from a randomly generated initial population within the specified minimum and maximum limits, three additional generations were produced with NSGA-II algorithm. In the section 5.1, the results of all individuals were given and the effect of each objective was evaluated separately. The relationships between objectives and parameters were investigated in the section 5.2. According to the results; prominent individuals were determined on the Pareto fronts for different performance criteria. Finally, the most favorable design individual (global optimum) in the optimization space was identified, and parametric studies were performed with it. The outcomes of these parametric studies were presented in the section 5.3.

5.1 Initial Population and Generation Results

The results of initial population is given in Table 5.1. Objectives of efficiency improvement target (Table 4.1) were combined to reduce the single objective “specific heat release” that is the ratio of the heat release rate to total fuel flow. Each objective was normalized according to its maximum and minimum values in the population. The normalized results of initial population is given in Table 5.2 and NSGA-II optimization was applied for the next generations then. Normalization was updated for every generation to keep up to date minimum and maximum normalized values.

The first and second generations are given in Table 5.3 and Table 5.4. Bold rows represents elite individuals from the previous generations. Elite individuals are tournament winners who carry on the strong traits of the previous generation. The third generation is the last generation in this study and its results were shown in Table 5.5 and Table 5.6. Between Table 5.1 and Table 5.6; the red fonts highlight the modified parameters of individuals.

The results of each design were investigated between sections 5.1.1 and 5.1.3. The objectives were examined with histogram diagrams and the convergence of the optimization was discussed.

Table 5.1 : Initial population results.

	PARAMETERS				OBJECTIVES		
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]	Specific Heat Release [kJ/kg] = Heat Release Rate [kW] / Total Fuel Flow [kg/s]	NO ₂ Emission [ppmV]	H ₂ Mass Flow Rate [kg/s]
Min Limit	0.5	6	-15	50/50			
Max Limit	2	12	40	100/0			
No	P1	P2	P3	P4	O1	O2	O3
D000	1	9	Base	50/50	7854.43	122.14	0.0545
D001	2	9	Base	50/50	8029.61	14.43	0.0545
D002	0.5	9	Base	50/50	7715.92	206.23	0.0545
D003	1	6	Base	50/50	7774.68	373.75	0.0545
D004	1	9	+30	50/50	7807.75	133.57	0.0545
D005	1	9	-10	50/50	7900.14	150.29	0.0545
D006	1	9	-15	50/50	7865.11	202.70	0.0545
D007	1	6	-15	50/50	7852.95	168.36	0.0545
D008	1	12	+40	50/50	7789.64	147.69	0.0545
D009	0.5	12	+40	70/30	5796.00	117.71	0.0310
D010	1	9	Base	80/20	5805.11	32.62	0.0218
D011	1.5	6	-15	60/40	7037.39	68.89	0.0436
D012	2	12	+10	50/50	8649.44	12.80	0.0545
D013	1.25	6	-5	75/25	5761.41	38.46	0.0272

Table 5.2 : Initial population results (normalized).

	PARAMETERS				OBJECTIVES (NORMALIZED)		
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]	Specific Heat Release [-]	NO ₂ Emission [-]	H ₂ Mass Flow Rate [-]
Min Limit	0.5	6	-15	50/50			
Max Limit	2	12	40	100/0			
No	P1	P2	P3	P4	O1	O2	O3
D000	1	9	Base	50/50	0.584	0.318	1.000
D001	2	9	Base	50/50	0.630	0.026	1.000
D002	0.5	9	Base	50/50	0.548	0.546	1.000
D003	1	6	Base	50/50	0.564	1.000	1.000
D004	1	9	+30	50/50	0.572	0.349	1.000
D005	1	9	-10	50/50	0.596	0.394	1.000
D006	1	9	-15	50/50	0.587	0.536	1.000
D007	1	6	-15	50/50	0.584	0.443	1.000
D008	1	12	+40	50/50	0.567	0.387	1.000
D009	0.5	12	+40	70/30	0.051	0.306	0.569
D010	1	9	Base	80/20	0.054	0.076	0.400
D011	1.5	6	-15	60/40	0.373	0.174	0.800
D012	2	12	+10	50/50	0.790	0.022	1.000
D013	1.25	6	-5	75/25	0.042	0.091	0.499

Table 5.3 : The first and second generation results.

	PARAMETERS				OBJECTIVES		
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]	Specific Heat Release [kJ/kg] = Heat Release Rate [kW] / Total Fuel Flow [kg/s]	NO ₂ Emission [ppmV]	H ₂ Mass Flow Rate [kg/s]
Min Limit	0.5	6	-15	50/50			
Max Limit	2	12	40	100/0			
No	P1	P2	P3	P4	O1	O2	O3
D014	1.00	9.00	-5.00	80/20	5628.90	32.27	0.0218
D015	0.50	12.00	40.00	70/30	5796.00	117.71	0.0310
D016	2.00	12.00	10.00	50/50	8649.44	12.80	0.0545
D017	1.50	6.00	-10.00	60/40	7086.66	77.84	0.0436
D018	2.00	9.00	0.00	50/50	8029.61	65.40	0.0545
D019	2.00	9.00	-5.00	50/50	9379.02	5.00	0.0545
D020	1.10	6.00	-10.00	50/50	7900.27	74.49	0.0545
D021	1.90	9.00	0.00	50/50	9460.45	4.76	0.0545
D022	1.05	9.00	-10.00	50/50	7921.10	122.27	0.0545
D023	1.45	6.00	-10.00	55/45	7549.94	75.12	0.0490
D024	1.25	6.00	0.00	75/25	5822.15	60.17	0.0272
D025	1.95	12.00	15.00	50/50	8253.84	48.96	0.0545
D026	1.00	9.00	0.00	80/20	5805.11	32.62	0.0218
D027	0.65	12.00	40.00	70/30	5822.75	125.29	0.0310
D028	1.90	9.00	0.00	50/50	9460.45	4.76	0.0545
D029	2.00	9.00	-5.00	50/50	9379.02	5.00	0.0545
D030	2.00	12.00	10.00	50/50	8649.44	12.80	0.0545
D031	1.00	9.00	0.00	80/20	5805.11	32.62	0.0218
D032	1.55	9.00	-5.00	65/35	5962.34	43.18	0.0381
D033	1.25	6.00	-10.00	90/10	5795.64	65.16	0.0109
D034	0.85	12.00	40.00	70/30	6051.93	117.96	0.0310
D035	1.75	12.00	15.00	50/50	8700.46	42.44	0.0545
D036	1.10	9.00	30.00	95/5	6037.43	61.17	0.0054
D037	1.35	12.00	0.00	80/20	5819.08	35.09	0.0218
D038	1.60	6.00	-5.00	75/25	5828.28	47.56	0.0272
D039	0.90	6.00	20.00	85/15	5810.18	170.70	0.0163
D040	1.45	12.00	5.00	60/40	7377.80	40.24	0.0436
D041	1.00	9.00	35.00	100/0	6037.43	65.34	0.0000

Table 5.4 : The first and second generation results (normalized).

	PARAMETERS				OBJECTIVES (NORMALIZED)		
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]	Specific Heat Release [-]	NO ₂ Emission [-]	H ₂ Mass Flow Rate [-]
Min Limit	0.5	6	-15	50/50			
Max Limit	2	12	40	100/0			
No	P1	P2	P3	P4	O1	O2	O3
D014	1.00	9.00	-5.00	80/20	0.008	0.075	0.400
D015	0.50	12.00	40.00	70/30	0.051	0.306	0.569
D016	2.00	12.00	10.00	50/50	0.790	0.022	1.000
D017	1.50	6.00	-10.00	60/40	0.385	0.198	0.800
D018	2.00	9.00	0.00	50/50	0.630	0.164	1.000
D019	2.00	9.00	-5.00	50/50	0.979	0.001	1.000
D020	1.10	6.00	-10.00	50/50	0.596	0.189	1.000
D021	1.90	9.00	0.00	50/50	1.000	0.000	1.000
D022	1.05	9.00	-10.00	50/50	0.601	0.318	1.000
D023	1.45	6.00	-10.00	55/45	0.505	0.191	0.899
D024	1.25	6.00	0.00	75/25	0.058	0.150	0.499
D025	1.95	12.00	15.00	50/50	0.688	0.120	1.000
D026	1.00	9.00	0.00	80/20	0.054	0.076	0.400
D027	0.65	12.00	40.00	70/30	0.058	0.327	0.569
D028	1.90	9.00	0.00	50/50	1.000	0.000	1.000
D029	2.00	9.00	-5.00	50/50	0.979	0.001	1.000
D030	2.00	12.00	10.00	50/50	0.790	0.022	1.000
D031	1.00	9.00	0.00	80/20	0.054	0.076	0.400
D032	1.55	9.00	-5.00	65/35	0.094	0.104	0.699
D033	1.25	6.00	-10.00	90/10	0.051	0.164	0.200
D034	0.85	12.00	40.00	70/30	0.118	0.307	0.569
D035	1.75	12.00	15.00	50/50	0.803	0.102	1.000
D036	1.10	9.00	30.00	95/5	0.114	0.153	0.099
D037	1.35	12.00	0.00	80/20	0.057	0.082	0.400
D038	1.60	6.00	-5.00	75/25	0.060	0.116	0.499
D039	0.90	6.00	20.00	85/15	0.055	0.450	0.299
D040	1.45	12.00	5.00	60/40	0.461	0.096	0.800
D041	1.00	9.00	35.00	100/0	0.114	0.164	0.000

Table 5.5 : The third generation results.

	PARAMETERS				OBJECTIVES		
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]	Specific Heat Release [kJ/kg] = Heat Release Rate [kW] / Total Fuel Flow [kg/s]	NO ₂ Emission [ppmV]	H ₂ Mass Flow Rate [kg/s]
Min Limit	0.5	6	-15	50/50			
Max Limit	2	12	40	100/0			
No	P1	P2	P3	P4	O1	O2	O3
D042	1.90	9.00	0.00	50/50	9460.45	4.76	0.0545
D043	1.00	9.00	0.00	80/20	5805.11	32.62	0.0218
D044	1.00	9.00	35.00	100/0	6037.43	65.34	0.0000
D045	1.45	12.00	5.00	60/40	7377.80	40.24	0.0436
D046	1.90	9.00	-5.00	60/40	7150.72	15.77	0.0410
D047	2.00	9.00	5.00	65/35	6242.83	13.01	0.0367
D048	1.80	9.00	0.00	70/30	5923.89	16.14	0.0315
D049	1.95	12.00	10.00	60/40	6886.46	11.03	0.0401
D050	1.85	12.00	15.00	65/35	6112.05	12.59	0.0353
D051	1.70	12.00	10.00	70/30	5890.53	14.21	0.0302
D052	1.75	12.00	5.00	60/40	7149.13	15.26	0.0397
D053	1.45	6.00	-5.00	75/25	5805.19	40.52	0.0277
D054	1.60	6.00	0.00	80/20	5598.05	28.86	0.0232
D055	1.35	9.00	0.00	75/25	5768.57	33.84	0.0262

Table 5.6 : The third generation results (normalized).

	PARAMETERS				OBJECTIVES (NORMALIZED)		
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]	Specific Heat Release [-]	NO ₂ Emission [-]	H ₂ Mass Flow Rate [-]
Min Limit	0.5	6	-15	50/50			
Max Limit	2	12	40	100/0			
No	P1	P2	P3	P4	O1	O2	O3
D042	1.90	9.00	0.00	50/50	1.000	0.000	1.000
D043	1.00	9.00	0.00	80/20	0.054	0.076	0.400
D044	1.00	9.00	35.00	100/0	0.114	0.164	0.000
D045	1.45	12.00	5.00	60/40	0.461	0.096	0.800
D046	1.90	9.00	-5.00	60/40	0.402	0.030	0.752
D047	2.00	9.00	5.00	65/35	0.167	0.022	0.673
D048	1.80	9.00	0.00	70/30	0.084	0.031	0.578
D049	1.95	12.00	10.00	60/40	0.334	0.017	0.736
D050	1.85	12.00	15.00	65/35	0.133	0.021	0.648
D051	1.70	12.00	10.00	70/30	0.076	0.026	0.554
D052	1.75	12.00	5.00	60/40	0.402	0.028	0.728
D053	1.45	6.00	-5.00	75/25	0.054	0.097	0.508
D054	1.60	6.00	0.00	80/20	0.000	0.065	0.426
D055	1.35	9.00	0.00	75/25	0.044	0.079	0.481

5.1.1 Specific heat release

According to the results given between Table 5.1 and Table 5.6; the more visual and understandable plots were generated for each objective results. In Figure 5.1; the specific heat release value of each individual was presented. While the initial population has a group with higher specific heat release, the last generation (Gen3) has a group with lower values. Since the initial population has random individuals, results of Gen1 and Gen2 has broadband results to search the global optimum point. This is the natural behavior of the genetic optimization algorithm. Re-grouping of the Gen3 results signs the convergence of optimization process. It is also seen from the histogram in Figure 5.2. The number of low heat release rate designs increase from

initial population to third generation. Although there are higher values on the last generation design space, the individual density of the results shows the tendency of population. This distribution seems like opposite to thesis objective which is the increase of specific heat release. However, since it is a multi-objective optimization, it must be evaluated together with other objectives due to its nature. Comparison of objectives and selection of objective based optimum design will be evaluated in the section 5.2.

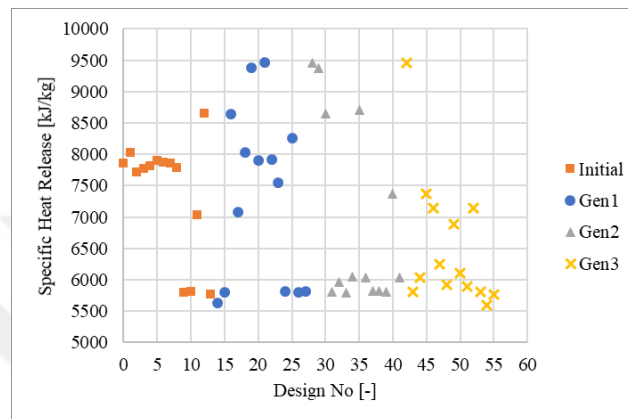


Figure 5.1 : Specific heat release of each design.

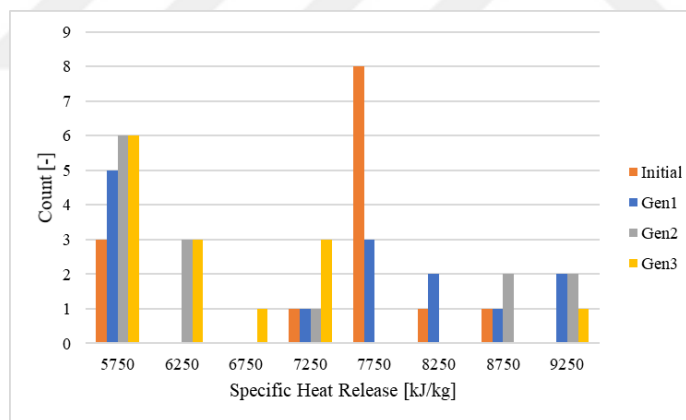


Figure 5.2 : Histogram of specific heat release.

5.1.2 NO₂ emission

Very similar to the previous section; the number of low NO₂ emission individuals increase from initial population to the last generation (Figure 5.3). While the initial population has various results, optimization focuses design space to target point. The convergence of the results can be seen very clear from Figure 5.4 also. In every generation; the optimization process drives the designs toward lower NO₂ levels.

Although this represents the achieved target when considered as a single objective, the advantages and drawbacks of each design will be discussed in section 5.2.

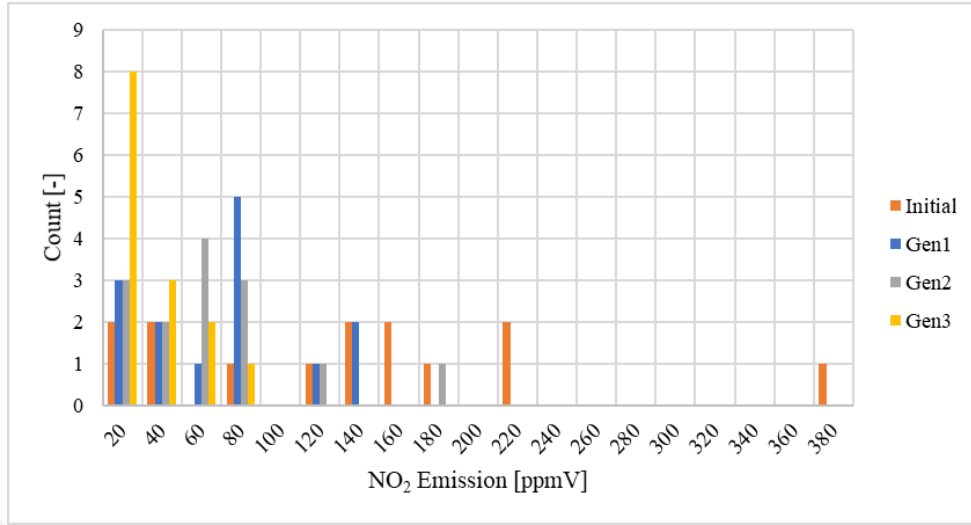


Figure 5.3 : Histogram of NO₂ emission.

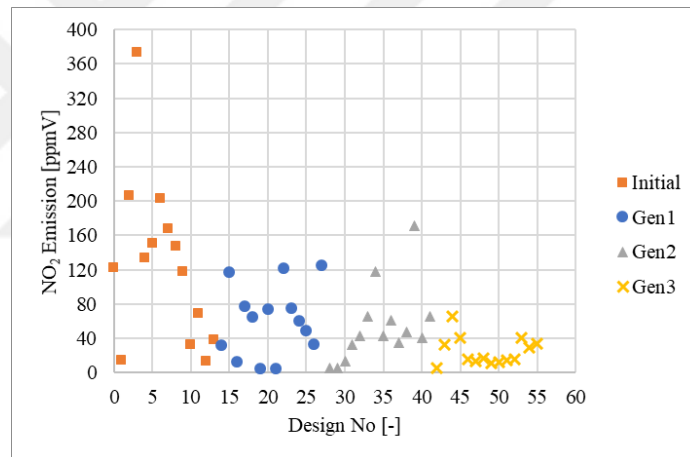


Figure 5.4 : NO₂ emission of each design.

5.1.3 H₂ mass flow rate

Initial population of H₂ mass flow rate does not have a good distribution on the design space (Figure 5.5). Although this is not a good starting point to optimization, NSGA-II extends its borders to entire design area. After a three generation, it can be seen that the model tends to reduce H₂ mass flow rate to lower levels. In Figure 5.6; there is only one individual that has a same H₂ mass flow rate with initial population. Similar to previous objectives, this objective will be evaluated in interaction with other objectives also.

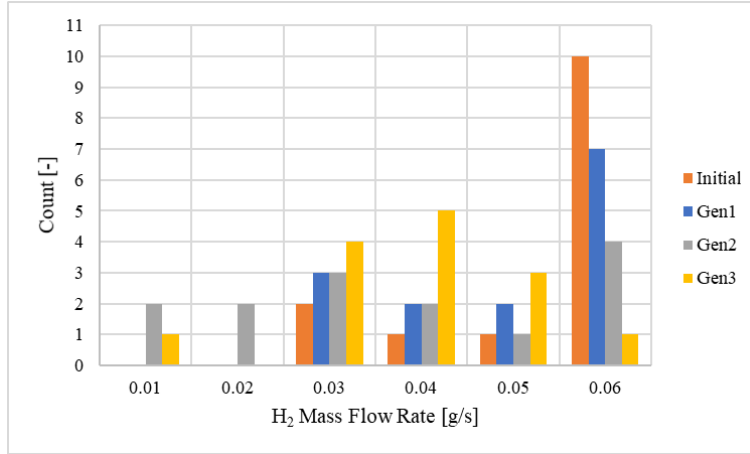


Figure 5.5 : Histogram of H₂ mass flow rate.

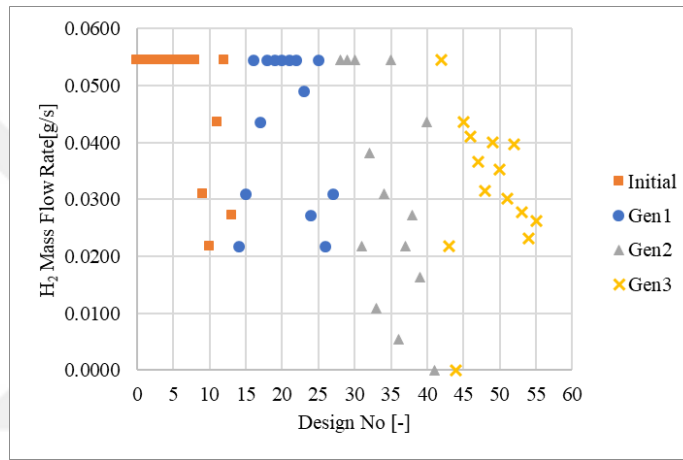


Figure 5.6 : H₂ mass flow rate of each design.

5.2 Relationships Between Objectives and Parameters

In this section; the normalized results of each objective were compared to understand the relationship between them. Also, the effect of each parameter on the objectives was investigated separately. According to the relationships between parameters and objectives; the global optimum and objective optimum models were selected. Advantages and drawbacks of optimum models were determined by comparing with base design.

Figure 5.7 shows the relationship between specific heat release (O1) and NO₂ emission (O2). Although the initial population does not have a good distribution on the design space, the third generation reached the optimum. It is clearly seen that the decrease of NO₂ requires the low specific heat release also. This conclusion is also consistent with the results presented in the Figure 5.8. Decrease of H₂ mass flow rate (O3) causes to

reduction of specific heat release also. As a result of this correlation; NO_2 decreases with lower H_2 usage (Figure 5.9). Same trend is available in Figure 1.6 also.

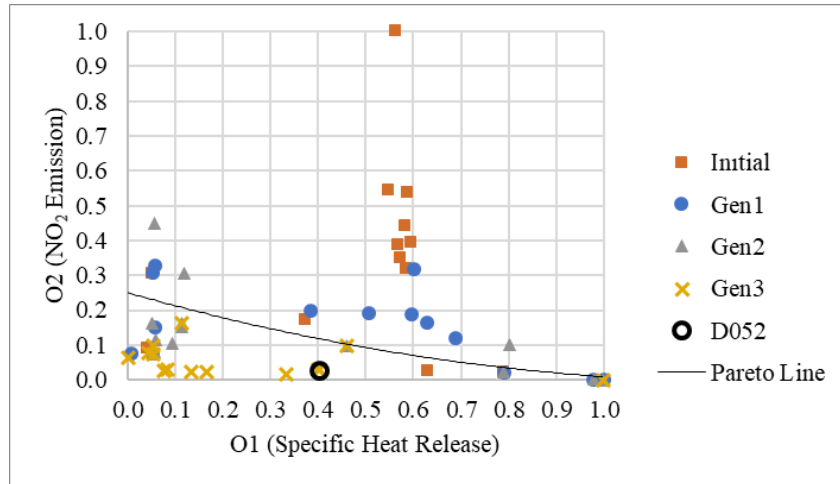


Figure 5.7 : Relationship between O1 and O2.

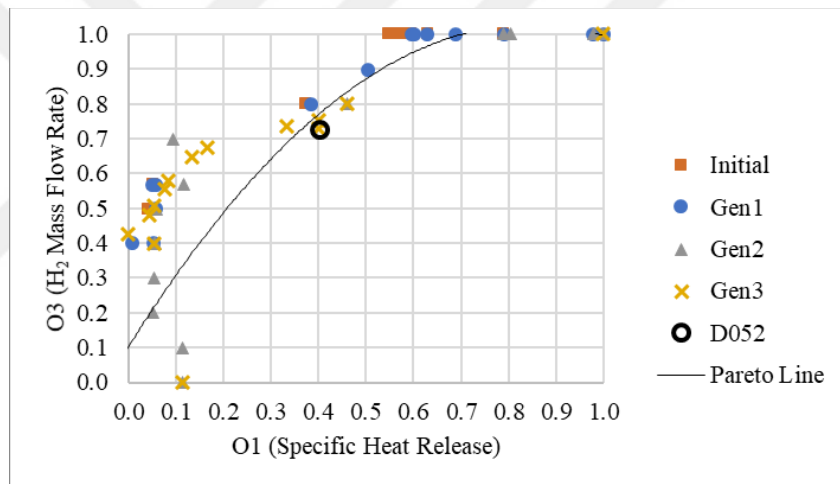


Figure 5.8 : Relationship between O1 and O3.

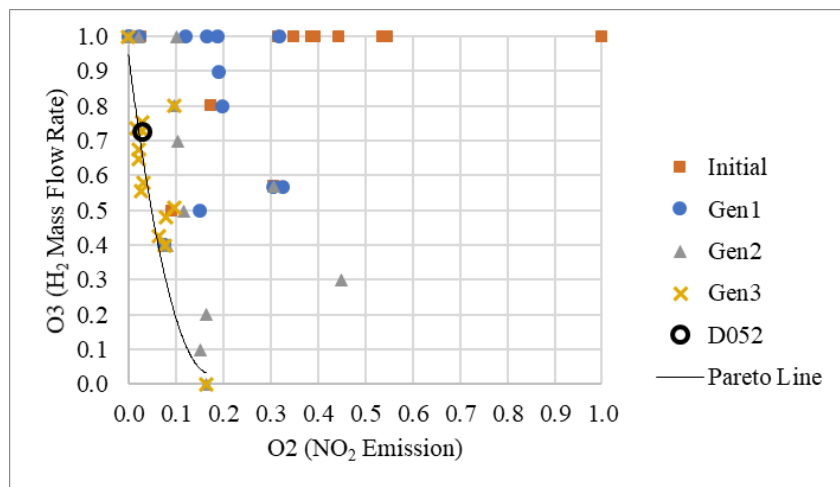


Figure 5.9 : Relationship between O2 and O3.

Figure 5.10 shows the response surface describing the relationship between specific heat release (O1), NO₂ emissions (O2), and H₂ mass flow rate (O3). The results indicate a clear trade-off among the objectives, where higher heat release is generally obtained at the expense of increased H₂ consumption and elevated NO₂ emissions. On the other hand, operating regions with lower NO₂ emissions are associated with reduced H₂ mass flow rates but also lower heat release levels. The non-uniform shape of the surface suggests a sensitive design space with competing performance targets, highlighting the need for a multi-objective optimization approach to identify balanced and feasible burner configurations.

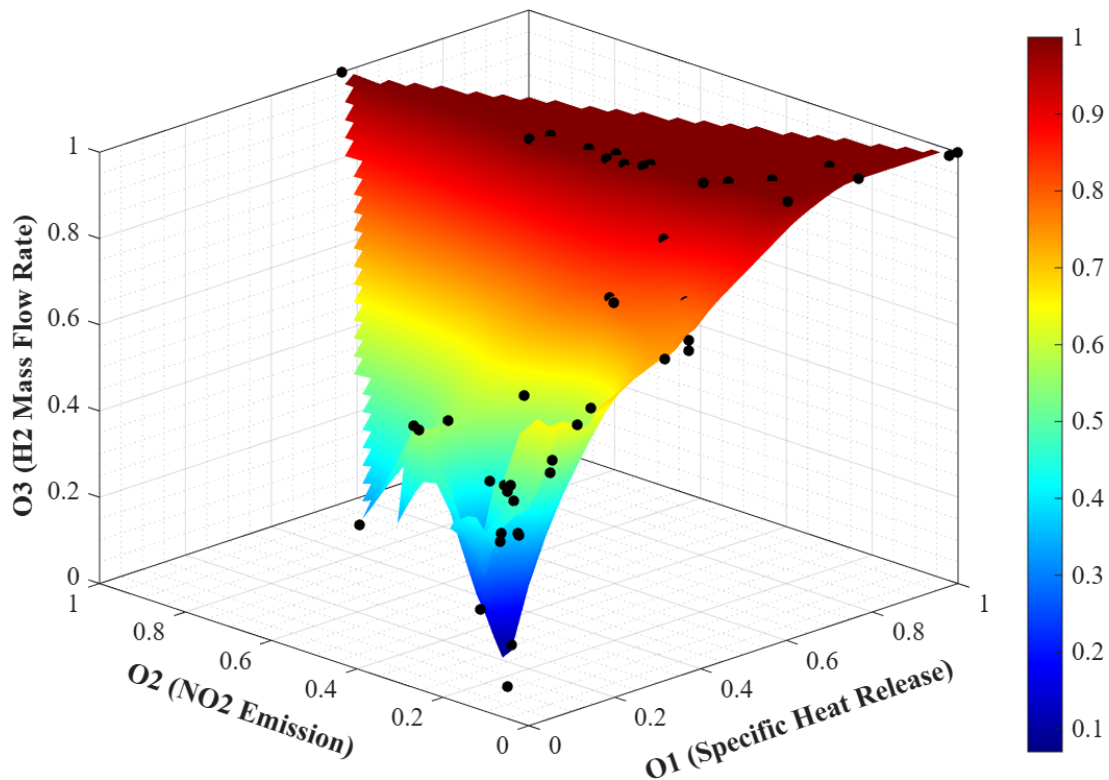


Figure 5.10 : Relationship between O1, O2 and O3.

In Figure 5.11; the effect of confinement ratio (P1) was investigated for three objectives. It can be said that the specific heat release increases and NO₂ emission decreases while the confinement ratio increases. However H₂ mass flow rate increases also. So here, when confinement ratio is increased, two objectives (O1, O2) are improved positively and H₂ mass flow rate (O3) is sacrificed.

In Figure 5.12; the same trade-off is available between objectives. It can be said that the specific heat release increases (O1) and NO₂ emission (O2) decreases while the number of vanes (P2) increase. However there is a drawback on the H₂ mass flow rate

(O3). Compared to confinement ratio (P1) results, it can be said that the relationship between number of vanes (P2) and objectives are weaker.

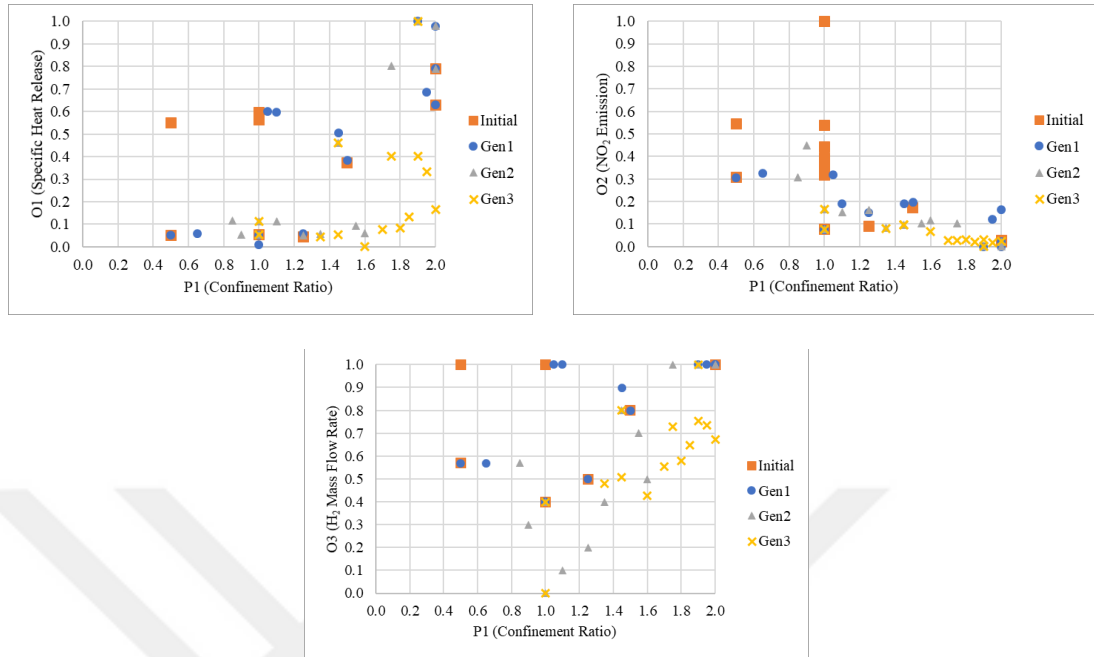


Figure 5.11 : Relationship between P1 and objectives.

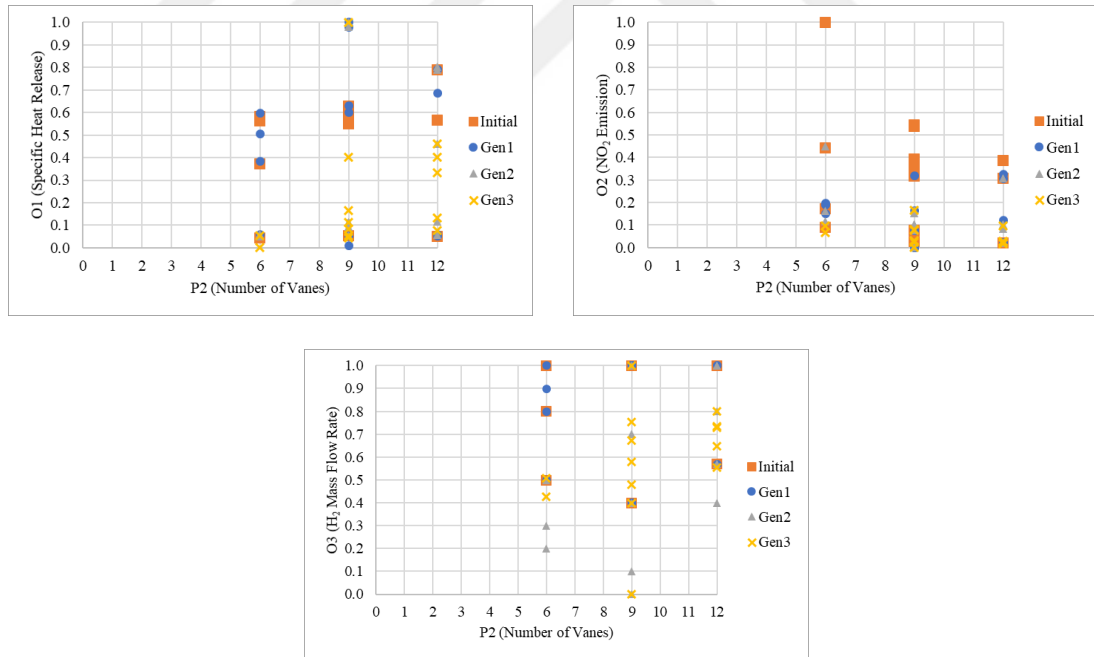


Figure 5.12 : Relationship between P2 and objectives.

Vane angle is in an opposite relationship with objectives compared to confinement ratio and number of vanes (Figure 5.13). The specific heat release decreases (O1) and NO₂ emission (O2) increases while the vane angle increase. As an important point; the H₂ mass flow rate (O3) decreases while the vane angle increases also. In summary;

we can say that: the higher vane angle gives a low H_2 designs in return relatively high NO_2 emission and low specific heat release.

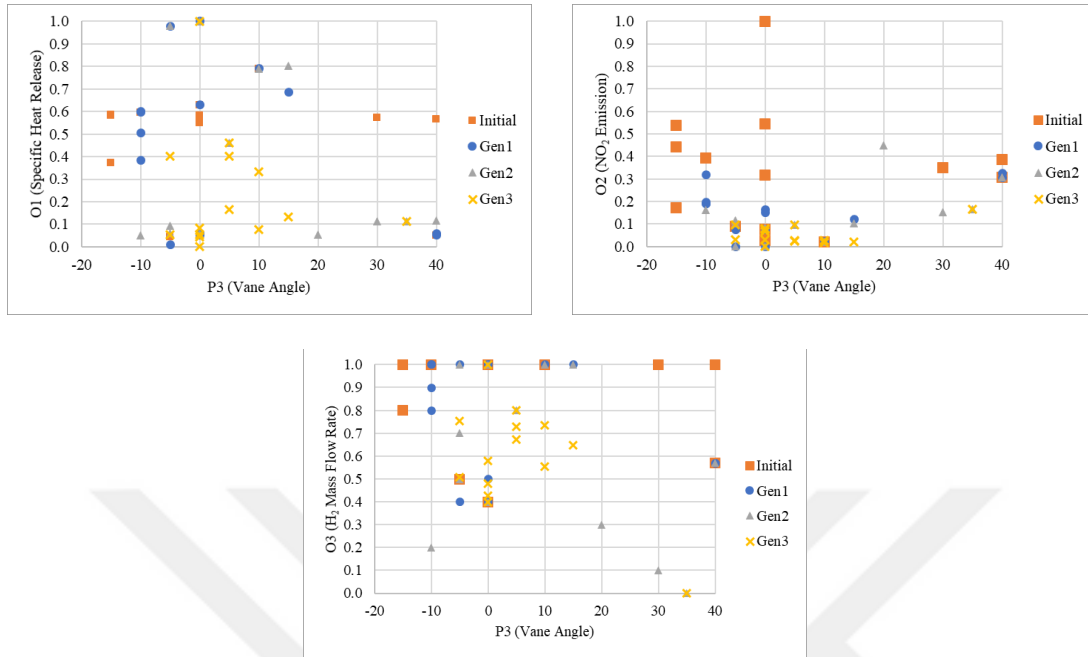


Figure 5.13 : Relationship between P3 and objectives.

In Figure 5.14; there is a linear relationship between H_2 mass flow rate (O3) and H_2 blend ratio (P4). Decrease of H_2 blend ratio decreases the specific heat release (OI) also. Although there is a weak relationship, NO_2 emissions seems like increase with H_2 blend ratio.

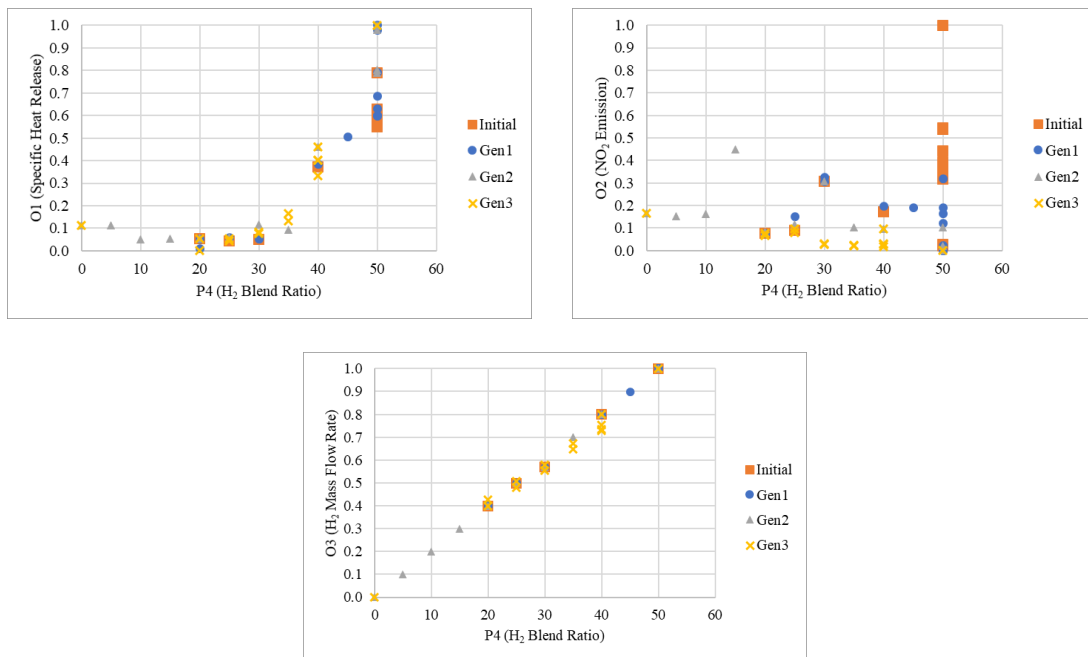


Figure 5.14 : Relationship between P4 and objectives.

The design space shows clear trade-offs among the three objectives and their relationships with four parameters. As a summary of the overall results; the design space forms two strong directions: a “high-performance but costly” region and a “fuel-saving but lower-performance” region.

In conclusion; the analysis shows that each objective points to a different design. For specific heat release (O1), the best design is D021. It gives the highest performance and keeps NO₂ at the minimum level. The drawback is its high hydrogen consumption. For NO₂ emissions (O2), D021 is again the optimum because it already has the lowest normalized NO₂ value. For H₂ mass flow rate (O3), the optimum becomes D041. This design uses no hydrogen, so O3 is minimized, but its heat-release performance is lower. When all objectives are considered together, the initial global optimum appears as D041 because it has zero hydrogen consumption and a low NO₂ level. However, this point is not practical in real operation. A 100% NH₃ flame is extremely difficult to ignite and stabilize under the same boundary conditions, and it usually requires external heating, pilot flames, or much higher inlet temperatures. In addition, the specific heat release performance of D041 is very low, and such a case would likely suffer from flame instability and high unburned NH₃ slip in an experimental setup. For these reasons, D041 should be seen as a theoretical limit rather than a realistic operating point. After removing this unrealistic case, a more feasible optimum design can be represented by D052. This design maintains low NO₂ emissions, provides acceptable heat release performance, and keeps hydrogen consumption at a reasonable level, making it a more balanced and realistic compromise among the three objectives.

These results should not be seen as exact final answers. They only show possible solution directions. Multi-objective optimization and Pareto front logic aim to identify non-dominated designs, not a single perfect point. Also, even a design that is not included in the dataset can be estimated by looking at the overall shape and trends of the Pareto fronts.

The results of base design (D000) and optimized design (D052) are summarized in Table 5.7. D052 leads to a moderate decrease (8.98%) in specific heat release. In contrast, NO₂ emissions are significantly reduced by 87.51%, while the H₂ mass flow rate decreases by 27.16%. These results highlight a clear trade-off between combustion performance and emission control. The substantial reduction in NO₂ formation, together with lower H₂ consumption, indicates that the selected geometric parameters

and fuel blend favor environmentally efficient operation. Accordingly, this configuration represents a viable low emission design option when emission reduction and H₂ utilization are prioritized over maximum heat release.

Table 5.7 : Comparison of base design and optimized design.

No	PARAMETERS				OBJECTIVES		
	Confinement Ratio [-]	Number of Vanes	Vane Angle [°]	NH ₃ /H ₂ Blend Ratio [%vol]	Specific Heat Release [-]	NO ₂ Emission [-]	H ₂ Mass Flow Rate [-]
	P1	P2	P3	P4	O1	O2	O3
D000	1	9	Base	50/50	7854.43	122.14	0.0545
D052	1.75	12.00	+5.00	60/40	7149.13 (-8.98%)	15.26 (-87.51%)	0.0397 (-27.16%)

In order to elucidate the physical mechanisms underlying the observed performance improvements, a detailed comparison between the base model D000 and the optimized configuration D052 was performed in terms of axial velocity, static pressure, temperature, and NO_x distributions. Rather than relying solely on global performance metrics, this comparison enables a spatially resolved assessment of how the optimization alters the internal flow structure and emission formation zones.

In Figure 5.15; the axial velocity distributions reveal a pronounced difference in the internal flow distribution between the base model D000 and the optimized configuration D052. In the base model, a strong jet-like structure is observed downstream of the injector, accompanied by a relatively confined central recirculation zone. This flow pattern indicates limited momentum redistribution and weaker interaction between the incoming jet and the surrounding recirculating flow. In contrast, the optimized configuration exhibits a more distributed axial velocity field with an expanded recirculation zone. The reduced jet penetration and enhanced radial momentum transfer promote stronger flow mixing and generate more effective swirl stabilization. This modification of the axial velocity field directly influences the downstream temperature and NO_x formation characteristics.

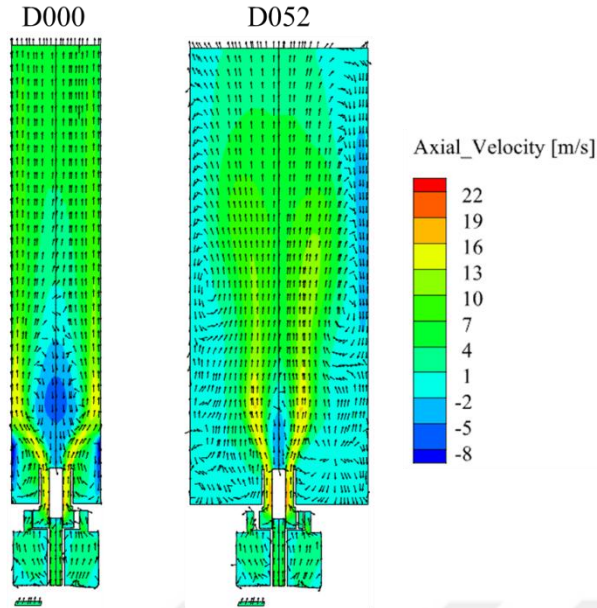


Figure 5.15 : Comparison of D000 and D052 – axial velocity.

The static pressure fields further support the differences observed in the axial velocity distributions (Figure 5.16). In the base model D000, higher pressure gradients are present near the injector region, suggesting increased local flow resistance and less efficient pressure recovery within the confinement zone. Such pressure characteristics are consistent with the strong jet-dominated flow structure observed in the axial velocity field in Figure 5.15. For the optimized configuration D052, the pressure distribution becomes more uniform along the combustor axis, with reduced pressure gradients downstream of the injector. This smoother pressure field indicates improved flow organization and reduced local losses, which contribute to a more stable recirculation structure.

The total temperature contours (Figure 5.17) demonstrate how the altered flow structure directly affects the combustion characteristics. In the base model D000, high temperature regions are localized near the injector and confined within a relatively narrow zone, indicating a compact but intense flame structure. This localized heat release is strongly influenced by the jet-dominated flow and limited recirculation observed in the velocity field. In the optimized configuration D052; the high temperature region becomes more uniformly distributed and extends further downstream. The broader temperature field reflects enhanced mixing and more effective utilization of the recirculation zone, resulting in a stable and spatially

distributed flame. This redistribution of the thermal field reduces localized peak temperatures, which is a critical factor in mitigating thermal NO₂ formation.

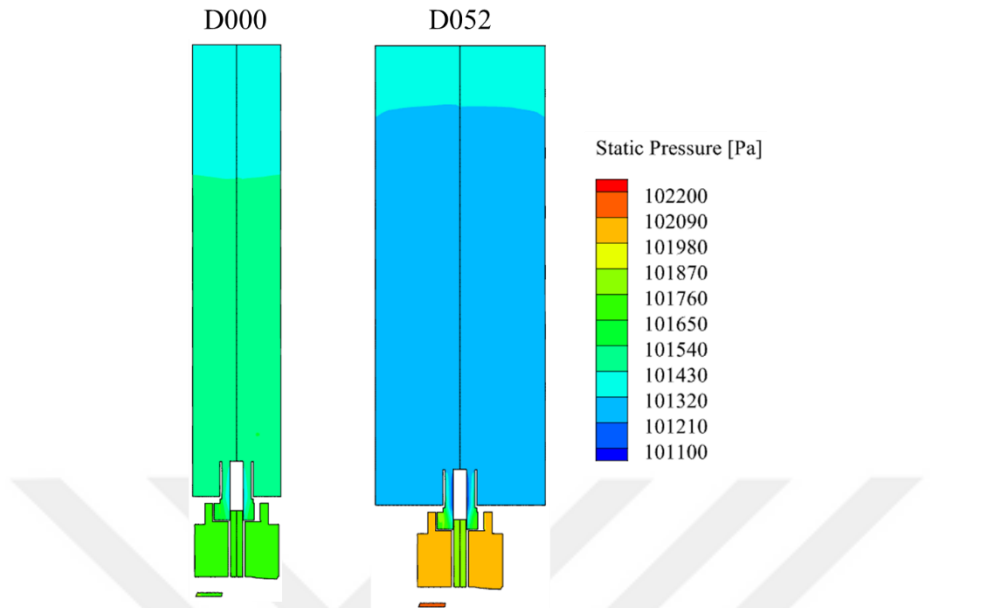


Figure 5.16 : Comparison of D000 and D052 – static pressure.

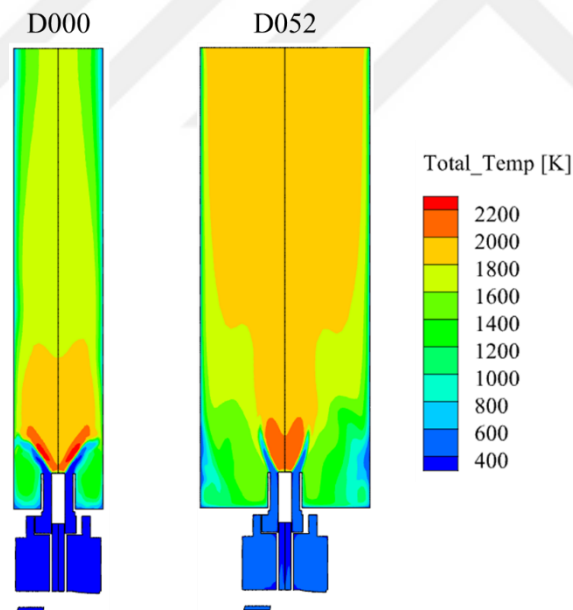


Figure 5.17 : Comparison of D000 and D052 – total temperature.

In Figure 5.18; the NO₂ distributions clearly illustrate the impact of the modified flow and thermal fields on emission formation. In the base model D000, elevated NO₂ concentrations are concentrated near the injector and along the high temperature shear layers, corresponding to regions of intense localized combustion and strong velocity gradients. These characteristics are consistent with the confined flame structure

observed in the temperature field. In contrast, the optimized configuration D052 exhibits significantly reduced NO_2 levels, with a more confined and downstream shifted formation region. The lower peak NO_2 concentrations are attributed to the combined effects of reduced local temperature peaks, improved mixing, and a more stable recirculation structure. This confirms that the optimization process not only improves global performance metrics but also fundamentally alters the combustion dynamics to suppress NO_x formation.

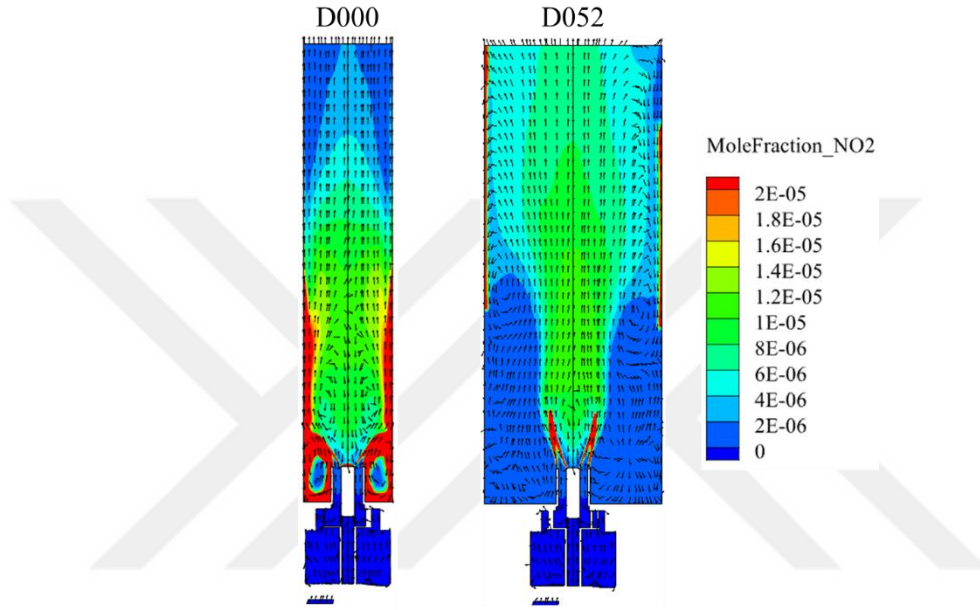


Figure 5.18 : Comparison of D000 and D052 – NO_2 emission.

Overall, the comparative analysis of axial velocity, static pressure, temperature, and NO_2 distributions demonstrates that the optimization process leads to a fundamental reorganization of the internal flow and combustion characteristics of the burner. The optimized configuration D052 exhibits improved flow uniformity, enhanced recirculation zone and a more distributed thermal field, which collectively contribute to reduced peak temperatures and suppressed NO_2 formation.

While these results confirm the effectiveness of the optimization under the prescribed operating conditions, practical combustion systems are inherently subject to variations in inlet temperature and pressure. Therefore, it is essential to evaluate the robustness of the optimized configuration under changing boundary conditions. In the following section, a parametric investigation is conducted to systematically assess the sensitivity of the optimized burner design to inlet temperature and pressure variations.

5.3 Parametric Study with Inlet Conditions

According to the optimization results; the parametric inlet conditions were changed to determine the burner's sensitivity to the inlet conditions. A parametric analysis was performed by varying the inlet temperature and inlet pressure in order to investigate the sensitivity of the D052 configuration to operating conditions. In this stage, the geometric parameters and fuel blend ratio were kept constant, and only the boundary conditions were modified. In this way, the influence of temperature and pressure on the performance of a burner design was systematically assessed (Table 5.8).

Table 5.8 : Parametric study results.

	INLET PARAMETERS		RESULTS		
	Inlet Temperature [K]	Outlet Pressure [Bara]	Specific Heat Release [kJ/kg] = Heat Release Rate [kW] / Total Fuel Flow [kg/s]	NO ₂ Emission [ppmV]	H ₂ Mass Flow Rate [kg/s]
D052_Base	300	1	7149.13	15.26	0.0397
D052_Temp	600	1	7718.16	59.7	0.0397
D052_Press	300	5	7386.22	92.32	0.0397

The results show that increasing the inlet temperature enhances flame stability and reaction intensity. As the inlet temperature is raised, the chemical reaction rates increase, and the overall heat release rises. This leads to a more robust and anchored flame, which is advantageous for stable operation under varying load conditions. However, the analyses also indicate that beyond a certain level, higher inlet temperatures tend to promote NO_x formation due to elevated peak temperatures in the reaction zone. This suggests that, for practical applications, an optimum inlet temperature range should be identified that provides sufficient stability and efficiency without causing excessive NO_x emissions.

The effect of inlet pressure exhibits an even stronger chemical sensitivity compared to temperature. With increasing pressure, the frequency of molecular collisions rises, which accelerates the reaction pathways responsible for NO_x formation. As a result, even mixtures with relatively low hydrogen content can produce noticeable NO₂ levels at high pressures.

Overall, the parametric study demonstrates that operating conditions are just as critical as geometric design and fuel composition for achieving low emission and stable combustion in ammonia–hydrogen swirl burners. Simply optimizing the burner geometry and fuel blend is not sufficient; inlet pressure, inlet temperature and the overall operating window must also be carefully controlled. These findings highlight the need for advanced control strategies and condition dependent operating guidelines in future industrial implementations of ammonia–hydrogen combustion systems.





6. CONCLUSIONS AND RECOMMENDATIONS

Ammonia presents several advantages as a hydrogen carrier and alternative fuel due to its carbon-free molecular structure and high hydrogen content per unit volume when liquefied [4]. It can be efficiently produced from both conventional and renewable resources, making it an economically feasible option [1-4]. Compared to pure hydrogen, ammonia offers significantly safer storage and distribution, with its distinct odor for leak detection and currently established infrastructure [1]. Additionally, it can be utilized in various energy applications, including engines and fuel cells, with relatively minor modifications required for existing combustion systems [5]. These attributes position ammonia as a promising energy vector for decarbonizing the energy sector and enhancing the market penetration of hydrogen-based technologies.

Recent studies have explored the use of ammonia as a clean fuel and pointed out not only its advantages but also the practical challenges it brings. These include slow flame speeds, long ignition delays, and issues like NO_x emissions and unburned ammonia in the exhaust [77]. To overcome these problems, researchers have suggested advanced solutions such as staged combustion, exhaust gas recirculation, and selective catalytic reduction systems. There is also growing interest in optimizing burner design and fuel blending, especially for applications like industrial boilers and internal combustion engines. Based on these findings, the present study provides a comprehensive investigation of ammonia-hydrogen combustion in an industrial scale swirl burner under both rich and lean conditions. By combining cold flow validation, reacting flow simulations and multi-objective optimization, the performance of different reaction mechanisms and burner configurations is systematically evaluated. The resulting insights clarify the main challenges of ammonia combustion and support the development of cleaner and more efficient burner designs for practical applications.

In the cold flow study, the LDA experiments and CFD simulations showed consistent agreement in terms of velocity distribution and the formation of the recirculation zone. This consistency confirms that the selected turbulence model can reliably predict the swirl dominated flow structures that govern flame stabilization in the reacting regime.

In addition, the AMR approach successfully captured the swirl induced velocity gradients by refining the mesh only in regions of high flow complexity, thereby reducing computational cost while maintaining accuracy. This validation ensured that the subsequent reacting flow simulations relied on a trustworthy aerodynamic and numerical foundation.

In the reacting flow study, the results show that the numerical models could predict temperature distributions with a maximum error of approximately 9%, indicating that the proposed numerical framework is sufficiently accurate for analyzing ammonia–hydrogen combustion. These findings highlight the importance of validating numerical models with experimental data to ensure reliability, particularly for swirl stabilized flames where flow chemistry interactions are complex. Furthermore, the study demonstrates that advanced CFD simulations can effectively support the optimization of ammonia–hydrogen burners by reducing the dependence on extensive experimental campaigns, thereby accelerating the development process for ammonia based combustion systems. Despite the overall promising performance, the observed discrepancies in NH_3 and NO_2 predictions indicate that current reaction mechanisms still require refinement to accurately represent ammonia chemistry under different operating conditions.

In the light of cold flow and reacting flow studies; a three-objective NSGA-II optimization was carried out to simultaneously maximize specific heat release, minimize NO_2 emissions, and minimize H_2 consumption. The CFD–Dakota coupling and the AMR supported CFD framework provided an efficient modeling strategy, allowing systematic exploration of the design space without requiring an extensive DOE study. The generated Pareto fronts clearly illustrated the conflicting nature of the objectives. The feasible global optimum was determined as D052, providing a balanced combination of acceptable specific heat release performance, moderate hydrogen demand, and low NO_2 emissions.

The optimized configurations demonstrated significant improvements compared to the initial baseline geometry (D000). The specific heat release increased by up to 20% in some optimized designs, while NO_2 emissions were reduced by nearly an order of magnitude in the best performing cases. In addition, the optimization model successfully identified configurations that required significantly less hydrogen. This result shows that simple geometric adjustments, such as increasing the confinement

ratio or modifying the vane angle, can improve overall efficiency. Compared with the baseline model, D052 also provided a more stable flame structure and lower emission levels, making it a more reliable reference point for further parametric evaluations.

Based on the optimization results, a parametric study was conducted to evaluate the burner's sensitivity to operating conditions. By varying only the inlet temperature and inlet pressure while keeping the geometry and fuel composition constant, the influence of operating conditions on burner performance was systematically examined. The results show that increasing the inlet temperature strengthens flame anchoring and enhances reaction intensity; however, excessively high temperatures promote NO_2 formation, indicating the need for defining an optimal temperature window that balances stability and emissions. Inlet pressure has a stronger chemical influence: higher pressures accelerate NO_x formation pathways and can lead to noticeable NO_2 levels. Overall, the parametric study confirms that operating conditions are as critical as geometric design and fuel blending in determining the behavior of ammonia–hydrogen swirl burners. Therefore, achieving low-emission and stable combustion requires careful control of inlet temperature, inlet pressure and the overall operating envelope, highlighting the importance of advanced control strategies in future industrial implementations.

This study does not aim to deliver a single exact “true” solution. Instead, it provides a set of plausible and physically meaningful design directions. Multi-objective optimization and Pareto front logic are based on identifying non-dominated solutions, where improving one objective necessarily worsens another. Therefore, the best design depends on the specific performance targets of the user and operational priorities. Moreover, even if a design does not physically exist in the current dataset, its potential behavior can still be inferred from the Pareto fronts. This allows the performance of intermediate or unevaluated configurations to be predicted with reasonable confidence.

The results of this study provide valuable insights into the numerical validation and optimization of an ammonia–hydrogen swirl burner. The improved understanding of combustion efficiency and emission formation, particularly NO_x reduction, contributes to cleaner burner operation and supports compliance with increasingly strict environmental regulations. These findings have practical implications for industrial boilers, heating systems, HVAC applications, and internal combustion engines where

low carbon operation and improved thermal efficiency are crucial. The ability to predict and minimize NO_x emissions while maintaining stable combustion also supports the transition from conventional fossil-fuel burners to ammonia-based systems. In addition, the validated numerical models can enhance the integration of ammonia combustion with waste-heat recovery and advanced thermal-management strategies, contributing to more sustainable thermal engineering solutions.

More powerful and comprehensive reaction mechanisms that can represent ammonia and ammonia-hydrogen combustion over a wider range of conditions should be investigated. Performing the optimization with a more extensive mechanism would improve predictive accuracy and yield more reliable results.

With the development of AI assisted modeling, future studies may incorporate AI supported optimization frameworks and reaction mechanism reduction techniques. Such approaches could enhance accuracy while significantly reducing computational cost. Extending the current methodology to higher fidelity turbulence models such as LES, DNS, or hybrid RANS–LES would provide deeper insight into turbulence–chemistry interactions that cannot be captured by RANS alone. Over the long term, advances in computational power, including quantum-accelerated and mesh-free numerical methods, may enable detailed 3D ammonia combustion simulations with unprecedented resolution.

Validated numerical models generated through such approaches could be used to optimize next-generation burners with fewer experimental requirements, reducing development time and cost. These improvements will support the wider adoption of ammonia as a carbon-free fuel and contribute to the decarbonization of thermal energy systems.

REFERENCES

- [1] **Herbinet, O., Bartocci, P., & Grinberg Dana, A.** (2022). On the use of ammonia as a fuel – a perspective. *Fuel Communications*, 11, 100064. <https://doi.org/10.1016/j.jfueco.2022.100064>
- [2] **Elbaz, A. M., Wang, S., Guiberti, T. F., & Roberts, W. L.** (2022). Review on the recent advances on ammonia combustion from the fundamentals to the applications. *Fuel Communications*, 10, 100053. <https://doi.org/10.1016/j.jfueco.2022.100053>
- [3] **Ishikawa, Y., Hayashi, J., Takeishi, H., Okanami, T., Yamamoto, Y., Iino, K., & Akamatsu, F.** (2018). Study on flame stability in oxygen-enriched ammonia/N₂/O₂ laminar diffusion flame. *Transactions of the JSME (in Japanese)*, 84(859). <https://doi.org/10.1299/transjsme.17-00526>
- [4] **Erdemir, D., & Dincer, I.** (2020). A perspective on the use of ammonia as a clean fuel: Challenges and solutions. *International Journal of Energy Research*, 45(4), 4827–4834. <https://doi.org/10.1002/er.6232>
- [5] **Li, J., Lai, S., Chen, D., Wu, R., Kobayashi, N., Deng, L., & Huang, H.** (2021). A review on combustion characteristics of ammonia as a carbon-free fuel. *Frontiers in Energy Research*, 9, 760356. <https://doi.org/10.3389/fenrg.2021.760356>
- [6] **Dunbar, B.** (2015, May 6). Technology readiness level. NASA. https://www.nasa.gov/directorates/heo/scan/engineering/technology/technology_readiness_level/
- [7] **Kobayashi, H., Hayakawa, A., Somarathne, K. D. K. A., & Okafor, E. C.** (2019). Science and Technology of Ammonia Combustion. *Proceedings of the Combustion Institute*, 37(1), 109–133. <https://doi.org/10.1016/j.proci.2018.09.029>
- [8] **Hayakawa, A., Arakawa, Y., Mimoto, R., Somarathne, K. D. K., Kudo, T., & Kobayashi, H.** (2017). Experimental investigation of stabilization and emission characteristics of ammonia/air premixed flames in a swirl combustor. *International Journal of Hydrogen Energy*, 42(19), 14010–14018. <https://doi.org/10.1016/j.ijhydene.2017.01.046>
- [9] **Franco, M. C., Rocha, R. C., Costa, M., & Yehia, M.** (2021). Characteristics of NH₃/H₂/air flames in a combustor fired by a swirl and bluff-body stabilized burner. *Proceedings of the Combustion Institute*, 38(4), 5129–5138. <https://doi.org/10.1016/j.proci.2020.06.141>

- [10] **Lee, J. H., Kim, J. H., Park, J. H., & Kwon, O. C.** (2010). Studies on properties of laminar premixed hydrogen-added ammonia/air flames for hydrogen production. *International Journal of Hydrogen Energy*, 35(3), 1054–1064. <https://doi.org/10.1016/j.ijhydene.2009.11.071>
- [11] **Li, J., Huang, H., Kobayashi, N., He, Z., & Nagai, Y.** (2014). Study on using hydrogen and ammonia as fuels: combustion characteristics and NO_x formation. *International Journal of Energy Research*, 38(9), 1214–1223. <https://doi.org/10.1002/er.3141>
- [12] **Nozari, H., & Karabeyoğlu, A.** (2015). Numerical study of combustion characteristics of ammonia as a renewable fuel and establishment of reduced reaction mechanisms. *Fuel*, 159, 223–233. <https://doi.org/10.1016/j.fuel.2015.06.075>
- [13] **Valera-Medina, A., Pugh, D. G., Marsh, P., Bulat, G., & Bowen, P.** (2017). Preliminary study on lean premixed combustion of ammonia-hydrogen for swirling gas turbine combustors. *International Journal of Hydrogen Energy*, 42(38), 24495–24503. <https://doi.org/10.1016/j.ijhydene.2017.08.028>
- [14] **Xiao, H., Valera-Medina, A., & Bowen, P. J.** (2017). Modeling combustion of ammonia/hydrogen fuel blends under gas turbine conditions. *Energy & Fuels*, 31(8), 8631–8642. <https://doi.org/10.1021/acs.energyfuels.7b00709>
- [15] **Mathieu, O., & Petersen, E. L.** (2015). Experimental and modeling study on the high-temperature oxidation of ammonia and related NO_x chemistry. *Combustion and Flame*, 162(3), 554–570. <https://doi.org/10.1016/j.combustflame.2014.08.022>
- [16] **da Rocha, R. C., Costa, M., & Bai, X.-S.** (2019). Chemical kinetic modelling of ammonia/hydrogen/air ignition, premixed flame propagation and NO emission. *Fuel*, 246, 24–33. <https://doi.org/10.1016/j.fuel.2019.02.102>
- [17] **Ichikawa, A., Hayakawa, A., Kitagawa, Y., Kunkuma Amila Somarathne, K. D., Kudo, T., & Kobayashi, H.** (2015). Laminar burning velocity and Markstein length of ammonia/hydrogen/air premixed flames at elevated pressures. *International Journal of Hydrogen Energy*, 40(30), 9570–9578. <https://doi.org/10.1016/j.ijhydene.2015.04.024>
- [18] **Valera-Medina, A., Mashruk, S., Xiao, H., Chiong, M.-C., & Chong, C.T.** (2020). Ammonia/hydrogen blends for zero-carbon energy. Paper presented at the *8th International Conference on Fluid Mechanics*, Virtual, September 25–28, 2018.
- [19] **Pacheco, G. P., Rocha, R. C., Franco, M. C., Mendes, M. A., Fernandes, E. C., Coelho, P. J., & Bai, X.-S.** (2021). Experimental and kinetic investigation of stoichiometric to rich NH₃/H₂/air flames in a swirl and bluff-body stabilized burner. *Energy & Fuels*, 35(9), 7201–7216. <https://doi.org/10.1021/acs.energyfuels.0c03872>

- [20] **Munteanu, N., & Amzaini, S. M.** (2018). Prediction of pollutant emissions from Bluff-body stabilised nonpremixed flames. *Journal of Combustion*, 2018, 1–11. <https://doi.org/10.1155/2018/8924370>
- [21] **Di Mauro, A., Ravetto, M., Goel, P., Baratta, M., Misul, D. A., Salvadori, S., Rothbauer, R., & Gretter, R.** (2021). Modelling aspects in the simulation of the diffusive flame in a bluff-body geometry. *Energies*, 14(11), 2992. <https://doi.org/10.3390/en14112992>
- [22] **Meraner, C., Li, T., Ditaranto, M., & Løvås, T.** (2018). Cold flow characteristics of a novel Bluff Body Hydrogen Burner. *International Journal of Hydrogen Energy*, 43(14), 7155–7168. <https://doi.org/10.1016/j.ijhydene.2018.02.062>
- [23] **Sudarma, A. F., Al-Witry, A., & Morsy, M. H.** (2017). RANS numerical simulation of lean premixed bluff-body stabilized combustor: Comparison of turbulence models. *Journal of Thermal Engineering*, 3(3), 1561–1573. <https://doi.org/10.18186/journal-of-thermal-engineering.321093955>
- [24] **Muppala, S. P. R., Manickam, B., & Dinkelacker, F.** (2015). A comparative study of different reaction models for turbulent methane/hydrogen/air combustion. *Journal of Thermal Engineering*, 1(5), 367–380. <https://doi.org/10.18186/jte.76780>
- [25] **Rajak, U., Nashine, P., Chaurasiya, P. K., & Verma, T. N.** (2021). A numerical investigation of the species transport approach for modeling of gaseous combustion. *Journal of Thermal Engineering*, 7(Supplement 14), 2054–2067. <https://doi.org/10.18186/thermal.1051312>
- [26] **Okafor, E. C., Somarathne, K. D. K. A., Hayakawa, A., Kudo, T., Kurata, O., Iki, N., & Kobayashi, H.** (2019). Towards the development of an efficient low-NO_x ammonia combustor for a micro gas turbine. *Proceedings of the Combustion Institute*, 37(4), 4597–4606. <https://doi.org/10.1016/j.proci.2018.07.083>
- [27] **Cai, T., Zhao, D., & E, J.** (2020). Bluff-body effect on thermal and NO emission characteristics in a micro-planar combustor fueled with premixed ammonia-oxygen. *Chemical Engineering and Processing - Process Intensification*, 153, 107979. <https://doi.org/10.1016/j.cep.2020.107979>
- [28] **Rocha, R. C., Costa, M., & Bai, X.-S.** (2020). Combustion and emission characteristics of ammonia under conditions relevant to modern gas turbines. *Combustion Science and Technology*, 193(14), 2514–2533. <https://doi.org/10.1080/00102202.2020.1748018>
- [29] **Mendiara, T., & Glarborg, P.** (2009). Ammonia chemistry in oxy-fuel combustion of methane. *Combustion and Flame*, 156(10), 1937–1949. <https://doi.org/10.1016/j.combustflame.2009.07.006>

- [30] **Zhang, M., Wei, X., Wang, J., Huang, Z., & Tan, H.** (2021). The blow-off and transient characteristics of co-firing ammonia/methane fuels in a swirl combustor. *Proceedings of the Combustion Institute*, 38(4), 5181–5190. <https://doi.org/10.1016/j.proci.2020.08.056>
- [31] **Okafor, E. C., Naito, Y., Colson, S., Ichikawa, A., Kudo, T., Hayakawa, A., & Kobayashi, H.** (2019). Measurement and modelling of the laminar burning velocity of methane-ammonia-air flames at high pressures using a reduced reaction mechanism. *Combustion and Flame*, 204, 162–175. <https://doi.org/10.1016/j.combustflame.2019.03.008>
- [32] **Honzawa, T., Kai, R., Okada, A., Valera-Medina, A., Bowen, P. J., & Kurose, R.** (2019). Predictions of NO and CO emissions in ammonia/methane/air combustion by LES using a non-adiabatic flamelet generated manifold. *Energy*, 186, 115771. <https://doi.org/10.1016/j.energy.2019.07.101>
- [33] **Valera-Medina, A., Gutesa, M., Xiao, H., Pugh, D., Giles, A., Goktepe, B., Marsh, R., & Bowen, P.** (2019). Premixed ammonia/hydrogen swirl combustion under rich fuel conditions for gas turbines operation. *International Journal of Hydrogen Energy*, 44(16), 8615–8626. <https://doi.org/10.1016/j.ijhydene.2019.02.041>
- [34] **Vigueras-Zúñiga, M. O., Tejeda-del-Cueto, M. E., Mashruk, S., Kovaleva, M., Ordóñez-Romero, C. L., & Valera-Medina, A.** (2021). Methane/ammonia radical formation during high temperature reactions in Swirl Burners. *Energies*, 14(20), 6624. <https://doi.org/10.3390/en14206624>
- [35] **Vigueras-Zúñiga, M.-O., Tejeda-del-Cueto, M.-E., Vasquez-Santacruz, J.-A., Herrera-May, A.-L., & Valera-Medina, A.** (2020). Numerical predictions of a swirl combustor using complex chemistry fueled with ammonia/hydrogen blends. *Energies*, 13(2), 288. <https://doi.org/10.3390/en13020288>
- [36] **Okafor, E. C., Naito, Y., Colson, S., Ichikawa, A., Kudo, T., Hayakawa, A., & Kobayashi, H.** (2018). Experimental and numerical study of the laminar burning velocity of CH₄-NH₃-Air premixed flames. *Combustion and Flame*, 187, 185–198. <https://doi.org/10.1016/j.combustflame.2017.09.002>
- [37] **Pugh, D., Bowen, P., Valera-Medina, A., Giles, A., Runyon, J., & Marsh, R.** (2019). Influence of steam addition and elevated ambient conditions on NO_x reduction in a staged premixed swirling NH₃/H₂ flame. *Proceedings of the Combustion Institute*, 37(4), 5401–5409. <https://doi.org/10.1016/j.proci.2018.07.091>
- [38] **Runyon, J., Marsh, R., Bowen, P., Pugh, D., Giles, A., & Morris, S.** (2018). Lean methane flame stability in a premixed generic Swirl Burner: Isothermal flow and atmospheric combustion characterization.

Experimental Thermal and Fluid Science, 92, 125–140.
<https://doi.org/10.1016/j.expthermflusci.2017.11.019>

- [39] Mikulčić, H., Baleta, J., Wang, X., Wang, J., Qi, F., & Wang, F. (2021). Numerical simulation of ammonia/methane/air combustion using reduced chemical kinetics models. *International Journal of Hydrogen Energy*, 46(45), 23548–23563.
<https://doi.org/10.1016/j.ijhydene.2021.01.109>
- [40] Valera-Medina, A., Marsh, R., Runyon, J., Pugh, D., Beasley, P., Hughes, T., & Bowen, P. (2017). Ammonia–methane combustion in tangential swirl burners for gas turbine power generation. *Applied Energy*, 185, 1362–1371. <https://doi.org/10.1016/j.apenergy.2016.02.073>
- [41] Wiseman, S., Rieth, M., Gruber, A., Dawson, J. R., & Chen, J. H. (2021). A comparison of the blow-out behavior of turbulent premixed ammonia/hydrogen/nitrogen-air and methane–Air Flames. *Proceedings of the Combustion Institute*, 38(2), 2869–2876.
<https://doi.org/10.1016/j.proci.2020.07.011>
- [42] Somarathne, K. D., Hatakeyama, S., Hayakawa, A., & Kobayashi, H. (2017). Numerical study of a low emission gas turbine like combustor for turbulent ammonia/air premixed swirl flames with a secondary air injection at high pressure. *International Journal of Hydrogen Energy*, 42(44), 27388–27399. <https://doi.org/10.1016/j.ijhydene.2017.09.089>
- [43] Somarathne, K. D., Colson, S., Hayakawa, A., & Kobayashi, H. (2018). Modelling of ammonia/air non-premixed turbulent swirling flames in a gas turbine-like combustor at various pressures. *Combustion Theory and Modelling*, 22(5), 973–997.
<https://doi.org/10.1080/13647830.2018.1468035>
- [44] Somarathne, K. D., C. Okafor, E., Hayakawa, A., Kudo, T., Kurata, O., Iki, N., & Kobayashi, H. (2019). Emission characteristics of turbulent non-premixed ammonia/air and methane/air swirl flames through a rich-lean combustor under various wall thermal boundary conditions at high pressure. *Combustion and Flame*, 210, 247–261.
<https://doi.org/10.1016/j.combustflame.2019.08.037>
- [45] Somarathne, K. D., Hayakawa, A., & Kobayashi, H. (2016). Numerical investigation on the combustion characteristics of turbulent premixed ammonia/air flames stabilized by a swirl burner. *Journal of Fluid Science and Technology*, 11(4).
<https://doi.org/10.1299/jfst.2016jfst0026>
- [46] Miller, J. A., Smooke, M. D., Green, R. M., & Kee, R. J. (1983). Kinetic modeling of the oxidation of ammonia in flames. *Combustion Science and Technology*, 34(1-6), 149–176.
<https://doi.org/10.1080/00102208308923691>

- [47] **Alnasif, A., Mashruk, S., Shi, H., Alnajideen, M., Wang, P., Pugh, D., & Valera-Medina, A.** (2023). Evolution of ammonia reaction mechanisms and modelling parameters: a review. *Applications in Energy and Combustion Science*, 15, 100175. <https://doi.org/10.1016/j.jaecs.2023.100175>
- [48] **Alnasif A., Mashruk S., Hayashi M., J'ojka J, Shi H., Hayakawa A., & Valera-Medina A.** Performance investigation of currently available reaction mechanisms in the estimation of NO Measurements: a comparative study. *Energies*, 16, 3847. <https://doi.org/10.3390/en16093847>
- [49] **Duynslaegher C., Contino F., Vandooren J., & Jeanmart H.** (2012). Modeling of ammonia combustion at low pressure. *Combustion and Flame*, 159, 2799–2805. <https://doi.org/10.1016/j.combustflame.2012.06.003>
- [50] **Nakamura H., Hasegawa S., & Tezuka T.** (2017). Kinetic modeling of ammonia/air weak flames in a micro flow reactor with a controlled temperature profile. *Combustion and Flame*, 185, 16–27. <https://doi.org/10.1016/j.combustflame.2017.06.021>
- [51] **Alnasif A., Zitouni S., Mashruk S., Brequigny P, Kovaleva M., Mounaim-Rousselle C., & Valera-Medina A.** (2023). Experimental and numerical comparison of currently available reaction mechanisms for laminar flame speed in 70/30 (%vol.) NH₃/H₂ flames. *Applications in Energy and Combustion Science*, 14, 100139. <https://doi.org/10.1016/j.jaecs.2023.100139>
- [52] **Stagni A., Cavallotti C., Arunthanayothin S., Song Y., Herbinet O., Battin-Leclerc F., & Faravelli, T.** (2020). An experimental, theoretical and kinetic-modeling study of the gas phase oxidation of ammonia. *Reaction Chemistry & Engineering*, 5, 696–711. <https://doi.org/10.1039/c9re00429g>
- [53] **Kurata, O., Iki, N., Matsunuma, T., Inoue, T., Tsujimura, T., Furutani, H., Kobayashi, H., & Hayakawa, A.** (2017). Performances and emission characteristics of NH₃–air and NH₃–CH₄–air combustion gas-turbine power generations. *Proceedings of the Combustion Institute*, 36(3), 3351–3359. <https://doi.org/10.1016/j.proci.2016.07.088>
- [54] **Thompson, J. S., Walton, S., Hassan, O., Rolland, S. A., & Sienz, J.** (2017). The use of CFD and multi-objective optimisation techniques to customise an industrial pre-mixer. *Structural and Multidisciplinary Optimization*, 55(6), 2339–2351. <https://doi.org/10.1007/s00158-016-1643-7>
- [55] **Khelladi, F. Z., Alliche, M., Rebhi, R., Lorenzini, G., Ahmad, H., & Menni, Y.** (2021). The effect of bluff body shape on flame stability in a non-premixed hydrogen-methane-air mixture combustion. *Annales De Chimie - Science Des Matériaux*, 45(5), 385–392. <https://doi.org/10.18280/acsm.450504>

- [56] **Kashir, B., Tabejamaat, S., & Jalalatian, N.** (2015). The impact of hydrogen enrichment and bluff-body lip thickness on characteristics of blended propane/hydrogen bluff-body stabilized turbulent diffusion flames. *Energy Conversion and Management*, 103, 1–13. <https://doi.org/10.1016/j.enconman.2015.06.028>
- [57] **Deger, M. D.** (2019). *Sentez gaz yanmasında parametrik çalışma ve hedeflenen çıktıkların genetik algoritmayla optimizasyonu* [Master's thesis, Istanbul Technical University]
- [58] **Baej, H., Valera Medina, A., Syred, N., Marsh, R. & Bowen, P. J.** (2015). CFD predictions of swirl burner aerodynamics with variable outlet configurations. In *Proceedings of the Global Conference on Energy and Sustainable Development (GCESD2015)*, Coventry University Technology Park, UK, 24-26 February 2015 (pp. 2307-2312).
- [59] **Mashruk, S., Kovaleva, M., Alnasif, A., Chong, C. T., Hayakawa, A., Okafor, E. C., & Valera-Medina, A.** (2022). Nitrogen oxide emissions analyses in ammonia/hydrogen/air premixed swirling flames. *Energy*, 260, 125183. <https://doi.org/10.1016/j.energy.2022.125183>
- [60] **Mashruk S., Kovaleva M., Chong C. T., Hayakawa A., Okafor E., & Valera-Medina A.** (2021). Nitrogen oxides as a by-product of ammonia/hydrogen combustion regimes. *Chemical Engineering Transactions*, 89, 613–618. <https://doi.org/10.3303/CET2189103>.
- [61] **Mashruk, S., Okafor, E. C., Kovaleva, M., Alnasif, A., Pugh, D., Hayakawa, A., & Valera-Medina, A.** (2022). Evolution of N₂O production at lean combustion condition in NH₃/H₂/air premixed swirling flames. *Combustion and Flame*, 244, 112299. <https://doi.org/10.1016/j.combustflame.2022.112299>
- [62] **Mashruk, S., Zhu, X., Roberts, W. L., Guiberti, T. F., & Valera-Medina, A.** (2023). Chemiluminescent footprint of premixed ammonia-methane-air swirling flames. *Proceedings of the Combustion Institute*, 39(1), 1415–1423. <https://doi.org/10.1016/j.proci.2022.08.073>
- [63] **Richards, K. J., Senecal, P. K., & Pomraning, E.** (2024). *CONVERGE 3.0*. Convergent Science.
- [64] **Shaddix, C. R.** (2017). A new method to compute the proper radiant heat transfer correction of bare-wire thermocouple measurements. In *10th U.S. National Combustion Meeting* (Ed.).
- [65] **British standards Institution.** (1996). *BS ISO 11042-1:1996 Gas turbines - Exhaust gas emission*.
- [66] **Gulsan, M. A., & Boke, Y. E.** (2024). CFD validation of unconfined low swirl burner under cold flow conditions. In *Proceedings of INCOS 2024: International Combustion Symposium* (pp. 65–77). Uludağ University, Bursa, Turkey.

- [67] **Eriksson, P.** (2007). The Zimont TFC model applied to premixed bluff-body stabilized combustion using four different RANS turbulence models. In *Proceedings of the ASME Turbo Expo 2007* (Paper No. GT2007-27480). <https://doi.org/10.1115/GT2007-27480>
- [68] **Adams, B.M., Bohnhoff, W.J., Dalbey, K.R., Ebeida, M.S., Eddy, J.P., Eldred, M.S., Hooper, R.W., Hough, P.D., Hu, K.T., Jakeman, J.D., Khalil, M., Maupin, K.A., Monschke, J.A., Ridgway, E.M., Rushdi, A.A., Seidl, D.T., Stephens, J.A., Swiler, L.P., & Winokur, J.G.** (2021). *Dakota, a multilevel parallel object-oriented framework for design optimization, parameter estimation, uncertainty quantification, and sensitivity analysis: version 6.15 user's manual* (SAND2020-12495). Sandia National Laboratories.
- [69] **Deb, K., Pratap, A., Agarwal, S., & Meyarivan, T.** (2002). A fast and elitist multiobjective genetic algorithm: NSGA-II. *IEEE Transactions on Evolutionary Computation*, 6(2), 182-197. <https://doi.org/10.1109/4235.996017>
- [70] **Oh, J.-T., & Chien, N. B.** (2018). Optimization design by coupling computational fluid dynamics and genetic algorithm. In *Computational Fluid Dynamics - Basic Instruments and Applications in Science*. IntechOpen. <https://doi.org/10.5772/intechopen.72316>
- [71] **Li, S., Deng, Z., Liu, J., & Liu, D.** (2022). Multi-objective optimization of plate-fin heat exchangers via non-dominated sequencing genetic algorithm (NSGA-II). *Applied Sciences*, 12(22), 11792. <https://doi.org/10.3390/app122211792>
- [72] **Sukumar, S., Kar, S. P., Swain, A., Sarangi, R. K., & Sekhar, P. C.** (2020). A combined CFD, ANFIS and NSGA-II model for repetitive pulse laser drilling process. *Lasers in Manufacturing and Materials Processing*, 7(4), 449–477. <https://doi.org/10.1007/s40516-020-00127-x>
- [73] **Santhanakrishnan, M. S., Tilford, T., & Bailey, C.** (2021). Multi-objective NSGA-II based shape optimisation of the cross-sectional shape of passively cooled heat sinks. *International Journal of Numerical Methods for Heat & Fluid Flow*, 32(3), 1025–1045. <https://doi.org/10.1108/hff-10-2020-0656>
- [74] **Gao, G., Gao, C., Guo, Z., Wu, H., Lyu, H., Niu, F., & Liu, Y.** (2024). Optimization study of lead-based reactor heat exchangers based on Dakota Coupling CFD. *International Journal of Advanced Nuclear Reactor Design and Technology*, 6(2), 67–77. <https://doi.org/10.1016/j.jandt.2024.05.001>
- [75] **Url-1 Wolf Dynamics.** (2021). *OpenFOAM Workshop 2021 Training Manual*. <https://www.wolfdynamics.com/training/OF_WS2021/OFWS2021.pdf>

- [76] **Url-2 Sandia National Laboratories.** (2023). *Coupling Dakota to simulation codes.* <<https://snl-dakota.github.io/docs/6.18.0/users/usingdakota/introduction/couplingtcouplingtosi.html>>
- [77] **Alnajideen, M., Shi, H., Northrop, W., Emberson, D., Kane, S., Czyżewski, P., Alnaeli, M., Mashruk, S., Rouwenhorst, K., Yu, C., Eckart, S., & Valera-Medina, A.** (2024). Ammonia combustion and emissions in practical applications: A review. *Carbon Neutrality*, 3(1), 13. <https://doi.org/10.1007/s43979-024-00088-6>





APPENDICES

APPENDIX A: Burner Variants





APPENDIX A

1. Initial Population and First Iteration Designs

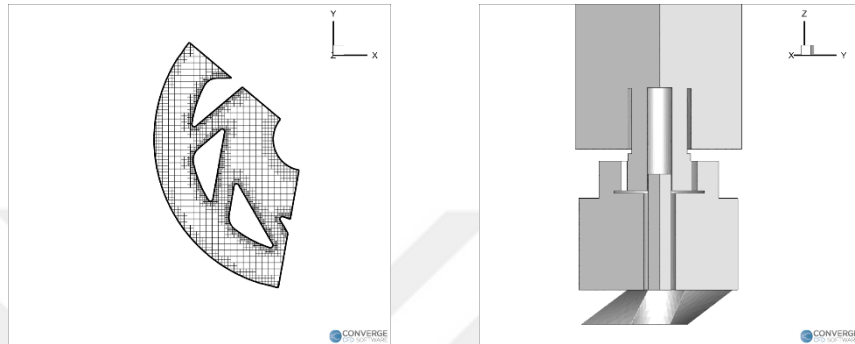


Figure A.1 : Design D000.

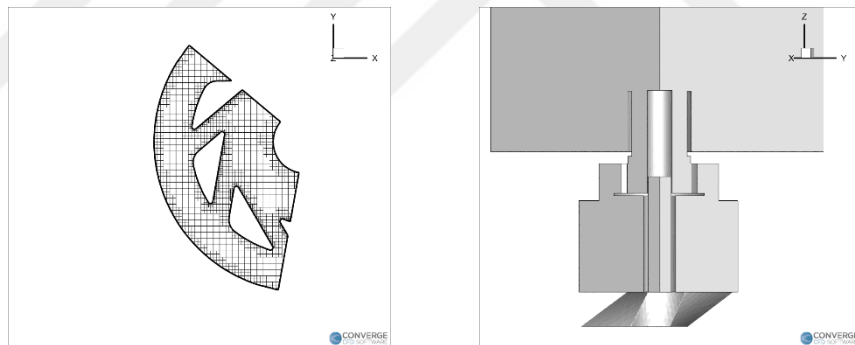


Figure A.2 : Design D001.

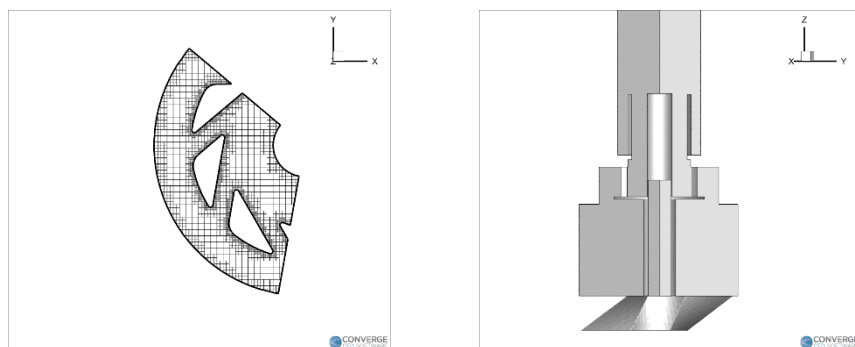


Figure A.3 : Design D002.

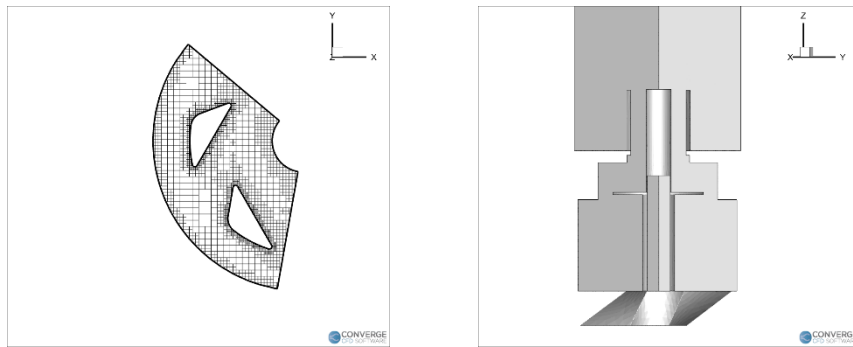


Figure A.4 : Design D003.

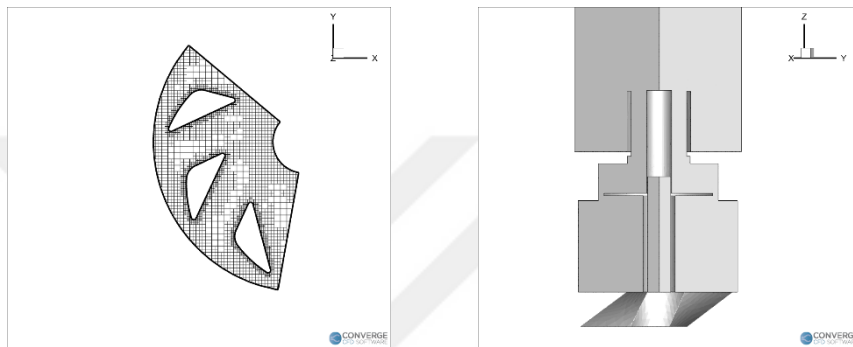


Figure A.5 : Design D004.

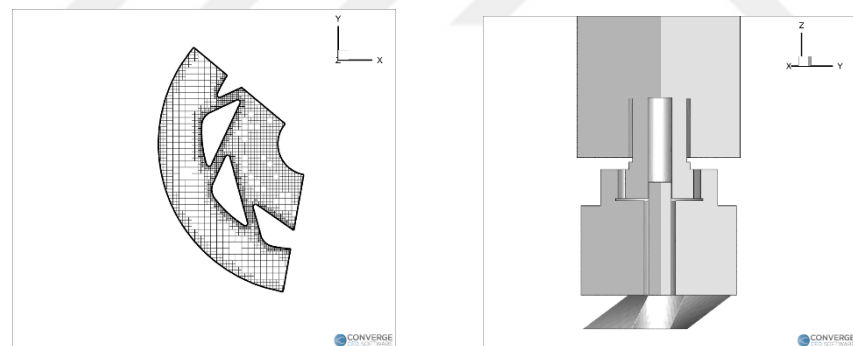


Figure A.6 : Design D005.

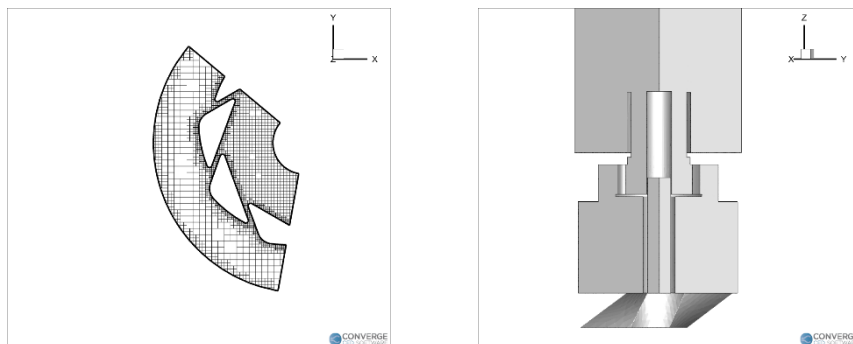


Figure A.7 : Design D006.

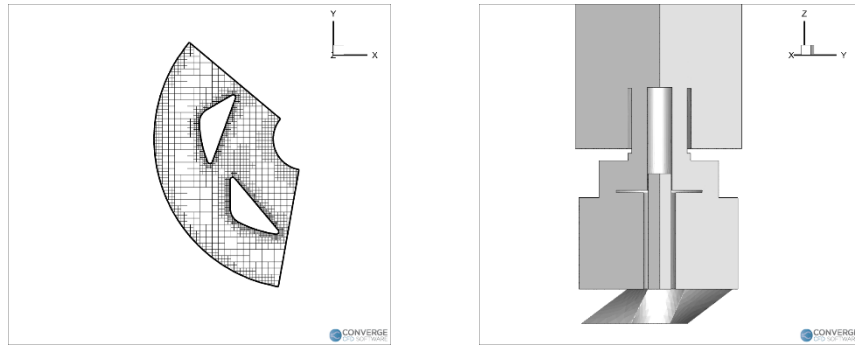


Figure A.8 : Design D007.

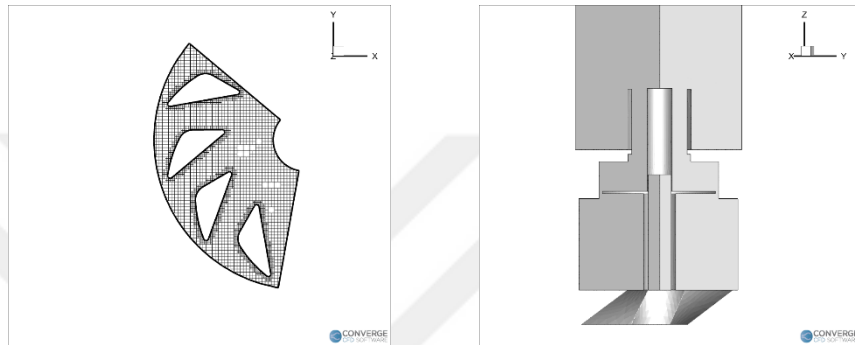


Figure A.9 : Design D008.

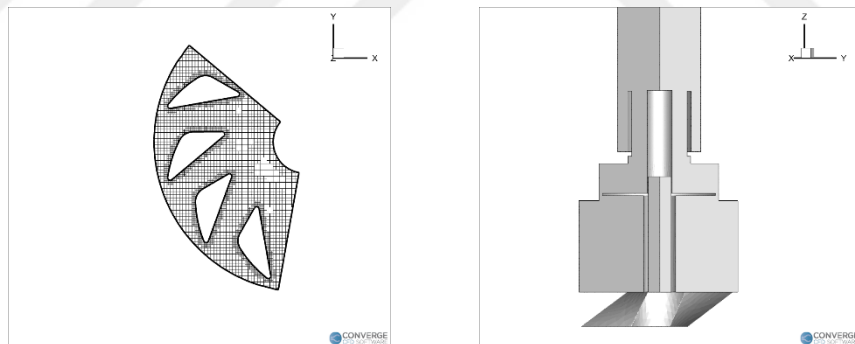


Figure A.10 : Design D009.

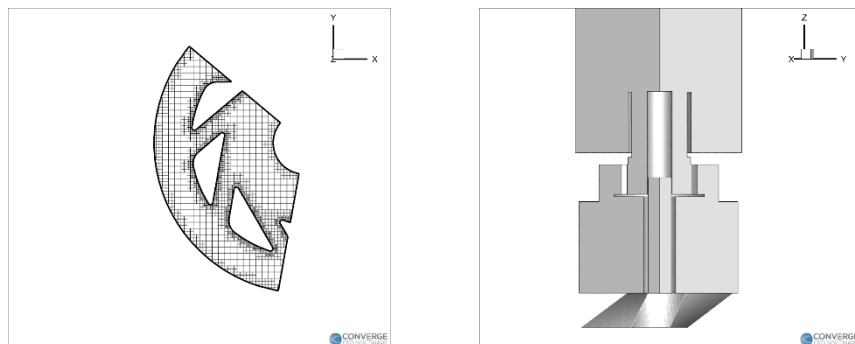


Figure A.11 : Design D010.

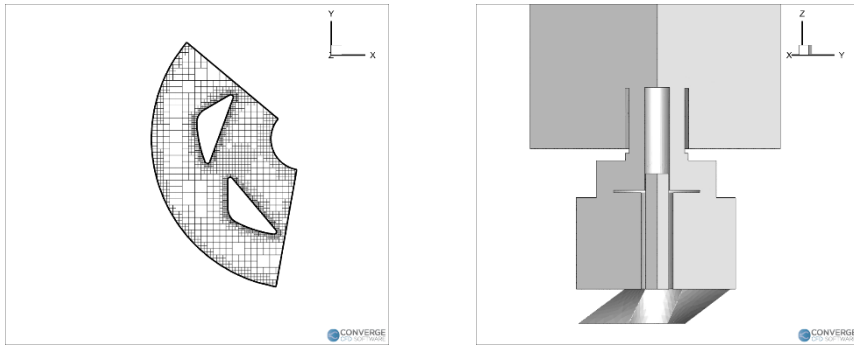


Figure A.12 : Design D011.

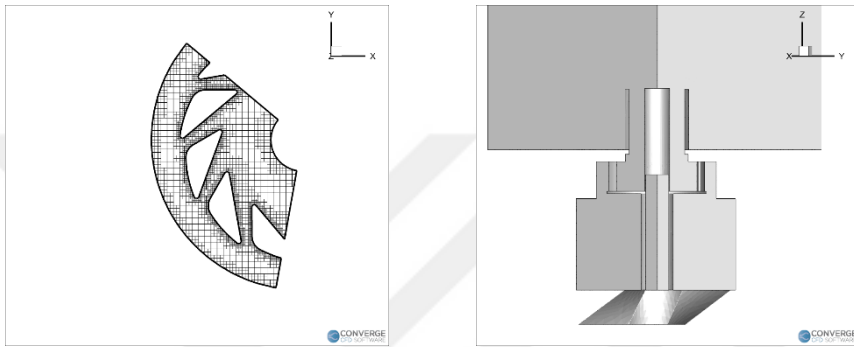


Figure A.13 : Design D012.

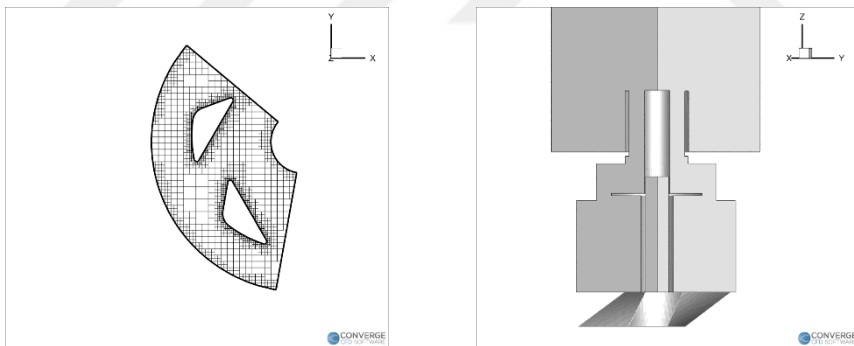


Figure A.14 : Design D013.

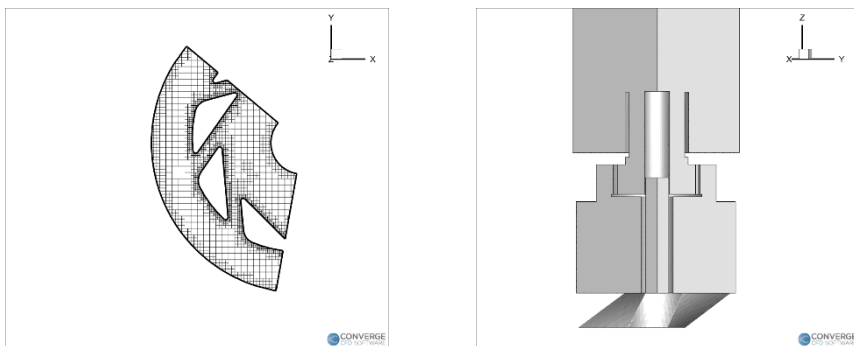


Figure A.15 : Design D014.

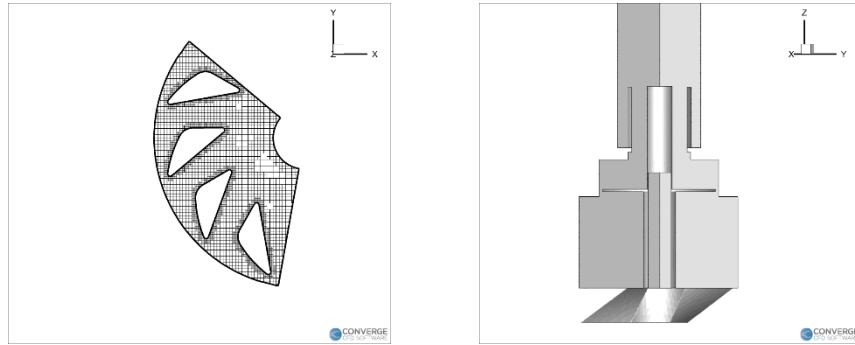


Figure A.16 : Design D015.

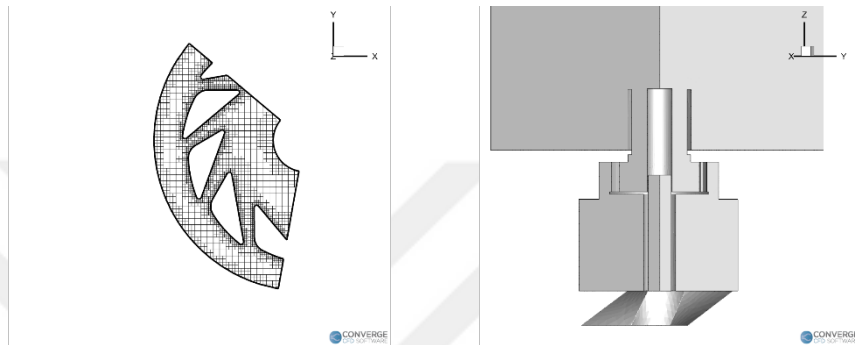


Figure A.17 : Design D016.

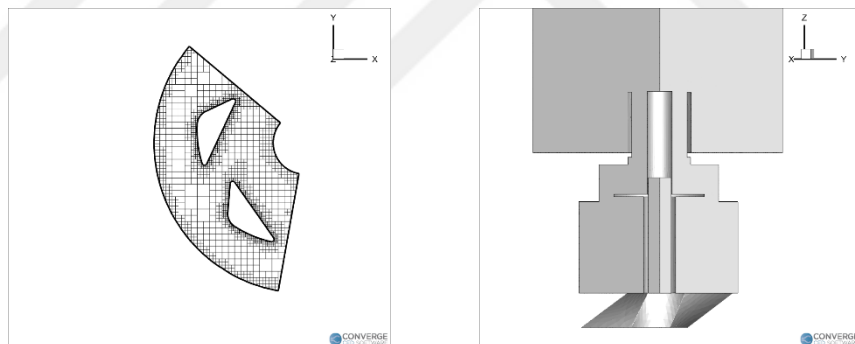


Figure A.18 : Design D017.

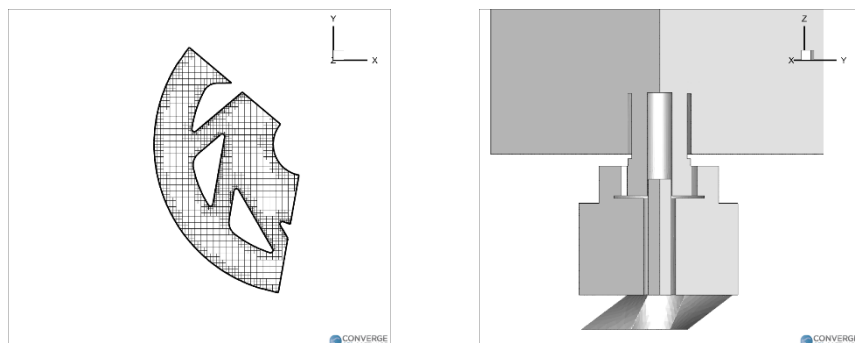


Figure A.19 : Design D018.

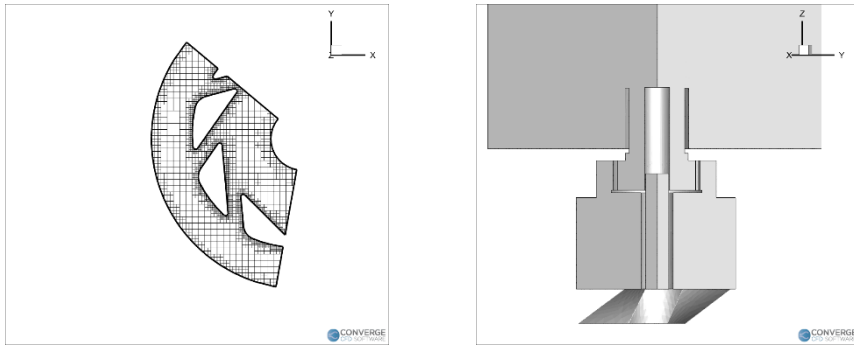


Figure A.20 : Design D019.

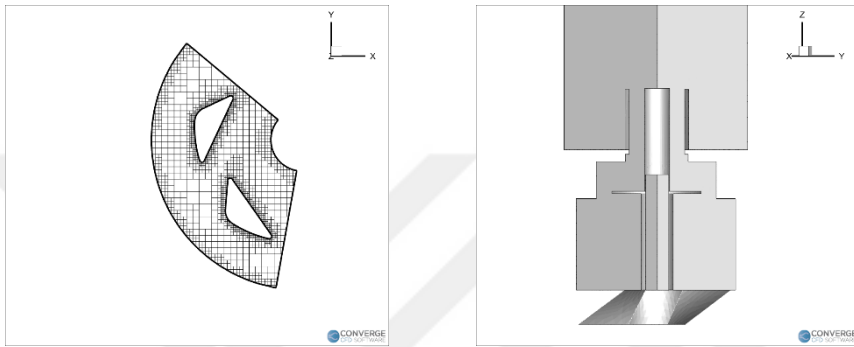


Figure A.21 : Design D020.

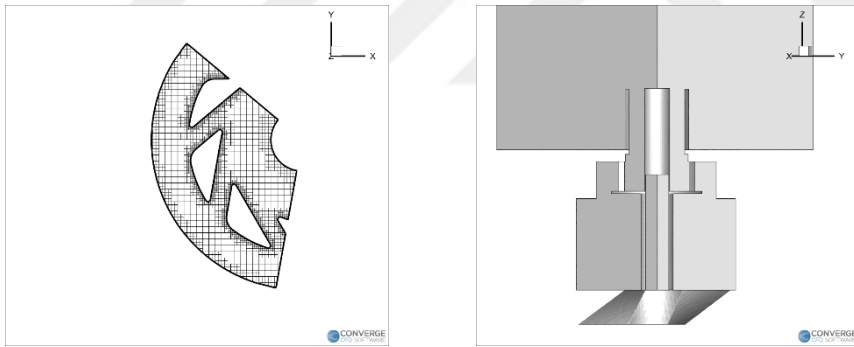


Figure A.22 : Design D021.

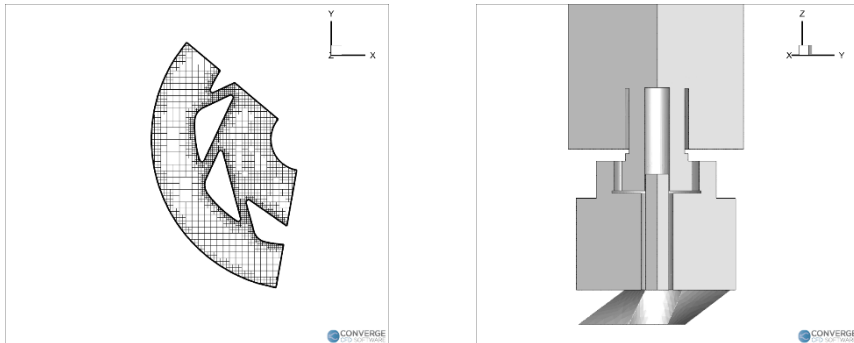


Figure A.23 : Design D022.

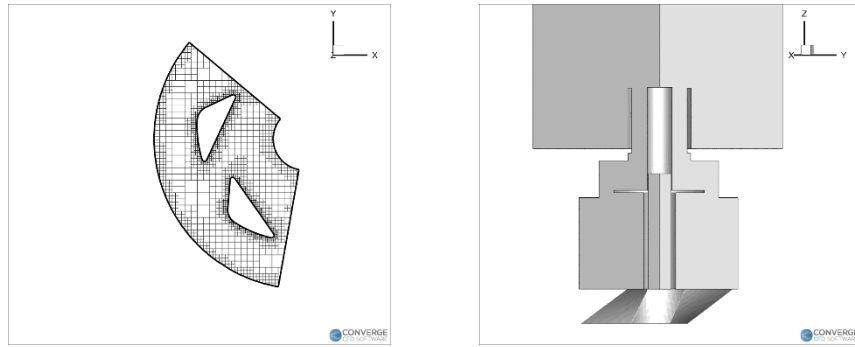


Figure A.24 : Design D023.

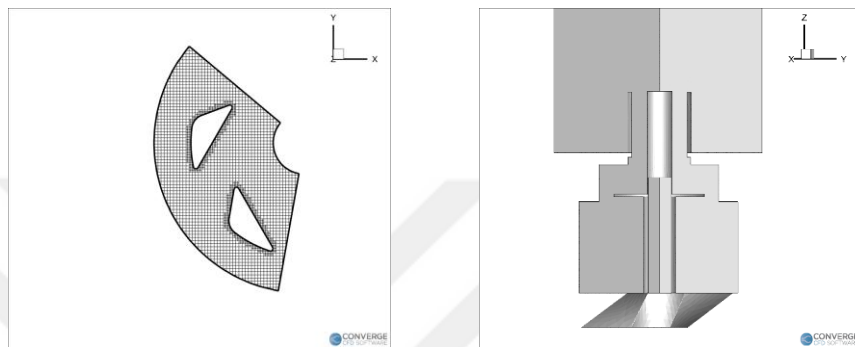


Figure A.25 : Design D024.

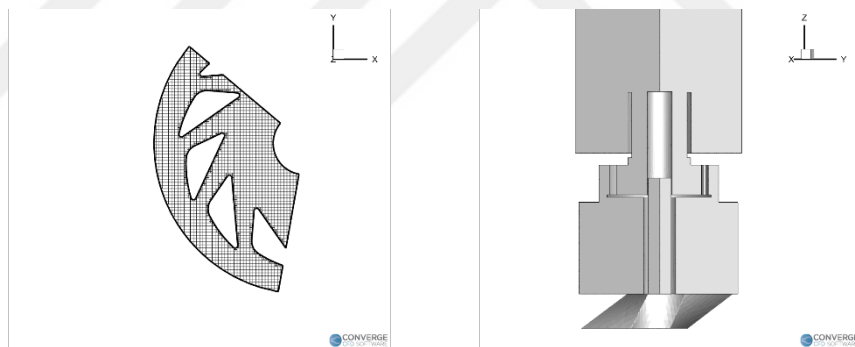


Figure A.26 : Design D025.

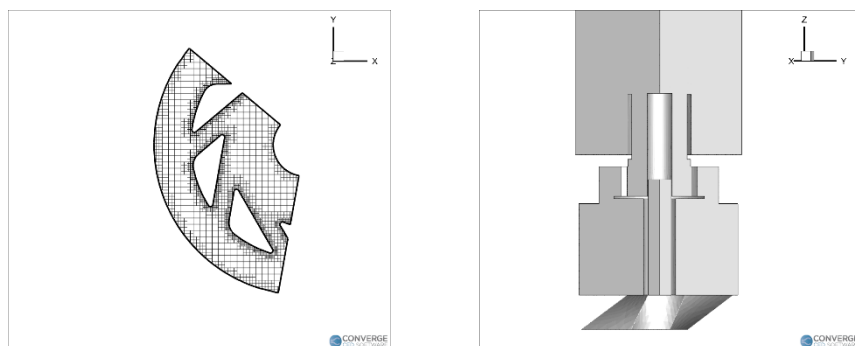


Figure A.27 : Design D026.

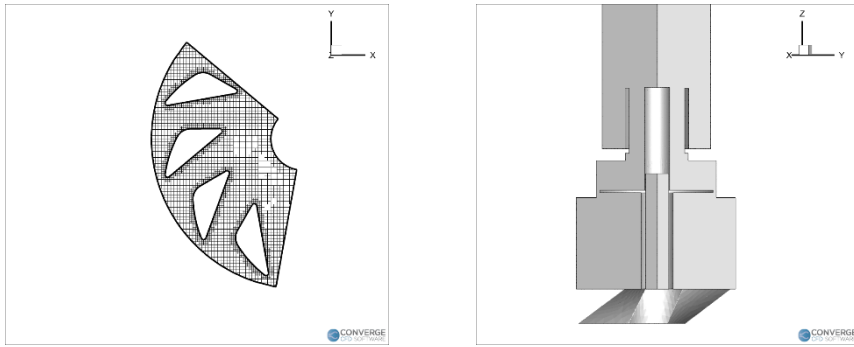


Figure A.28 : Design D027.



CURRICULUM VITAE

Name Surname : Mehmet Anıl Gülşan

EDUCATION :

- **B.Sc.** : 2016, İstanbul Technical University, Mechanical Engineering Faculty, Mechanical Engineering Dep.
- **M.Sc.** : 2018, İstanbul Technical University, Mechanical Engineering Faculty, Heat-Fluid Program

PROFESSIONAL EXPERIENCE AND REWARDS:

- 2016-2018 R&D Project Engineer at Arcelik Co.
- 2018-2023 Senior CFD Engineer at BMC Power Engine & Control Systems Co.
- 2023-On Advanced Lead Engineer at TUSAŞ Engine Industry Co.

PUBLICATIONS, PRESENTATIONS AND PATENTS ON THE THESIS:

- **Gulsan, M. A., & Boke, Y. E.** (2024). CFD Validation of Unconfined Low Swirl Burner Under Cold Flow Conditions. In *Proceedings of INCOS 2024: International Combustion Symposium* (pp. 65–77). Uludağ University, Bursa, Turkey, September 19–21, 2024. ISBN: 978-625-6443-27-3
- **Gulsan, M. A., & Boke, Y. E.** (in press). Numerical Investigation of an Ammonia Hydrogen Swirl Burner. *Journal of Thermal Engineering*

OTHER PUBLICATIONS, PRESENTATIONS AND PATENTS:

- **Gülşan, M. A., Tokgoz, S., & Onbaşıoğlu, S.** (2023). ANALYTICAL STUDY OF HEMISPHERICAL ICE SUBLIMATION IN ENCLOSURES WITH HUMIDITY AND FORCED CONVECTION. *Isı Bilimi Ve Tekniği Dergisi*, 43(2), 207-215. <https://doi.org/10.47480/isibted.1391429>