

# Comparison of Response Surface-Based Preliminary Design Methodologies for a Gas Turbine Combustor

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## ABSTRACT

The preliminary design of gas turbine combustors is a multi-objective optimization problem. The methodology to be used at the preliminary design stage depends on the freedom of design choices available. In this article, we explore three preliminary design methodologies for gas turbine combustor - M1: combustion liner design for a given casing; M2: combustion liner design without the casing and M3: coupled design of combustion liner and casing. A workflow for the automated design space exploration of gas turbine combustors using response surface methodology is presented. Computational fluid dynamics studies along with central composite design for the design of experiments and genetic aggregation for response surface generation are used to quantify the combustor performance in design space. A comparison of three different design methodologies (M1, M2, and M3) is made to show how the choice of design methodology changes the available design space and limits/expands combustor performance. Candidate optimal designs and associated trade-offs from the optimization study are also presented. This study can aid combustor design engineers in choosing the most suitable preliminary design methodology for their specific use case.

**Keywords:** Preliminary design; CFD; Combustor design; Response surface optimization; Blow-off.

## NOMENCLATURE

$S_N$	: Swirl number
$D_{sec}$	: Secondary hole diameter
$D_{dil}$	: Dilution hole diameter
$\dot{m}_{swirl}$	: Mass flow rate through the swirler
$\dot{m}_{sec}$	: Mass flow rate through the secondary holes
$\dot{m}_{dil}$	: Mass flow rate through the dilution holes
$AR$	: Annulus area ratio
$\eta_c$	: Combustion efficiency
$\Delta P$	: Pressure drop
$PF$	: Pattern factor
$Y_{co}$	: CO mass fraction
$Y_{NOx}$	: NOx mass fraction
$D_i$	: Swirler inner diameter
$D_o$	: Swirler outer diameter

## 1. INTRODUCTION

In recent years, requirements to meet tighter emission norms, decarbonization, and sustainable fuel goals have created the need to improve preliminary design methodologies of gas turbine combustors. This involves the use of computational models and tools whose predictive capabilities have improved manifolds in the last few decades. The use of Computational Fluid Dynamics (CFD) in the preliminary design of gas turbine combustors has been explored extensively in the literature and is reviewed here.

Motsamai<sup>1</sup>, *et al.* used CFD design runs with a Dynamic-Q optimization algorithm to improve the exit temperature profile of a combustor. Several studies<sup>2-5</sup> have used Reynolds Averaged Navier Stokes (RANS) based CFD simulations combined with the Design of Experiments (DOE) algorithms to improve combustor performance by varying geometric and operational design variables. Automated CFD design study workflow presented by Briones<sup>6</sup>, *et al.* and Thomas<sup>7</sup>, *et al.* is used for the design space exploration and optimization of a gas turbine combustor. They use DOE algorithms along with adaptive multi-objective optimization algorithms for exploring the design space. Pegemanyfar<sup>8-9</sup>, *et al.* discuss a combustor design tool that uses a combination of empirical design rules, network solvers, and CFD solvers for preliminary combustor design. More recently, machine learning methods have been incorporated into the search for optimal engine designs. Owoyele<sup>10-11</sup>, *et al.* used a machine learning-based design space exploration and optimization strategy to optimize the design parameters of an internal combustion engine. Compared to conventional optimization techniques, optimal designs are obtained with up to 80 % fewer CFD runs with this strategy.

All these design methodologies differ not just in the methods, tools, and algorithms being used but also in the freedom of choosing design variables. The choice of design variables and associated constraints are driven by design requirements and may not be the same for all cases. A systematic comparison that brings out the effect of these choices and constraints is missing from the literature. In this

study, three different preliminary design methodologies for gas turbine combustors are tested and compared:

- M1: Design of combustion liner for a given casing
- M2: Design of combustion liner decoupled from the casing
- M3: Coupled design of combustion liner and casing

The performance parameters considered here for all three design methodologies are: combustion efficiency, pattern factor, total pressure drop, CO mass fraction and NOx mass fraction. The design variables are different for each of the three design methodologies and are shown in Table 1.

**Table 1. Design variables and their range for three different design methodologies**

Design variable	Range
<b>M1: Design of combustion liner for a given casing</b>	
Swirl number	0.6 – 2.0
Secondary hole diameter	5 – 15 [mm]
Dilution hole diameter	5 – 20 [mm]
<b>M2: Design of combustion liner without the casing</b>	
Swirl number	0.6 – 2.0
Secondary hole diameter	5 – 15 [mm]
Dilution hole diameter	5 – 20 [mm]
Primary air mass flow rate	2 – 20 %
Secondary air mass flow rate	2 - 40 %
<b>M3: Coupled design of combustion liner and casing</b>	
Swirl number	0.6 – 2.0
Secondary hole diameter	5 – 15 [mm]
Dilution hole diameter	5 – 20 [mm]
Annulus area ratio	0.5 - 0.9

Here, the annulus area ratio (AR) is defined as the ratio of liner cross-sectional area to casing cross-sectional area. For methodology M1, AR is kept constant at 0.7. The air mass flow rate through the porous walls is assumed to be constant for all cases. Primary and secondary airflow rates for M2 are defined as percentages of the total airflow rate at the combustor inlet i.e. 0.1 kg/s. Thus, the dilution air flow rate is a linearly dependent variable and is not considered as an independent design variable in M2.

The three preliminary design methodologies discussed here come with their own set of advantages and disadvantages. The choice lies with the design team and is dependent on specific design requirements and constraints.

When the design team is looking to modify an existing combustor to meet a different set of requirements, there exist tight constraints on the casing size. This may also be the case when a new component/modification is being tested for the combustor. Methodology M1 allows us to work within these constraints and make informed trade-off decisions to meet the new set of requirements. The assumption of a given casing design puts a constraint on the possible airflow distribution through different zones in the combustor. This shrinks the feasible design space in comparison to the other two methodologies.

When a combustor is being designed from scratch for a gas turbine, there is a lot of freedom in design choices and

sizing. Here, methodology M2 can be useful as it works with the least number of constraints. The freedom of choosing the mass flow distribution allows a lot more control over performance parameters. Modern techniques for directing airflow to different combustor zones may meet the required objective but will certainly be accompanied by trade-offs in pressure losses and sizing. Hence, care must be taken to ensure that these parameters are considered for casing design at a later stage.

Methodology M3 is a middle ground between the methodologies M1 and M2. It assumes some freedom in the design of the casing. This allows the elimination of mass flow rates as design variables and replaces them with sizing of the annulus area between the casing and liner. Thus, the design space expands compared to M1 but is still smaller than M2.

Response surface method combined with an automated CFD workflow is used for design space exploration and optimization of a can-type gas turbine combustor for all three methodologies. Qualitative and quantitative comparisons between the design methodologies show the differences in design space and performance possibilities. This will allow designers to choose a methodology that is best suited to their design requirements.

## 2. METHODOLOGY

Although the geometry, validation, and workflow have been discussed earlier<sup>12-13</sup>, the main ideas are summarized here and changes required for the current study are discussed.

### 2.1 Geometry, Mesh and Workflow

The design study is performed on a typical can-type combustor shown in Fig. 1(a) whose geometry is well described by Bicen<sup>14</sup>, *et al.* It consists of a swirler, secondary and dilution holes, and a conical fuel injector. The combustor liner walls are made of a porous material that allows cooling air to go through. These walls are represented by hemispherical, cylindrical, and nozzle inlet boundaries in Fig. 1(b). As shown in Fig. 1(c), the geometry is simplified by removing the swirler and replacing it with a swirl boundary condition in the CFD solver. The mesh consists of polyhedral cells (~0.95 M) and has been finalized following a mesh independence study. There are 12-15 cells across the diameter of fuel and air inlet holes. The grid in the primary zone and secondary air inlets are refined using a sphere of influence (cell size of ~ 1.5 mm) to capture the swirling flow physics.

As shown in Fig. 2, an automated workflow for design space exploration and optimization of gas turbine combustors based on CFD is developed. The workflow automates the entire workflow which consists of parametric geometry modification, meshing, boundary condition modification, CFD solution, and post-processing of results. The parametric geometry modification is done with Solidworks and then passed to the ANSYS meshing tool for grid generation. Flownex, a 1D flow network solver in conjunction with spreadsheet software modifies the boundary conditions based on the geometry. The mesh and boundary conditions are then passed onto ANSYS Fluent - a CFD solver for calculating the reacting flow solution. The output parameters are then calculated and stored for the

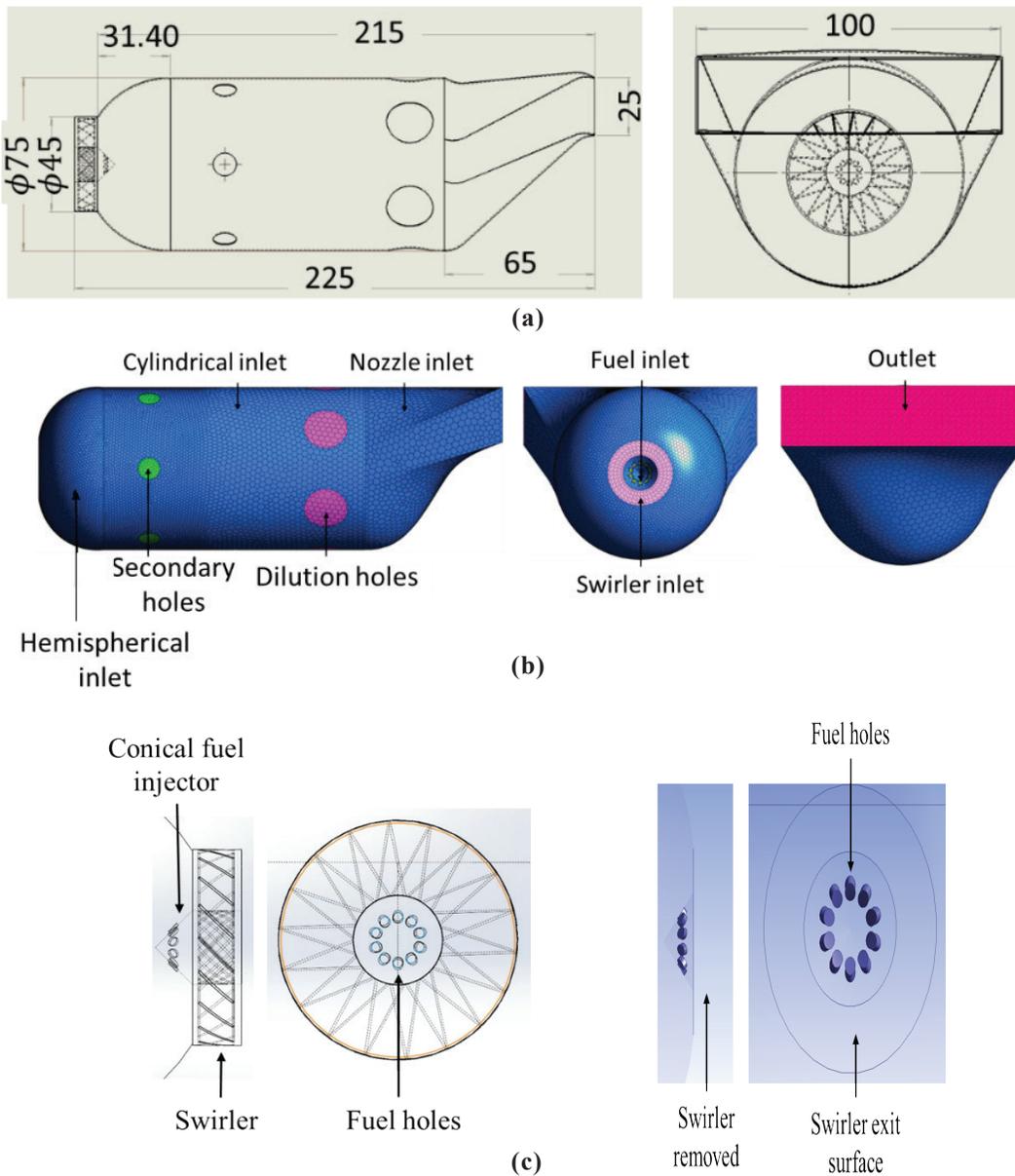


Figure 1. (a) Geometry [all units in mm]; (b) CFD domain for can type gas turbine combustor; and (c) Swirler and fuel hole modification.

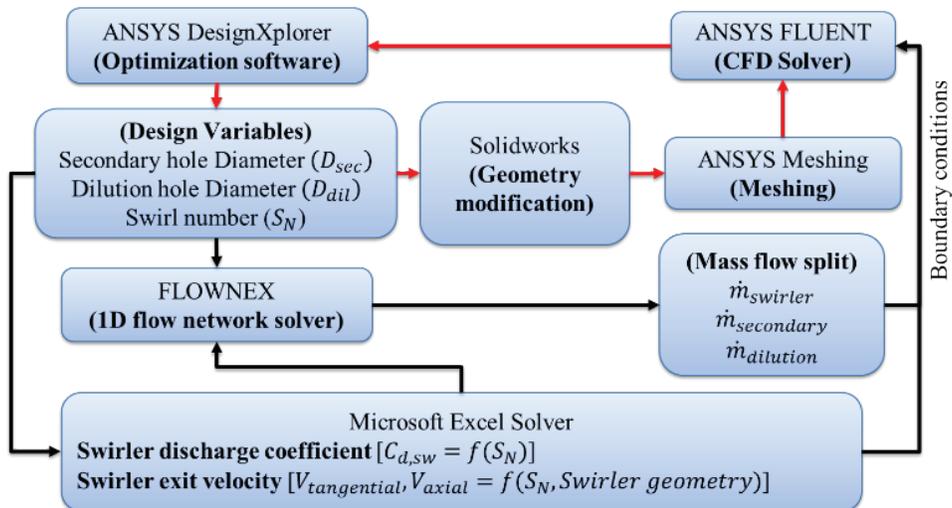


Figure 2. Automated workflow for CFD-based preliminary design of gas turbine combustor.

design point. ANSYS DesignXplorer controls the flow through different solvers for each design iteration.

The calculation of the swirler boundary condition and discharge coefficient based on the swirl number is completed using an Excel solver. Based on the swirler geometry and swirl number,  $\theta$  parameter is calculated as:

$$\theta = \tan^{-1} \left[ \frac{3}{2} S_N \left( \frac{1 - (D_i / D_o)^2}{1 - (D_i / D_o)^3} \right) \right] \quad (1.1)$$

Thereafter,  $\cos\theta$  and  $\sin\theta$  become the tangential and axial components of flow direction, while the radial flow component is 0 at the swirler exit. Combined with the mass flow rate and swirler exit area specification, the swirl boundary condition is now fully defined. The discharge coefficient modification is based on the swirler data available from Ishak et al.<sup>15</sup> since no experimental data is available for the specific swirler used in this geometry.

This workflow was developed for methodology M1 and requires some modifications for M2 and M3. For M3, the annulus area ratio is also used by Flownex for the calculation of boundary conditions. For M2, the Flownex component is completely removed from the workflow, and swirler and secondary air mass flow rates become independent design variables.

## 2.2 CFD Solver Setup

For the CFD solution of reacting flow in the combustor, we use ANSYS Fluent 2020 R2<sup>16</sup>. For turbulence modeling, RANS (Reynolds Averaged Navier Stokes) simulations are carried out using the Shear Stress Transport (SST)  $k-\omega$  turbulence model. The SST  $k-\omega$  model blends the standard  $k-\omega$  formulation in the near wall region with the  $k-\epsilon$  model in the freestream region. Also, in the definition of turbulent viscosity the SST  $k-\omega$  model considers the transport of shear stresses. A partially premixed Flamelet Generated Manifold (FGM) model combined with the Zimont turbulent flame speed model is used to model combustion. The thermochemical states have been parametrized by mixture fraction, un-normalized progress variable, and enthalpy. Steady diffusion flamelets are generated for scalar dissipation rate starting from 0.01/s with increments of 1/s until flame extinction. We use the San Diego Mechanism<sup>17</sup> to generate the diffusion flamelets for modeling the combustion chemistry of gaseous Propane. The laminar flame solutions are then convoluted with the assumed joint probability density function (PDF). These values are then tabulated and stored in a PDF table which is used during CFD calculations. CO predictions are taken from the flamelet PDF results while the NOx calculations are obtained by solving a decoupled transport equation for NOx in ANSYS Fluent that accounts for thermal NOx. We tested a reactor network model as well for predicting pollutants from the reacting flow results and found that this will almost double the computational cost associated with each simulation. Since it is a design optimization study and we are focusing on performance trends rather than accurate performance numbers, we did a trade-off to keep the simulation time for each run feasible enough to run 100s of design iterations.

For the baseline design with  $S_N=1.01$ ,  $D_{sec}=10$  mm and  $D_{dil}=20$ mm, the air mass flow rate is distributed into the swirler

inlet (6.9 %), hemispherical inlet (6.6 %), cylindrical inlet (13.8 %), secondary holes (13.6 %), dilution holes (53.3 %) and nozzle inlet (5.8 %). The total air mass flow rate is 0.1 kg/s coming to the combustor at an inlet temperature of 315 K, same as the fuel inlet temperature. The gaseous fuel Propane is injected through the conical injector at a mass flow rate of 0.0012 kg/s. The primary zone is rich with equivalence ratio,  $\phi=2.0$ , the secondary zone at  $\phi=0.6$  and the dilution zone at  $\phi=0.2$ . The outlet is defined as a pressure outlet boundary condition at standard atmospheric conditions.

Validation is carried out using the numerical models discussed above by comparing the experimental temperature measurements with CFD predictions at different axial locations<sup>13</sup>. The prediction accuracy from the numerical models is found to be adequate for the current design study.

## 2.3 Design of Experiments (DOE) and Response Surface Methodology (RSM)

For all three design methodologies, the design space is assumed to be continuous in the chosen design variables. Sampling points within this design space for CFD runs are chosen based on a central composite design (CCD) algorithm with Variance Inflation factor (VIF)-optimality criteria<sup>18-19</sup>. VIF is a measure of non-orthogonality which is minimized in the current CCD method. It is a 5-level design where the determination of alpha relies on this minimization. Based on the design variables and their range defined earlier, the DOE algorithm generates 15, 27, and 25 sampling points for methodology M1, M2, and M3, respectively.

CFD runs on the DOE design points are carried out. This is followed by the generation of response surface predictions using the genetic aggregation (GA) algorithm. GA algorithm automatically generates the most suitable response surface from a combination of the following response surfaces: full 2<sup>nd</sup>-order polynomial, moving least squares, Kriging, and non-parametric regression. This is based on a genetic algorithm that solves response surfaces in parallel and generates different populations with fitness functions associated with each response surface. This is used to determine the best combination of response surfaces for each output parameter.

The accuracy of response surface predictions is improved by adding 100 additional samples in the design space using Non-Linear Programming by Quadratic Lagrangian (NLPQL)<sup>20</sup> algorithm based on the maximum predicted error in combustion efficiency. This is carried out for all three design methodologies.

## 3. RESULTS AND DISCUSSIONS

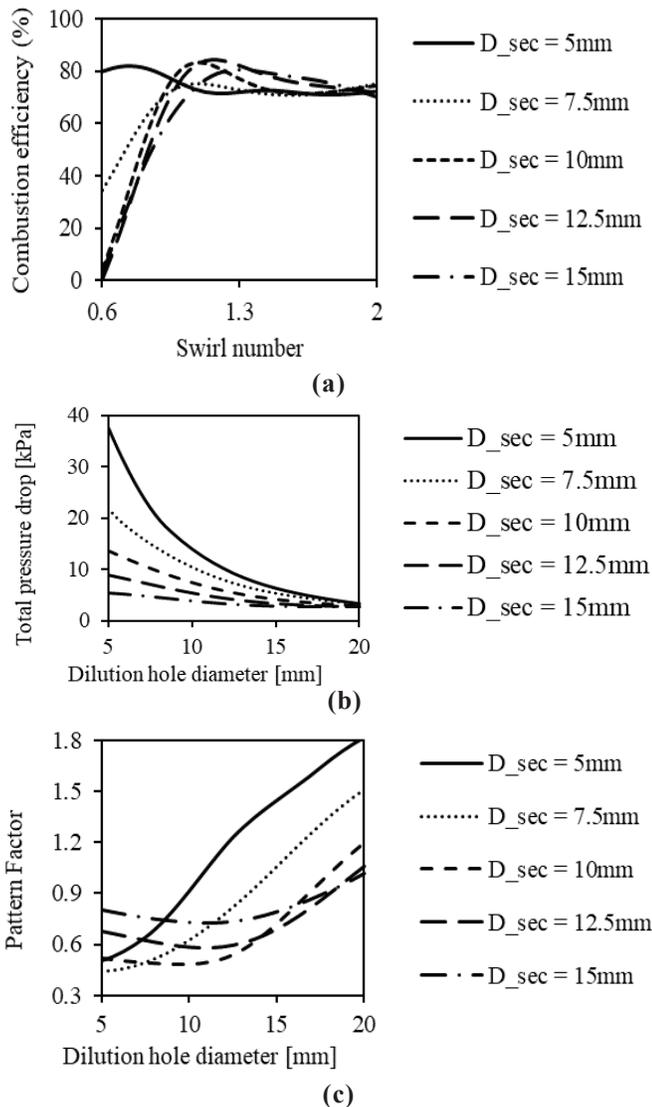
The results obtained with DOE, response surface generation, and optimization for the three design methodologies are presented and compared in this section.

### 3.1 M1: Design of Combustion Liner for a Given Casing

Combustion efficiency results from methodology M1 show that adequate fuel-air mixing for combustion requires moderate swirl strength combined with adequate secondary jet penetration. Figure 3(a) shows the combustion efficiency

response surface predictions obtained with M1. It can be observed that a swirl number of around 0.9 is required to completely cross the blow-off region. A peak in efficiency is achieved for  $S_N$  in between 0.9 -1.3, which then goes down for higher swirl numbers. This decrease in efficiency is a weak correlation and we could not identify any specific physics that stands out to explain this phenomenon. One hypothesis is that the excessive turbulent kinetic energy and associated mixing could be leaning out parts of the primary zone too fast toward the lean flammability limit. This might result in some of the fuel-air mixture escaping unburnt from the primary zone and being too lean to burn later in the combustor as well.

The total pressure drop response in Fig. 3(b) shows the variation with secondary and dilution hole size. Decreasing the hole diameter increases jet penetration in the combustor liner and hence increases the total pressure drop. These curves shift to higher pressure drop values as the swirl number increases. This trend captures the trade-off between fuel-air mixing and total pressure loss.



**Figure 3. Variation of performance parameters with design variables: (a) Combustion efficiency for  $D_{dil}=12.5$  mm (b) Total pressure drop for  $S_N=1.3$  and (c) Pattern Factor for  $S_N=1.3$ .**

Temperature uniformity at the combustor outlet is an important design criterion for gas turbine combustors. Pattern factor (PF), is a measure for this criterion and is defined in terms of maximum and average temperatures at the combustor outlet. Figure 3(c) shows the PF variation with dilution and secondary hole diameter. An increase in dilution hole size decreases the dilution jet penetration which reduces the mixing of combustion products with dilution air. This results in an increase in temperature non-uniformity and hence the pattern factor.

### 3.2 M2: Design of Combustion Liner Without the Casing

Combustor performance is a strong function of fuel-air mixing. The effect of dilution hole diameter on combustion is generally limited by its effect on the airflow distribution to primary and secondary zones. Hence, we can conclude that combustion in primary and secondary zones is controlled by the fuel-air mixing, which in turn is determined by the swirl strength ( $S_N$ ), primary ( $\dot{m}_{swirl}$ ) and secondary ( $\dot{m}_{sec}$ ) air flow rates and secondary jet penetration. Secondary jet penetration is a function of the secondary hole diameter ( $D_{sec}$ ) and secondary air flow rate ( $\dot{m}_{sec}$ ).

Higher air flow rates and smaller jet diameters result in greater jet penetration. When the airflow distribution is a function of annulus sizing (as in M1 and M3), it is observed that smaller secondary holes present a greater resistance in the flow network and hence allow smaller air flow rates. However, this is not necessarily the case with methodology M2. Since casing design is not considered, the airflow rate is independent of the hole sizing. High air flow rates through small holes can be set up to obtain greater jet penetration.

With five different input parameters, the response in the design space becomes difficult to visualize. Hence, we first divide our design space into low, moderate, and high swirl number regions defined for swirl numbers 0.6, 1.3, and 2.0, respectively. For each of these swirl numbers a low, moderate, and high value of secondary and dilution hole diameters are similarly selected. Contour plots of combustion efficiency as shown in Fig. 4 are then plotted with  $\dot{m}_{sec}$  and  $\dot{m}_{swirl}$  for each of these combinations.

With low swirl strength, achieving good combustion efficiency requires the secondary jet to contribute more to the fuel-air mixing. This can be achieved by smaller  $D_{sec}$  or higher  $\dot{m}_{sec}$ . For  $D_{sec}=5$  mm, high combustion efficiency can be achieved with a higher  $D_{dil}$  by keeping  $\dot{m}_{sec}\sim 15\%$  and  $\dot{m}_{swirl}\sim 12\%$ . This high-efficiency region, however, represents a local maximum and any small variation in mass flow rates may result in significantly lower efficiencies. For  $D_{sec}=10$ mm, prominent blow-off regions can be observed for moderate and high  $D_{dil}$ . However, high combustion efficiencies can be achieved by controlling the secondary and primary air flow rates carefully. For  $D_{sec}=15$ mm, the jet diameter is too big to achieve the required fuel air mixing and thus, the designs are limited to lower combustion efficiencies.

Moderate swirl strength maximizes the design space for high combustion efficiencies. With enough swirl strength, secondary jet diameter strength is no longer essential for high

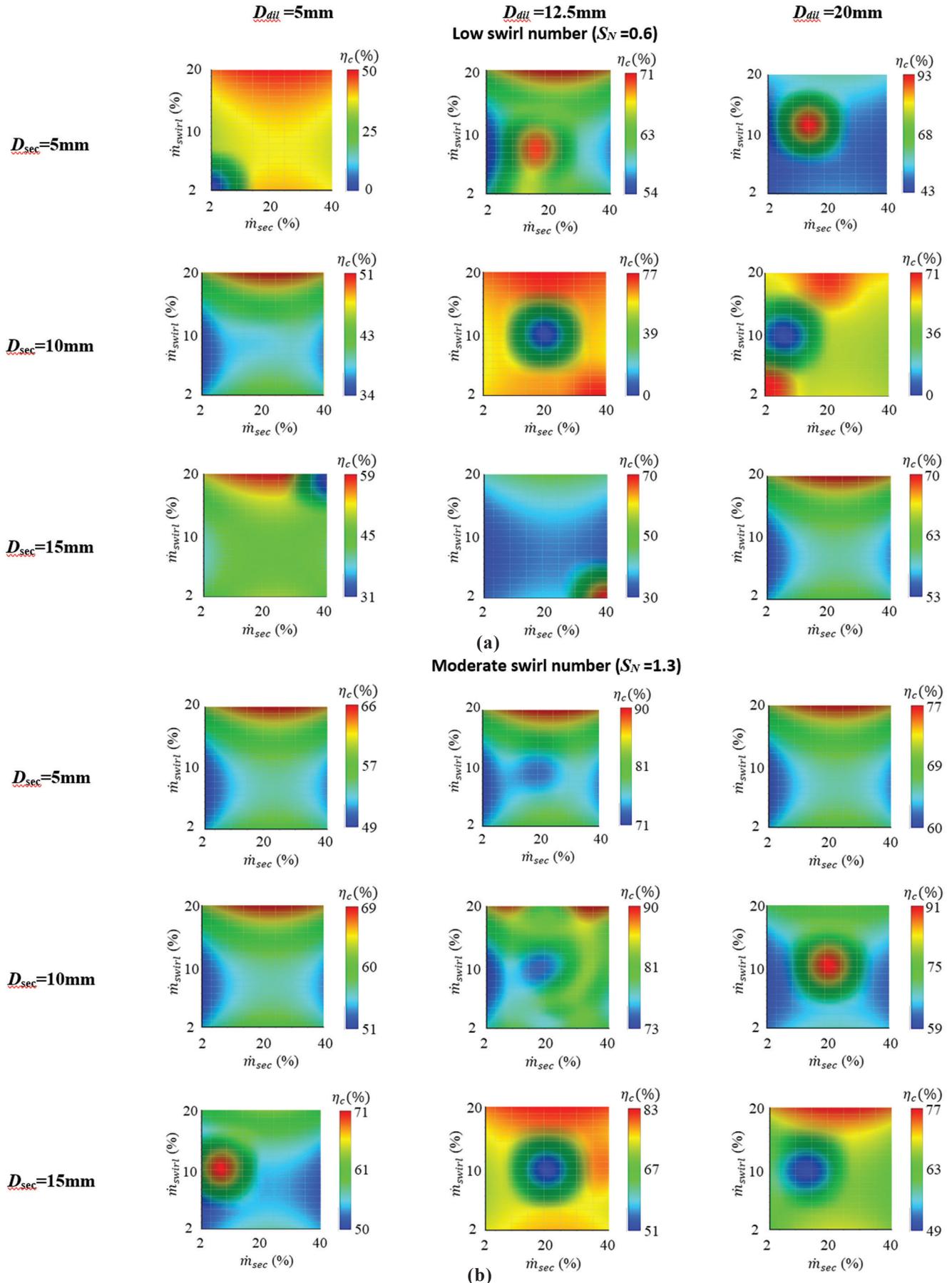


Figure 4. Variation of combustion efficiency in the design space with methodology M2 for (a) Low (b) Moderate and (c) High swirl numbers.

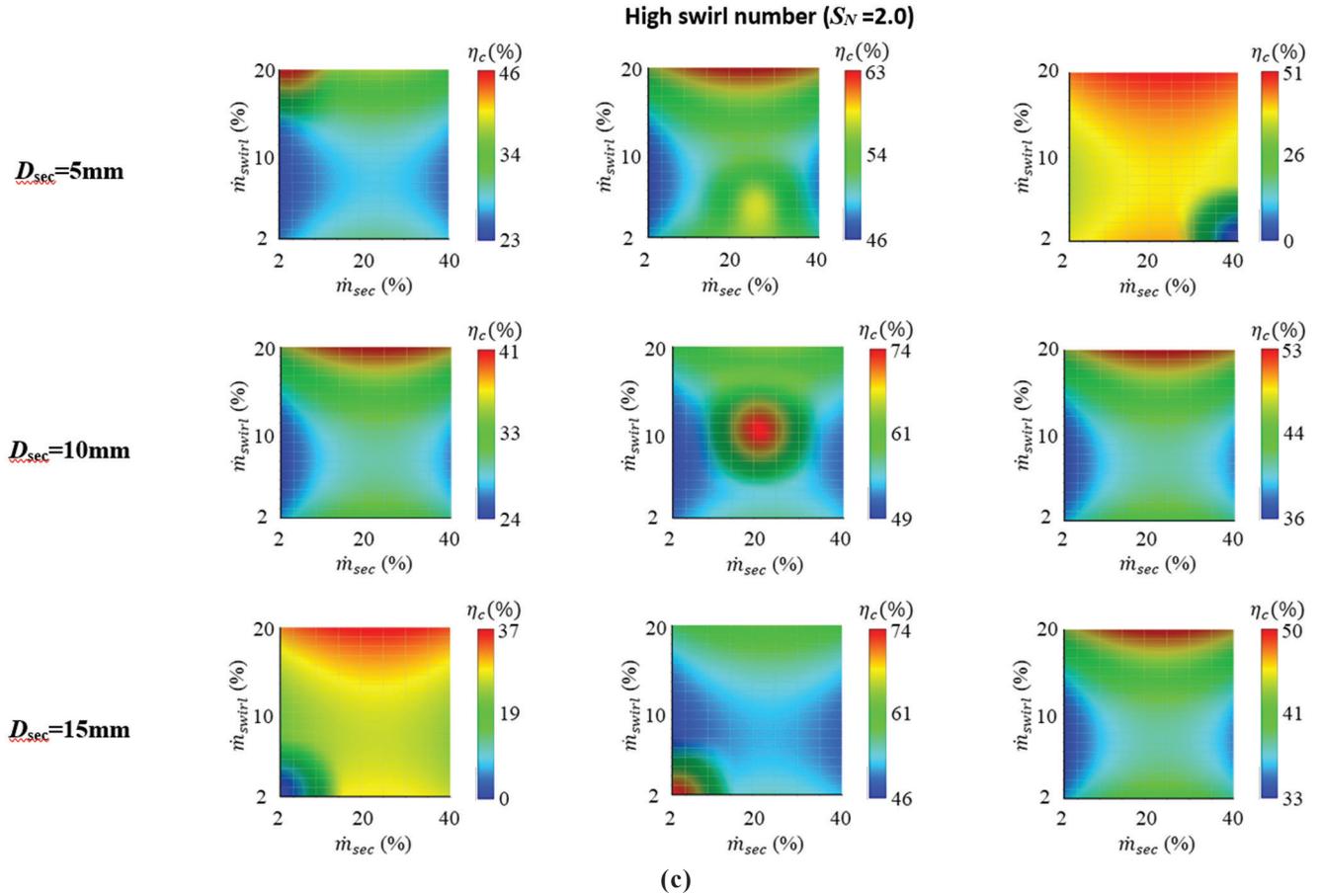


Figure 4. Variation of combustion efficiency in the design space with methodology M2 for (a) Low (b) Moderate and (c) High swirl numbers.

combustion efficiency. The highest efficiencies are observed for  $D_{sec}=10\text{mm}$ ;  $D_{dil}=20\text{mm}$ ;  $\dot{m}_{sec}\sim 21\%$ ;  $\dot{m}_{swirl}\sim 12\%$ . The blow-off region is absent in the moderate swirl design space. As observed from the design study with methodology M1, swirl numbers beyond a certain limit bring down the combustion efficiency. This is also seen very clearly with methodology M2, where for high swirl numbers, high combustion efficiency is limited only to moderate dilution hole diameter – with  $D_{sec}=10\text{mm}$ ;  $D_{dil}=20\text{mm}$ ;  $\dot{m}_{sec}\sim 22\%$ ;  $\dot{m}_{swirl}\sim 12\%$ .

One common observation for all three swirl regions is that smaller dilution hole diameter designs consistently gave a low combustion efficiency. As shown in Fig. 5(a), this can be attributed to the recirculation regions being formed in the secondary zone due to the strong dilution jet. This disturbs the air-fuel distribution in the secondary zone and limits combustion to the primary zone as shown in Fig. 5(b). Hence, a larger dilution hole diameter is essential to allow secondary combustion.

### 3.3 M3: Coupled Design of Combustion Liner and Casing

The only difference between methodology M1 and M3 is the addition of an annulus area between the liner and casing as a design variable in M3. This expands the design space by allowing more freedom in the mass flow distribution to different zones. To demonstrate how M3 differs from M1, we first focus on the effect of the annulus area on air flow through secondary

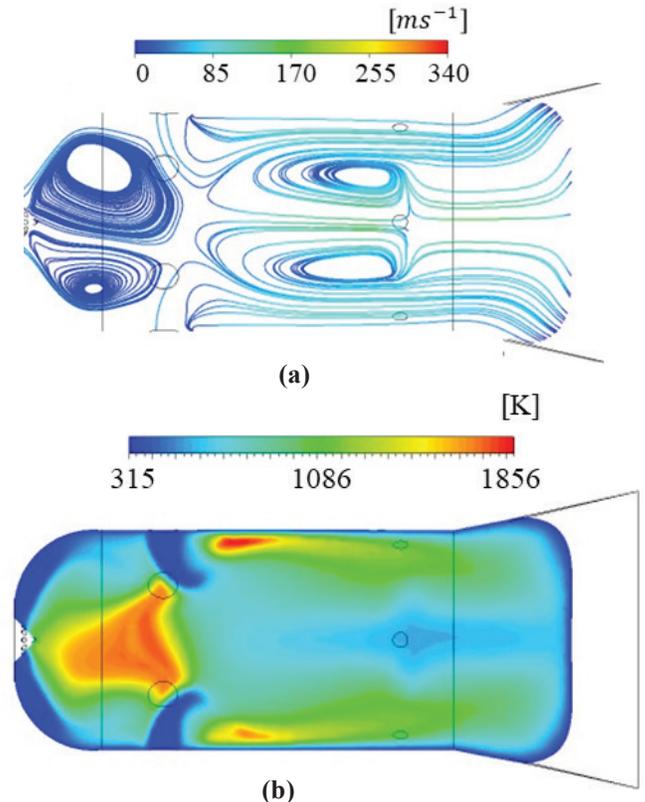
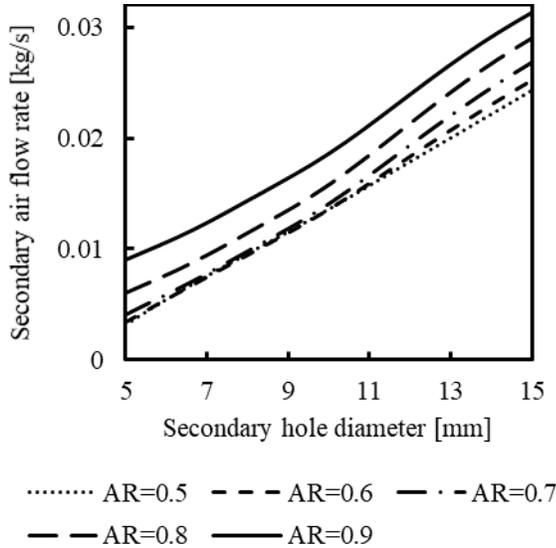


Figure 5. (a) Streamline and (b) temperature contour plot for a design point with  $D_{dil}=5\text{mm}$ .

holes. The entire combustor and casing arrangement can be seen as a resistance flow network. The airflow distribution to different zones of the combustor is decided by the resistances in this flow network. The annulus area is an important design parameter that can change the flow resistance and hence control airflow distribution. For methodology M1, we considered a casing with a constant annulus area ratio of 0.7. However, for M3 the annulus area ratio is chosen as a design variable varying between 0.5-0.9. This results in higher variation in air flow distribution. As observed from Fig. 6, the variation of  $\dot{m}_{sec}$  for M3 (AR = 0.5-0.9) allows a wider range of airflow rates as compared to M1 (AR=0.7).



**Figure 6. Variation of secondary air flow rate [kg/s] with secondary hole diameter for varying annulus area ratios.**

### 3.4 Pollutant Formation (CO and NOX)

CO and NOx emissions are the most important design criteria for gas turbine combustors. CO formation is a result of incomplete combustion. CO does not form in the blow-off region as there is no combustion. In the high-efficiency regions as well, CO goes down to negligible levels because of a complete CO burnout. In between these two regions, we see high CO emissions. This trend is similar for all three design methodologies considered.

For NOx predictions, the current study models only the thermal NOx, since it forms the major part of NOx emissions. The formation of thermal NOx is significant above  $\sim 1700$  K and thus it follows that designs with higher combustion efficiency will have local high-temperature regions which allow the formation of thermal NOx. The trend for all three design methodologies shows that NOx formation sees a sudden jump as the combustion efficiencies become greater than  $\sim 40$  %.

### 3.5 Multi-Objective Optimization

Once the response surface in the design space is generated, optimization can be carried out. Since this is a multi-objective design problem, we use a multi-objective genetic algorithm – a variant of a non-dominated sorting genetic algorithm (NSGA) – to search for optimal candidates in the feasible design space.

Pareto fronts representing the trade-offs between multiple objectives are generated and candidate designs can be chosen based on the design requirements. The objectives and their specifications are listed in Table 2. The priority and constraints are subjective and can be modified based on specific design requirements.

**Table 2. Optimization objectives and constraints**

Objective	Priority	Type	Constraints
Combustion efficiency	High	Maximize	>70%
Total pressure drop	High	Minimize	<3000 Pa
CO mass fraction	Normal	Minimize	< 20 E-6
NOx mass fraction	Normal	Minimize	<1.3 E-6
Pattern factor	Normal	Minimize	<1

Optimal candidate points obtained from each of the three design methodologies and their performance are shown in Table 3. We see that each methodology gives candidate optimal designs that show improvements in different performance parameters and the choice of the final design is based on application-specific design requirements.

**Table 3. Optimal candidate design points and their performance**

	Design variables		
	M1	M2	M3
$S_N$	1.00	1.10	1.87
$D_{sec}$ [mm]	12.24	11.02	14.09
$D_{dil}$ [mm]	15.26	15.69	16.83
$\dot{m}_{swirl}$ [kg/s]	-	0.0084	-
$\dot{m}_{sec}$ [kg/s]	-	0.0276	-
AR	-	-	0.59
Performance parameters			
$\eta_c$ (%)	89.43	85.39	84.43
$\Delta P_L$ [kPa]	2.92	2.01	2.86
CO [1e-6]	5.75	3.73	0.39
NOx [1e-6]	0.75	0.64	0.99
PF	0.67	0.90	0.8

## 4. CONCLUSIONS

This study presents an automated workflow for the preliminary design study and optimization of a gas turbine combustor. Three different design methodologies-M1: Design of combustion liner for a given casing; M2: Design of combustion liner decoupled from the casing and M3: Coupled design of combustion liner and casing - are discussed with implementation details.

We observe that the M2 methodology with five design variables provides the largest design space and freedom in preliminary design. We show that between M1 and M3, the variation of the annulus area ratio in M3 allows the expansion of design space in terms of airflow distribution. The pollutant formation in all three design methodologies shows similar trends where CO peaks for moderate combustion efficiencies and thermal NOx formation sees a sudden increase for combustion efficiencies greater than 40 %. Multi-objective optimization for the three design methodologies is carried

out. Candidate optimal design points from different design methodologies show improvements in different performance parameters.

The current work presents an overview of the implementation details and trade-offs associated with each of the three preliminary design methodologies for gas turbine combustors and can help in choosing the methodology to be adopted while designing a combustor.

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## ACKNOWLEDGEMENTS

We are thankful for the computational resources provided by the National Centre for Combustion Research and Development, IIT Madras.

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