

A COUPLED FLOW AND CHEMICAL REACTOR NETWORK MODEL FOR PREDICTING GAS TURBINE COMBUSTOR PERFORMANCE

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Gas turbine combustor performance was explored by utilizing a one-dimensional flow network model. To obtain the preliminary performance of combustion chamber, 3 different flow network solvers were coupled with a chemical reactor network scheme. These flow solvers were developed via simplified, segregated and direct solutions of the nodal equations. Flow models were utilized to predict the flow field, pressure, density and temperature distribution inside the chamber network. The network model followed a segregated flow and chemical network scheme, and could supply information about the pressure drop, nodal pressure, average temperature, species distribution and flow split. For the verification of the model's results, analyses were performed using computational fluid dynamics on a seven-stage annular test combustor from TUSAS Engine Industries, and the results were then compared with actual performance tests of the combustor. The results showed that the preliminary performance predictor code accurately estimated the flow distribution. Pressure distribution was also consistent with the computational fluid dynamics results, but with varying levels of conformity. The same was true for the average temperature predictions of the inner combustor at the dilution and exit zones; however, the reactor network predicted higher elemental temperatures at the entry zones.

Key words: flow network, chemical reactor network, turbulent combustion, combustor performance, combustor preliminary design, computational fluid dynamics.

1. Introduction

The design of a gas turbine combustor requires detailed planning as well as rig testing in the verification phases. In the preliminary design phase, analytical and semi-empirical models are used to produce a fast solution in the form of a reduced dimensional model of a combustion chamber. However, preliminary design tools are usually limited by semi-empirical design requirements [1-3]. In this phase, some of the important performance parameters include pressure drop, average exit temperature, flow split through liner holes and the Mach number along the gas path. In the detailed design step, complex Computational Fluid Dynamics (CFD) modelling of the combustor flow is performed utilising iterative computational cycles. In order to shorten the design cycle for combustors, preliminary tools are used in order to shape the design through a process of best estimation. A study of the literature [3-6] shows that there are many different preliminary design methods available. In this study, we developed a simplified performance prediction tool in which flow

network solver methods are coupled with a chemical reactor network and compared with a detailed three dimensional analysis of a prototype combustor.

2. Flow network solvers

Modelling the flow inside gas turbine combustors can be simplified by utilizing a 1-D pipe flow approach commonly known as the network flow approach. Pipe flow network solvers have a significant history and they have been refined a number of times in recent years. Flow network solvers are commonly categorized as loop, element and node solvers [4]. The loop method was the first network method, and was presented by Hardy Cross in 1936 [5-6]. This method groups the several branches inside the flow loops and solves a general mass flow conservation equation. The method was especially suitable in cases where computational resources were limited; however, it came with several disadvantages, such as the defining of the loop structure for complicated cases and the conservation of the initial flow distribution during initialization phase [5]. The element method, although reported to be better converged [7], defines the loop structures separately and so requires more computational resources. Node methods, in contrast, have a couple of important advantages. They require fewer computational resources and can be adapted to different boundary conditions [4]. System initiation can also be performed without initial conserved flow values and the loops. Nodal equations can also be solved directly or through simplifications. The former approach results in the solution of a large system matrix composed of linear node flow equations and non-linear head loss equations. The solution of the non-linear system both satisfies the head loss and continuity equations. This method was described in the works of Costa et al. [8]. The simplified solution of the nodal equations is based on the Linear Theory Method (LTM). The non-linear equations in the direct solution of the flow network system are linearised according to the LTM and a simplified nodal set of equations are solved by basic matrix algebra [9-11]. Extensive works on nodal methods are available in the literature [12-14]. The direct solution of the nodal approach is widely used in gas pipelines, discussions on which can be found in various sources [15-16].

The size of the flow network depends on the complexity of the geometry. The reduced dimensional approach only considers a section of the flow domain. In Stutttaford [6], the size of the flow domain is around 70 elements, whereas in a similar study [13], the size of the network is 17. The full network model used in this study included 31 elements and the improved version that focused on the cooling aspects included 41 elements [17].

2.1. Reactor networks

Chemical Reactor Networks (CRN) can be used in predicting the preliminary performance of gas turbines. Computational reactors replicate small reactors that have inlet and outlet ports. The reactors can be connected in series to simulate successive hole rows and mass flow injections. They can also be connected in a parallel configuration to simulate recirculation regions. The different uses of CRN models are widely described in the work of Murthy [18]. In his study, he developed a semi-empirical 1-D flow and thermal model to predict the equilibrium composition inside a combustor. The flow information from CFD analysis can be combined with CRN models with an equivalent processing approach [19], which is a fast method to obtain chemical species concentrations and temperature in the complex domain. Equivalent reactor modelling from CFD was also utilized to predict a target species inside a combustor [20-21]. Chen et al [22], utilized CRN to design and

optimize a gas turbine combustor. The target temperature and concentration of critical species were examined by changing the flow distribution among the holes. A combination of perfectly stirred reactors, plug flow reactors and mixers were utilized to model the reactor network. A CRN application on lean-premixed burners and two phase combustion inside wood dust burners was performed by Novosselov [23]. Other efforts utilizing CRN networks can be found in the literature [24-27]. Gas turbine combustors are also widely investigated by numerical methods; similar combustor modelling efforts are also available in the literature [28-29].

3. Theory

3.1. Flow equations

The flow network fundamental equations for a single-phase compressible flow are given in Eqs. (1) - (3) for the two sections shown in Fig. 1, Liu [5].

$$\text{continuity: } \rho_1 V_1 A_1 = \rho_2 V_2 A_2 = \text{const.} \quad (1)$$

$$\text{energy: } \frac{V_1^2}{2} + \frac{P_1}{\rho_1} + gz_1 = \frac{V_2^2}{2} + \frac{P_2}{\rho_2} + gz_2 + hf \quad (2)$$

$$\text{momentum: } F = \rho_2 V_2^2 A_2 - \rho_1 V_1^2 A_1 \quad (3)$$

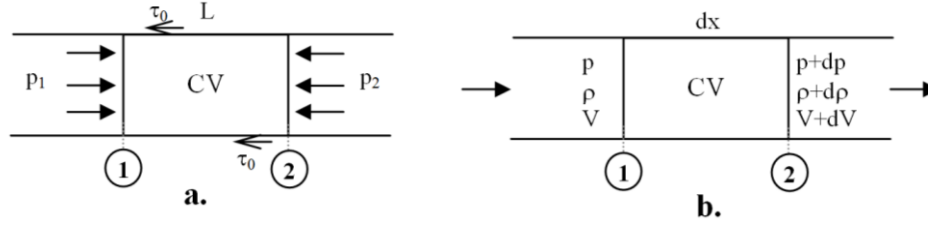


Fig. 1 A pipe element

The simplified version of the pressure drop equation can be rewritten for a pipe section, Liu [5].

$$\frac{dP}{\rho V^2} + \frac{fdx}{2D} = 0 \quad (4)$$

$$P_1 - P_2 = \frac{fL}{D} \frac{\rho V^2}{2} \quad (5)$$

3.2. Reactor theory

In this work, a 0-D perfectly stirred reactor (PSR) model [30] was used. The state variables were the mass inside the reactor, the reactor volume, the total internal energy of the mixture and its mass fraction. The governing mass conservation, species conservation and energy conservation equations are given in Eqs. (6) - (8).

$$\frac{dm}{dt} = \sum_{in} \dot{m}_{in} - \sum_{out} \dot{m}_{out} \quad (6)$$

$$\frac{d(mY_k)}{dt} = \sum_{in} \dot{m}_{in} Y_{k,in} - \sum_{out} \dot{m}_{out} Y_k + \dot{m}_{k,gen} \quad (7)$$

$$\frac{d(U)}{dt} = -P \frac{dV}{dt} - \dot{Q} + \sum_{in} \dot{m}_{in} h_{in} - h \sum_{out} \dot{m}_{out} \quad (8)$$

4. Numerical methods

The computational flow network mapping approach used in this study is based on the method described by Greyvenstein et al. [4]. A network schematic for a sample system is given in Fig. 2. The nodes are the element junctions and they are mainly used for storing pressure data. The elements represent the “virtual pipe” itself by holding the diameter, length, friction factor, temperature, density, flow rate and any other section related data. The flow passes through elements 1-2 and 1-3-4. Both of these paths are active. To obtain a solution to the network system, at least two boundary conditions are necessary.

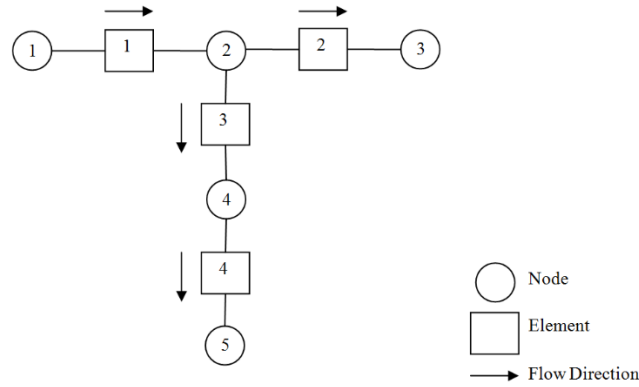


Fig. 2 A sample flow network

4.1. Linear method

The linear method is based on the pressure loss equation, given in Eq. (9).

$$Q_{ij} = \sqrt{\frac{P_{ni-1} - P_i}{\left(\frac{f_{ij} l_{ij}}{d_{ij}}\right) (\rho_{ij} \kappa_{ij})}} \quad (9)$$

The equation can be written around the nodes in the system, n_i . Grouping the constant terms allows the equation to be expressed in a more general form, as in Eq. (10). The linear set of equations can be easily solved by matrix methods.

$$(P_{ni-1} - P_i)C_{ij} - (P_i - P_{ni+1})C_{ij+1} = 0 \quad (10)$$

4.2. Segregated method

This method is based on the continuity and pressure drop equations given in Eqs. (11) – (12). However, it is based on the SIMPLE algorithm of Patankar and Spalding. It includes an iterative corrective scheme and modifies the solution on every iteration. The corrections are applied to pressure, flow rate and density, as given in Eq. (13).

$$\sum_{j=1}^J \rho_{ij} Q_{ij} s_{ij} = -d_i \quad (11)$$

$$\Delta P_{ij} = P_{nij} - P_i = s_{ij} H_{ij} g_{ij} f_{ij} \quad (12)$$

$$P = P^* + P', \quad Q = Q^* + Q', \quad \rho = \rho^* + \rho' \quad (13)$$

4.3. Non-linear method

The non-linear method is based on the pressure loss given in Eq. (14). Rearranging this equation yields Eq. (15). It should be noted that the mass flow conservation is written for the nodes of the system as described in Eq. (16).

$$P_i^2 - P_{ni+1}^2 = \rho_{ij} P_{ij} V_{ij}^2 \left[2 \ln \frac{V_{ni+1}}{V_i} + \frac{f_{ij} L_{ij}}{d_{ij}} \right] \quad (14)$$

$$F_i(P_i, P_{ni+1}) = P_i^2 - P_{ni+1}^2 - C_{ij} Q_{ij}^2 \quad (15)$$

$$F_i(Q_{ij}, Q_{ij+1}, d) = d + \rho_{ij} Q_{ij} - \rho_{ij+1} Q_{ij+1} \quad (16)$$

The set of nonlinear equations are grouped in each branch. The overall system can be solved by the Newton-Raphson method, which is quite effective and, with today's computational resources, able to present a solution for moderate sized networks in an insignificant amount of time.

5. The current model

5.1. Network model

A network model was generated for the TUSAS Engine Industries (TEI) experimental combustor, the schematics of which can be seen in Fig. 3. The TEI combustor is a through-flow type combustor. It has a pressure swirler structure at the liner front, which contains primary and secondary swirler holes. There are hole groups on the combustor liner, including primary, secondary, dilution-1

and dilution-2 hole groups. The holes in the swirler structure and the liner are assigned to hole elements in the network model.

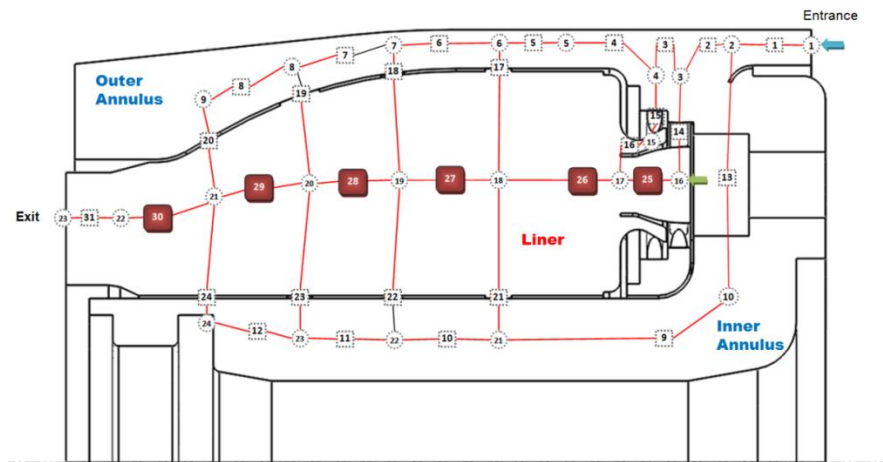


Fig. 3 Network map of the combustor

Elements also represent other flow regions in the model. These regions are the annulus and liner sections. The incoming air from element-1 moves towards the annulus elements of the combustor, passes into the liner holes and leaves the combustor by passing through the liner elements. The liner elements, assigned the numbers 25-30 and shown with a red background, are also registered as chemical reactors. The flow network system produces data for flow field variables. The inner liner reactor elements, part of the same system, get flow information from the flow network and generate chemical reactor outputs. Fuel is injected from the 16th node to the 25th element, which is the first element of the reactor network. Successive liner elements are fed from the previous reactor and hole flow elements. The solution sequence is shown in Fig. 4. The solution starts with the initiation of the model with the initial flow estimates. It is then followed by the calculation of the constant loss terms. As the solution progresses, the distribution of the flow field, pressure and density throughout the domain are obtained. By recalculating the constant loss terms, the second main loop is initiated. Following convergence, the final solution loop starts, in which reactors are activated. In this process, the reactors supply temperature, density and species concentration data at the corresponding elements. Following the completion of the CRN calculations, the temperature and density values are assigned to the related elements and the recalculation phase begins. By the end of the third main loop, the final solution is obtained. A similar 1-D solution approach is also utilized in the study of Al-Agha [31].

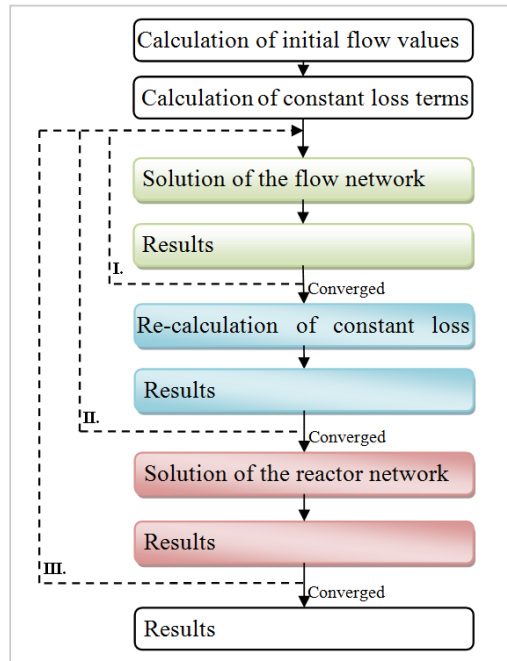


Fig. 4 Solution procedure for the network system

5.2. The loss models

The 1-D flow modelling approach requires the utilization of loss flow correlations and loss factors. An approximation can be used for the 2-D section shown in Fig. (3) because modelling all the loss elements inside the three dimensional domain is not feasible. An important loss element is the liner hole element loss factor [1], a modified orifice equation for liner holes. Sudden expansion and contraction elements also exist in the annulus flow region [32]. Other loss elements in the modelling are: (i) the gradual expansion for the expanding regions of the annulus (ii) the gradual contraction for the contracting regions of the liner internal elements and (iii) the 90 degree round section turn for the turning section of the annulus to the inner liner-connecting element.

5.3. The fuel surrogate models

Different fuels can be utilized in gas turbine engines. The well-known fuels are Jet A-1, standard commercial jet fuel, and JP-8, US military jet fuel. These two fuels are similar, but JP-8 includes 3 different additives. Colket et al. published an extensive report on different jet fuel samples, including the content of these samples [33]. With regard to the modelling of jet fuel combustion, different fuel surrogates were presented by Oldani [34]. In this study, a JP-8 fuel surrogate was selected for combustion modelling. The content of the selected fuel is a blend of 80 % n-Decane and 20 % 1, 2, 4-trimethylbenzene, which is known as the Aachen blend [34]. Detailed chemical mechanisms are used to model the fuel combustion. These mechanisms are utilized to calculate the combustion products and the temperature inside the combustors. In this study, 2 different detailed chemical mechanisms were utilized. The first one is the Aachen University mechanism, which includes 118 species and 527 reactions [35]. The second one is the Creck mechanism of Politecnico di Milano for Kerosene combustion, which has 121 species and 2673 reactions [36-37].

5.4. CFD analysis

Additional CFD analyses were carried out to compare internal characteristics of the combustor. In the CFD analysis, we only modelled a single sector out of the seven identical combustor sectors. Each sector has a dedicated, separate swirler unit. The section showing the combustor simulation model with the boundary locations is given in Fig. 5. The flow domain was analysed at different mesh densities before the mesh independency analysis was carried out. A total number of 19 M tetrahedral elements were used for the purpose of modelling. ANSYS Fluent was utilized to perform the simulations. A RANS model with a $k-\epsilon$ model was selected using the standard wall functions. The mesh was created to guarantee a y^+ value of 60 for the wall regions. For the modelling of the combustion, a non-premixed modelling approach was selected, meaning the fuel and oxidizer mix after entering the domain. A mixture-fraction-based approach was utilized in order to bypass the solution of the complex mechanism during the domain solution. This was achieved via a preliminary chemistry calculation stage.

The complex chemistry was solved by using the flamelet approach. It was at this stage that a flamelet library was generated, which was later incorporated into the CFD solution. The flamelet model included the assumption that a small flame structure inside the combustor domain reflects the character of an equivalent flamelet. The flamelet library provided information about the temperature and species distribution inside the domain. They were given as a function of the mixture fraction and scalar dissipation [39-40]. A flamelet library was generated for each of the chemical mechanisms used in this study. CFD averages are taken from the longitudinal cut section passing through the swirler center. Average values are taken by using multiple post-processing points. The analyses were completed in a 12 core workstation, each steady case with different chemistry took around 24 hours to converge. The solution residuals of temperature, velocity components and pressure went down to 1×10^{-4} . The residuals for the turbulence terms could only converge to 1×10^{-3} , due to flow complexity around the swirler.

6. Results and discussions

The 1-D network analyses were conducted for the TEI test combustor. The results were compared with a 3D CFD analysis and also with the available performance tests. The TEI experimental combustor is a through-flow type combustor, formed of seven sectors [38]. The test conditions of the combustor are given in Table 1. The experimental performance tests provided data for the inlet-outlet properties, such as inlet temperature, inlet total pressure, exit temperature, exit pressure and exit species concentrations. The internal characteristics of the combustor such as hole flow distribution, internal temperature and internal pressure were predicted by 3D CFD analysis.

The results of the 1-D study are presented for the three different network flow solvers that have the same CRN structure. The two chemical mechanisms mentioned were also utilized in the reactor networks. Therefore, a classification was also made based on the chemical mechanisms used. The pressure distribution inside the combustor was given for two regions of the combustor, and the average total pressure distribution is presented in Fig. 6 and Fig. 7. The LTM and segregated models predicted a lower pressure distribution in the outer annulus compared to the CFD results. However, the non-linear model predicted a higher distribution. The pressure values were higher than the CFD predictions

for all three models in the inner annulus nodes. As presented in Fig. 8, the total pressure distribution inside the liner was better predicted by all of the models.

Table 1 Combustion chamber test boundary conditions

Test Boundary Conditions	
Air mass flow rate (kg/s)	0.18
Combustor inlet temperature (K)	478
Combustor exit pressure	Open to atm.
Air/Fuel Ratio	49
Equivalence Ratio	3.27
Combustor Design Power	161 kW

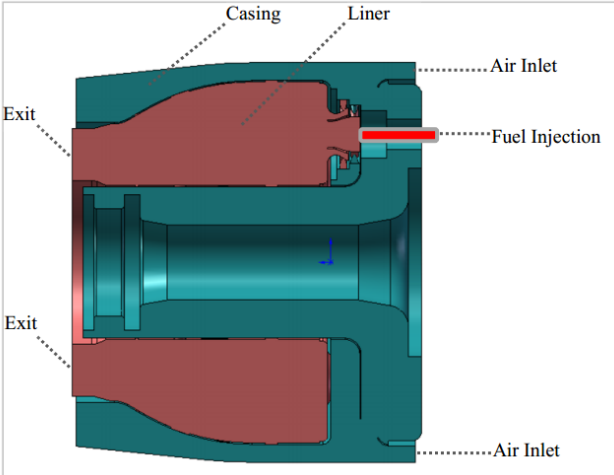


Fig. 5 The section of the combustor model

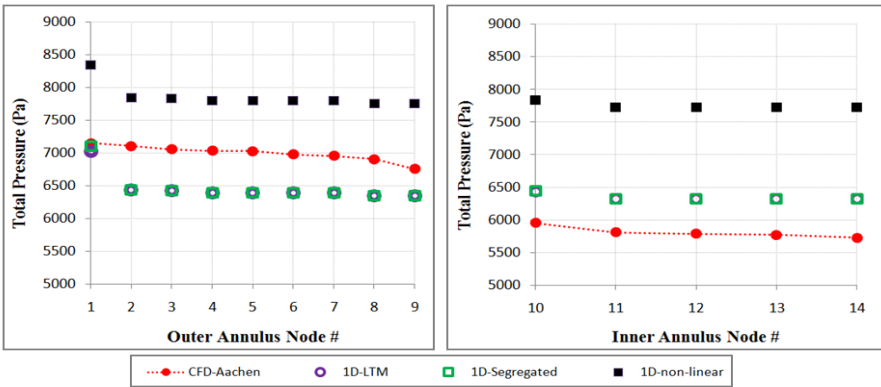


Fig. 6 Total pressure distribution at outer and inner annulus nodes - Aachen mechanism

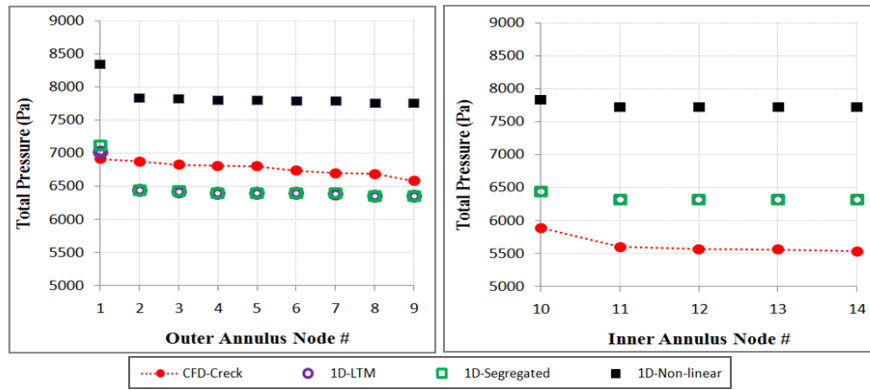


Fig. 7 Total pressure distribution at outer and inner annulus nodes - Creck mechanism

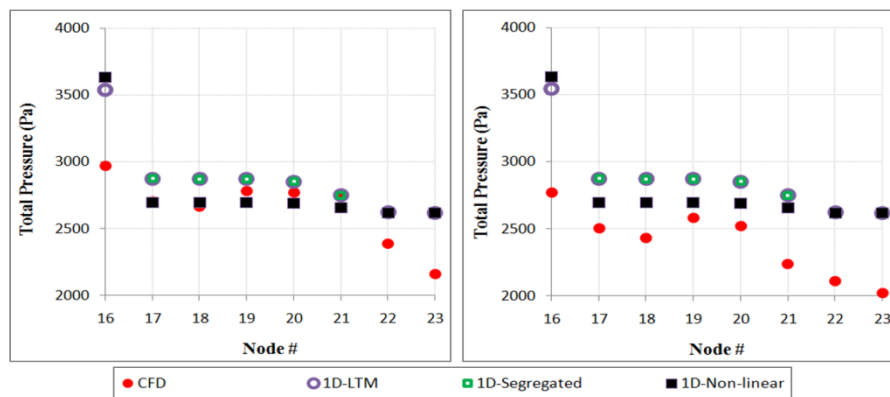


Fig. 8 Total pressure distribution - liner inner nodes - Aachen (left) and Creck (right) mechanism

Nodal temperature values are given for the inner liner elements of the combustor, which are the outputs of the reactor elements. According to Fig. 9, the temperature values are quite large at the primary and secondary zones compared to the CFD results; however, they get closer to the CFD predictions near the exit of the combustor.

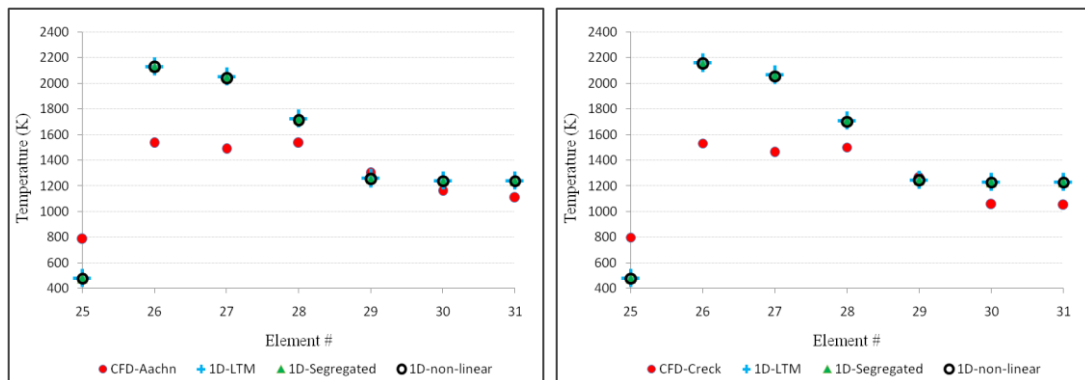


Fig. 9 Temperature distribution - liner elements - Aachen (left) -Creck (right) mechanism

The overall performance parameters of the combustor are presented in Table 2. The overall pressure drop values for the combustor varies with respect to the measured data. The 1-D predictions are in general lower than the experimental data, with the difference being around 20 %. The level of percentage deviation is within 10 % when compared to the CFD predictions. The non-linear model

predicts a higher overall pressure drop, which is very close to the real characteristics. Another important outcome of the code is the average exit temperatures. Average exit temperature data, given in Table 2, shows that the 1-D models generally predict a higher exit temperature compared to the real characteristics. This is due to the idealisation of the combustion CRN networks. On the other hand, the CFD findings are slightly lower than the real value, since these consider the mixing and the flow phenomena in much greater detail. The mass flow distribution percentage through the holes of the combustor is presented in Table 3 and Fig. 10. These are based purely on the Aachen mechanism since the chemical mechanism used in the analysis barely affects the mass flow distribution. The mass percentages passing through the combustor liner holes are similar among the network models. However, they deviate from the CFD findings depending on the positions and types of the holes. Nevertheless, the general distribution character of the combustor is still predicted well, given such a reduced dimensional approach.

Table 2 Combustor overall performance parameters

		COMBUSTOR PERFORMANCE PARAMETERS	
		Total Pressure Loss (Pa)	Average Exit Temperature (K)
Aachen Mechanism	Non-linear	5730	1239
	Segregated	4484	1238
	LTM	4406	1238
	CFD	4989	1109
Creack Mechanism	Non-linear	5730	1228
	Segregated	4504	1227
	LTM	4407	1227
	CFD	4896	1050
Experimental value		5725	1150

Table 3 Hole mass flow distribution percentages - Aachen Mechanism

Hole name	% CFD Aachen	% 1-D-LTM	% 1-D-Segregated	% 1-D-Non-linear
Primary swirler	7.9	8.9	8.8	9.6
Secondary swirler	14.5	15.9	15.9	15.9
Primary outer	5.4	6.5	6.5	6.5
Primary inner	5.2	4.6	4.6	4.6
Secondary outer	12.8	11.5	11.5	11.5
Secondary inner	5.9	6.8	6.8	6.7
Dilution 1 outer	32.2	27.3	27.3	27.0
Dilution 1 inner	11.5	15.1	15.1	14.9
Dilution 2 outer	4.0	2.4	2.4	2.3
Dilution 2 inner	0.7	1.1	1.1	1.1

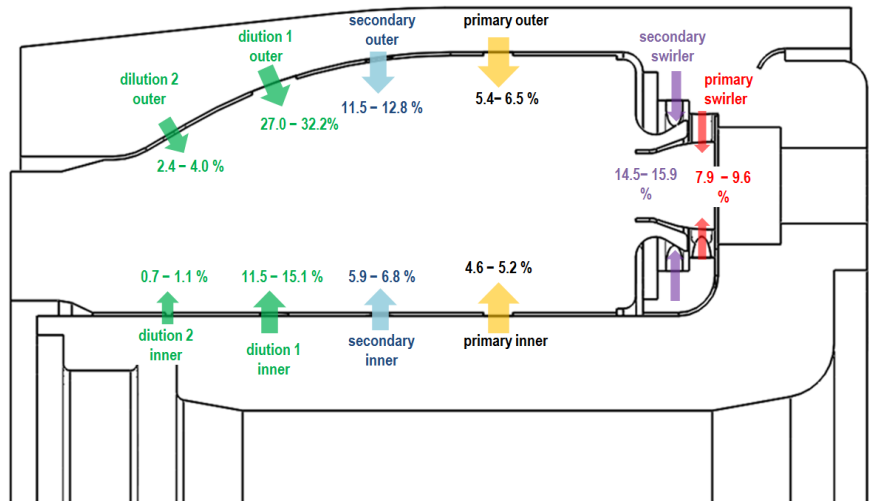


Fig. 10 Mass flow distribution through the combustor liner

The results in Table 3 show that the percentage of mass flow through the holes agrees well with the CFD predictions. The non-linear model predicts a 1.8 % higher mass flow through *primary swirler* holes, whereas other models predict only 1 % through this hole. It is also seen that all the models predict approximately 5 % less air flow from the *dilution 1 outer* hole group, whereas the *dilution 1 inner* hole prediction is 3.5 % higher. The deviations are therefore 3-5 %. The LTM and segregated model predictions agree very well with the mass flow split predictions, whereas the non-linear model deviates from the other two models. That peculiar behaviour is related with the extra terms included in the pressure loss equations. As previously mentioned, there is a great potential to improve and calibrate the hole flow models based on a measurement database. Two different detailed chemical mechanisms are used in this study and the results are presented for each mechanism. The pressure results show no significant change from altering the mechanism because the temperature levels in the liner are nearly the same. However, there is a small difference in the exit temperatures: the average exit temperature with the Aachen mechanism is 1238 K and it is 1227 K for the Creck mechanism. It can be seen that there is a considerable discrepancy when switching from the Aachen to Creck mechanism in the CFD results as the average exit temperature value deviates by up to 60 K. This is believed to be the effect of the thermal variations in the 3D flow domain.

The differences amongst the three solver models used in this study are discussed in terms of the basic performance parameters. The LTM and non-linear model convergences are not readily disrupted, which means that their structures can bear flow-pressure variations at the initial time steps. However, it was shown that the segregated model depends on the initial pressure distribution, which means that in cases where the initial values are not carefully set, the system may converge to a meaningless value which is not physically correct. In addition, low resistance lines may cause convergence problems for all the models considered in the study. As the convergence of the segregated method in high flow speed regions is problematic, an under-relaxation multiplier was applied to the pressure correction terms in this work.

7. Conclusion

In this work, a gas turbine combustor performance prediction model and the solution procedure is presented for three different flow network solvers that include the coupling of the chemical reactor

elements with the flow network elements. The solution behaviour is investigated for three different chemical mechanisms. Annulus and inner combustor regions are separated from each other by liner holes, and the flow through these holes is incorporated by the special orifice models. The total pressure figures show that the pressure levels are estimated with some error in the annulus. However, the liner inner nodes show consistency with the CFD predictions. The overall pressure drop values are compared with CFD findings and the available performance test data. The overall pressure drop shows 10-20 % of deviation among the different 1-D flow models. This is related with the hole flow discharge character, since the highest loss occurs while passing through the liner holes. The hole loss models are not calibrated based on the test results, and although not done in this study, they could be improved by modifying the models to enhance prediction performance. The non-linear method has an extra term in the pressure loss equation, which improves the prediction performance of the method. This shows promise as it consequently produces a much closer overall pressure drop figure.

The inner nodes in the network model are assigned reactor output temperatures directly, which is an idealization for a 1-D modelling application. In the 3-D model, however, the temperature varies in the combustor liner segments significantly. The local temperature at the hole exits are cooler than the core region temperatures. Inside the reactor network elements, the fuel and oxidizer mix perfectly, and this modelling idealization in the combustor liner is the main reason for the higher temperature predictions in comparison to the detailed spatial CFD predictions. Nevertheless, higher temperature figures at the primary and secondary zones of the combustor liner converge to reasonable values near the exit of the combustor, as presented in Fig. 9. Similarly, the average exit temperature predictions of the 1-D network models are slightly higher than the measured values due to the reduced dimensional simplifications of the reactor network. Reduced dimensional flow network models are a popular choice for the quick prototyping of combustors. Their simple nature allows the customization of the code for different combustor types and cooling technologies. Different flow modelling approaches and comprehensive chemical modelling techniques can enhance performance prediction capability. These methods provide a good starting point for more complex optimization steps. The models presented here lay out the basic steps with several options in this regard.

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Nomenclature

A	Element area, [m ²]
C	Constant terms grouped
D	Element diameter, [m]
dx	Infinitesimal pipe element
d	External mass flow, [kgs ⁻¹]
F	Body force, [N]
f	Friction factor

g	Gravitational acceleration, [Ns^{-1}]
hf	Flow loss head, [m^2s^{-2}]
h	Enthalpy, [J]
l, L	Length of the element, [m]
\dot{m}	Mass flow, [kgs^{-1}]
n_i	Node number i
P	Total pressure, [Pa]
\dot{Q}	Heat generated, [W]
s_{ij}	Direction indicator of the flow inside the element (i.e. 1 or -1)
T	Temperature, [K]
t	Time, [s]
U	Internal energy
V	Velocity, [m/s]
Y	Species mass fraction [kgkg^{-1}]
z	Elevation head, [m^2s^{-2}]
Greek Symbols	
ρ	Density, [kgm^{-3}]
τ_0	Shear stress, [Nm^{-2}]
κ	Dynamic pressure terms
Subscripts	
i	Global node number
j	Local branch number
Superscripts	
*	Tentative values
'	Corrections

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