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Preliminary combustor design using a network approach based on chemical reactor modeling

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ABSTRACT

Chemical Reactor Network approach has great advantages in emission prediction research and one-dimensional design of combustors. It can use detailed chemical reaction mechanism and substantially shorten the computing time. This paper uses it to calculate the optimum air distribution scheme of a low NOx annular combustor. The combustor is divided into several zones based on the flow filed characteristics. First, the total air amount is divided into two parts, the first half air flow of annular combustor including swirler and primary holes, and the last half air flow including cooling holes and dilution holes. Air flow of these two parts is confirmed. After analyzing all reactor data and comprehensively considering all aspects of the factors, air flow mass fraction of each zone is confirmed for the optimum air distribution scheme. The effective volume of each zone and the one-dimensional combustor lengths are calculated using Differential Element method. The NOx and CO emission under the optimum air distribution scheme and exact effective volumes are proved much lower than general level.

Key words: Chemical reactor network; combustor design; Differential Element method

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INTRODUCTION

As a core component of gas turbine, combustor works in an environment with high temperature, high pressure and high intensity. The internal flow field of combustor is very complicated and will directly influence gas turbine performance, which means that the design study of combustor is crucial for gas turbine.

In 1950s, researchers started to use network approach based on chemical kinetics model in combustor design. In 1980s, a series of commercial software of chemical reactions modules appeared, such as Chemkin, ModLink, Cantera and so on. They are all able to handle large-scale chemical reaction mechanism.

Chemical reactor network (CRN) approach is based on the distribution characters of the flow field in combustors, dividing the combustor into several zones. According to the characteristics of each zone, use different reactor module to simulate different zones. All reactor modules build the chemical reactor network. The streamlines between reactors simulate the flow characters of combustor.

Novosselov [1] simulated the gas turbine combustor through CRN approach and compared the results with the experimental data. He [2] also used the CRN approach to simulate the working process of the Dry Low Emission combustor in industrial gas turbines and predict emissions. There were 31 chemical reactors in his network and the combustor flow field was divided into 5 zones. Allaire [3] et al used both empirical formula approach and CRN approach to predict the NOx and CO emission of CIAM-M combustor. They compared the advantages and disadvantages of these two approaches. Russo [4] et al used CRN approach in ARI100 micro-gas turbine's operating characteristics research. All the calculated parameters were consistent with the experimental data.

Zakharov [5] et al has used CRN approach in emission research of hydrocarbon fuel combustion under different

pressures. The network used in his paper was universal and not complicated. Fichet [6] et al built a chemical reactor network based on the component concentration and temperature of the CFD numerical simulation results. It was shown that the NOx prediction value of CRN approach were consistent with the experimental data better.

Hu [7] built a CRN model for typical gas turbine combustor. He presented a new double-entrance double-mixed reactor model and confirmed its availability. Yang [8] has used CRN approach in NOx prediction research of a heavy-duty gas turbine combustor burning hydrogen-rich synthesis gas. He studied the NOx emission changing trend along with steam fraction of fuel. Yu [9] has used CRN approach in a can annular combustor research. She was the first one who used Differential Element (DE) method in combustor one-dimensional design research.

This paper is about an annular combustor of gas turbine, using CRN approach to analyze the combustion flow field. The flow field is divided into network partition according the work characteristics of conventional diffusion combustor and the structure of annular combustor. Parameter changing trend of each zone, especially the outlet parameters, is analyzed under different air distribution schemes. Air distribution scheme is optimized based on the lowest NOx and CO emission at the outlet. Then the DE method is used to calculate the one-dimensional characteristic length of this low emission annular combustor under this optimum air distribution scheme.

COMBUSTOR STRUCTURE

This paper simulates 1/20 of an annular combustor, including 1/20 of flame tube and a radial swirler. Figure 1 shows the geometry structure. The flame tube is 20cm long, 10cm high, and has 5 primary holes and 3 rows of cooling holes.

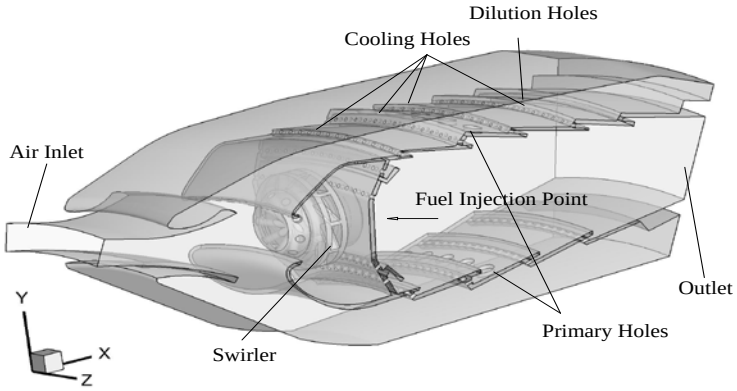


Fig.1: Geometry structure of combustor

COMBUSTOR NETWORK CONSTRUCTION

Chemical reactors

Chemkin® software is a commonly used computational tool in combustion area, usually used in combustion process, catalytic process, plasma and other reactions [10]. The reactor types used in this paper are as follows.

PSR, Perfectly Stirred Reactor, is the transient or steady-state perfectly stirred reactor. After flowing into the reactor, materials instantly disperse evenly throughout the reactor and are completely mixed with remain materials of the reactor. So the reaction rate is controlled by the chemical reaction rate not the mixing process.

PFR, Plug-flow Reactor, is the reactor where convection dominates transport. In this reactor, all materials flow along the flow direction, with no axial mixing and diffusion.

Gas Mixer is non-reactive gas mixer which accepts multiple inlets.

Gas Flow Splitter splits stream into multiple streams.

Reaction mechanism

Fuel used herein is n-heptane (C_7H_{16}). The detailed reaction mechanism of C_7H_{16} is from the LLNL website [11]. The mechanism includes 179 reactants and 876 elementary reactions, applied for 1000K-3000K temperature range. The mechanism contains all the elementary reactions of every stage in the gas combustion process. These elementary reactions and reaction rates are all based on the current reaction rate theories which have been accepted. Fuel mass flow is 0.0555kg/s, air mass flow is 3kg/s.

Network

According to the annular combustor flow characteristics, the flow field is divided into 6 parts: head combustion zone (PSR1), recirculation zone central region (PSR2), recirculation zone periphery including upper layer and lower layer (PSR3), wall cooling zone (PSR4), primary combustion zone (PSR5) and dilution zone (PFR1). All combustor zones and the flow between each zone are shown in Figure 2. This network assumes that: the combustion starts at head combustion zone; recirculation zone mainly carries out fuel cracking and mixing process; the cooling air flow is flowing close to the wall and its only effect is cooling the flame tube wall; the primary combustion zone mainly completes fuel combustion process; in the dilution zone all the chemical reactions have done. The network based on above zones is shown in Figure 3.

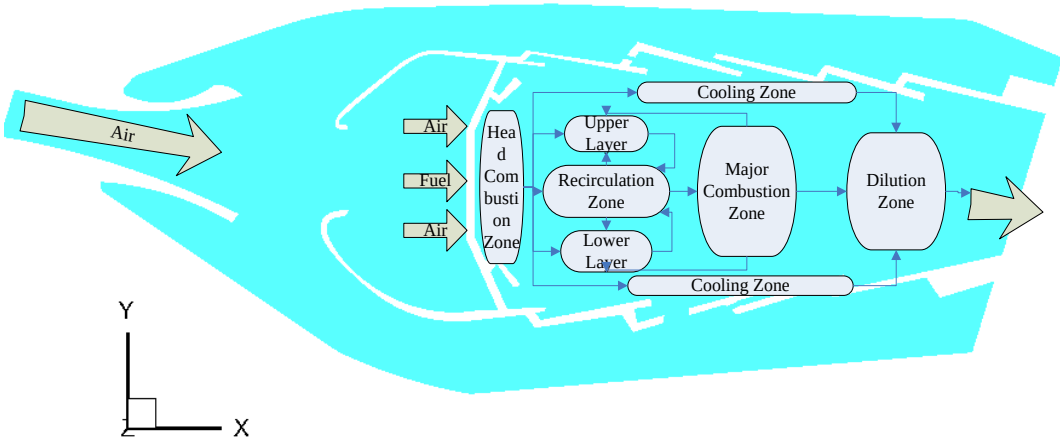


Fig.2: Annular combustor zones and flow

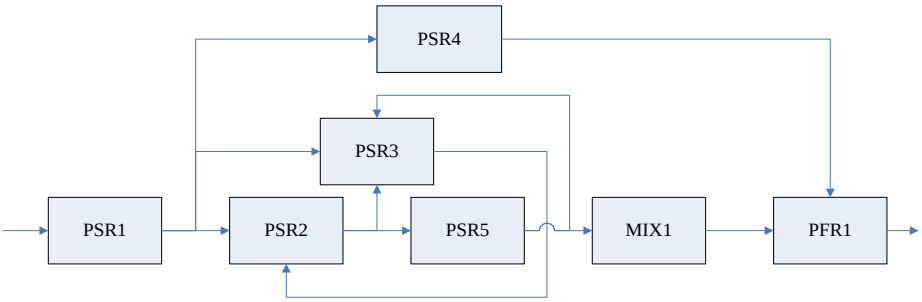


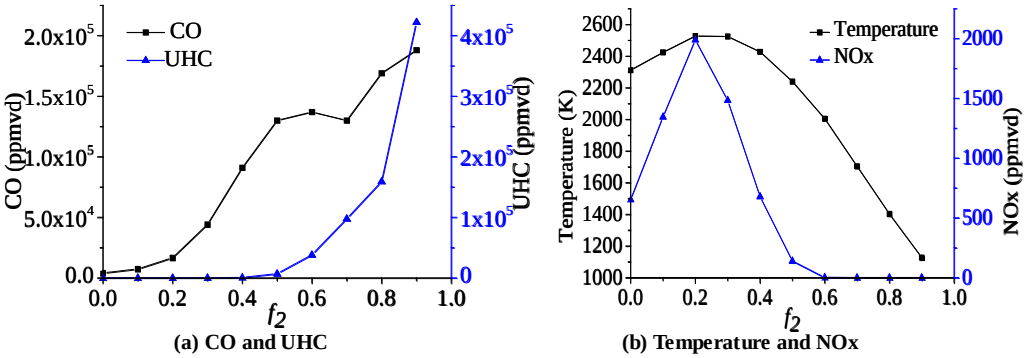
Fig.3: Annular combustor network

DATA ANALYSIS

Air distribution schemes

The initial flow rate distribution is based on the conventional annular combustor. In the first half combustor, the ratio of swirler air flow to primary holes air flow is 6:4. In the last half combustor, the ratio of dilution air flow to cooling air flow is also 6:4. At this air distribution, the air flow of the last half combustor varies from 0% to 100% mass fraction of the combustor inlet air flow. The changing trend of NOx CO temperature and unburned hydrocarbons (UHC) are analyzed as follows.

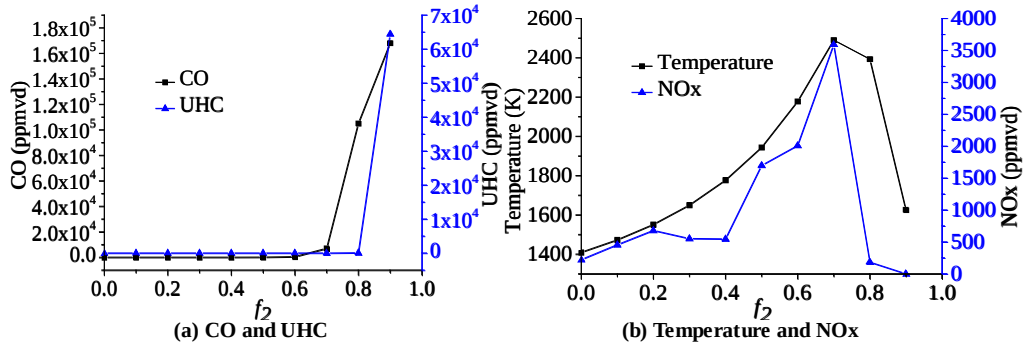
Figure 4 shows the data of PSR1. The total air flow is divided into two parts, the first half air flow of annular combustor including swirler and primary holes, and the last half air flow including cooling holes and dilution holes. In the next analysis, the ratio of the first half air flow to the total air flow is defined as f_1. The ratio of the last half air flow to the total air flow is defined as f_2. Figure 4(a) is the CO and UHC trend along with f_2. The CO and UHC are all increase as f_2 increasing. When f_2 increases, meaning f_1 decreases, air in PSR1 also decreases. The lean-burning environment in PSR1 changes into a rich-burning environment. As a result, more cracking fuel burning incompletely causes more CO and UHC residue in PSR1. Figure 4(b) is temperature and NOx trend along with f_2. NOx and temperature all increase at first and then start to decrease from f_2=0.2. At f_2=0~0.2 stages, the PSR1 is in super lean combustion state. Excess air flow will cool down flame and decrease temperature of combustion zone. Temperature effects NOx formation especially the Thermal-NOx a lot. So when f_2 changes from 0 to 0.2, the excess air flow decreases, temperature increases, NOx increases as well. For the same reason, temperature decreases from f_2=0.2 to f_2=0.9 and NOx decreases as well.



(a) CO and UHC **(b) Temperature and NOx**

Fig.4: CO UHC temperature and NOx trend of PSR1 (ppmvd: Parts per Million Volumetric Dry)

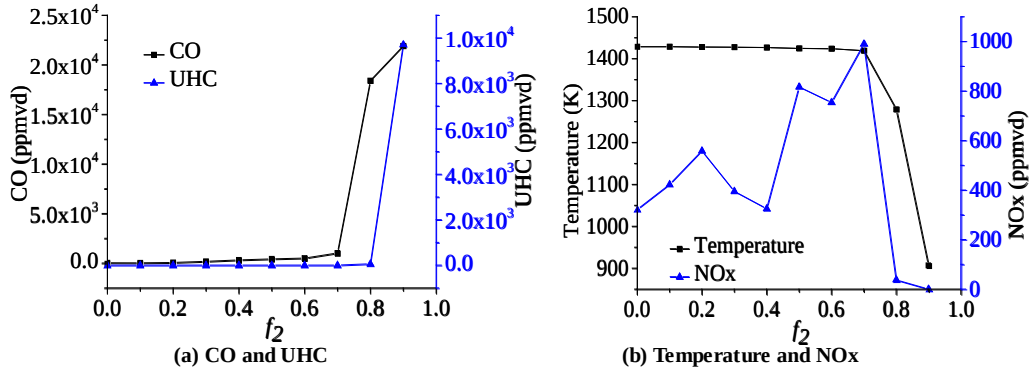
Figure 5 shows CO UHC temperature and NOx trend of PSR5. Figure 5(a) is the CO and UHC trend along with f_2. PSR5 is the major combustion zone. All unburned fuels from the head combustion zone and the recirculation zone finally mix with primary holes' air and burn here. So when f_2 varies from 0 to 0.6, the CO and UHC in PSR5 is little and the combustion is complete. At this condition, the decreasing air flow in PSR5 will certainly increase temperature and NOx formation, as seen in Figure 5(b). Within this, NOx formation is not so large because temperature is lower than 1800K at f_2=0~0.4. When temperature goes larger than 1800K, NOx formation increases obviously faster. When f_2 varies from 0.7 to 0.9, the PSR5 is in rich fuel state, the combustion is incomplete, and then the CO and UHC content increases rapidly. At this time, temperature decrease immediately as few fuels are burned. Along with temperature's decreasing, NOx formation of PSR5 decreases fast as well.



(a) CO and UHC **(b) Temperature and NOx**

Fig.5: CO UHC temperature and NOx trend of PSR5

The CO and UHC emission at outlet are close to PSR5 data, as seen in Figure 6(a). These two almost remain the same until f_2=0.6 then increases rapidly at f_2=0.7~0.9. But temperature and NOx emission at outlet are quite different, as seen in Figure 6(b). Figure 5(b) is the temperature changing trend of primary combustion zone, which is the highest temperature zone of the whole combustor. While at the combustor outlet, the high temperature gas has been diluted in the dilution zone. Temperature has been cooled down to 1428K, shown in Figure 6(b). NOx emission has decreased into magnitude order of 10^2. The total NOx trend is fluctuant, increasing at f_2=0~0.2 first, decreasing at f_2=0.2~0.4, then increasing again at f_2=0.4~0.7 and finally decreasing at f_2=0.7~0.9. Within the result NOx is in a low level both at f_2=0~0.4 and f_2=0.8~0.9. But the data of f_2=0.8~0.9 shows that there are few chemical reactions in the combustor, which means the flame goes out. So the lowest NOx air distribution scheme is within f_2=0~0.4.



(a) CO and UHC **(b) Temperature and NOx**

Fig.6: CO UHC temperature and NOx trend of combustor outlet

The ratio of last half air flow to the total combustor air flow, f_2, is 0~0.4, which means the ratio of first half air flow to the total combustor air flow, f_1, is 0.6~1.0. It still needs to confirm the swirler air flow and the primary holes air flow. Define the ratio of swirler air flow to first half combustor air flow as f_{11}. In Figure 7, the X axial is f_{11}, the Y axial is NOx emission at combustor outlet and the Z axial is f_2. The general NOx emission trend is increasing along with the Z axial f_2. It shows that the lowest NOx emission is near f_{11}=1.0 and f_2=0.1~0.2. Considering the detail temperature of PSR4 (cooling zone), the NOx CO and UHC emission at outlet, the optimum air distribution is at f_2=0.14 and f_{11}=1.0. That means there are 0.86 of total air flow goes through swirler, 0.14 of total air flow goes into the cooling zone and dilution zone, and no air goes through primary holes.

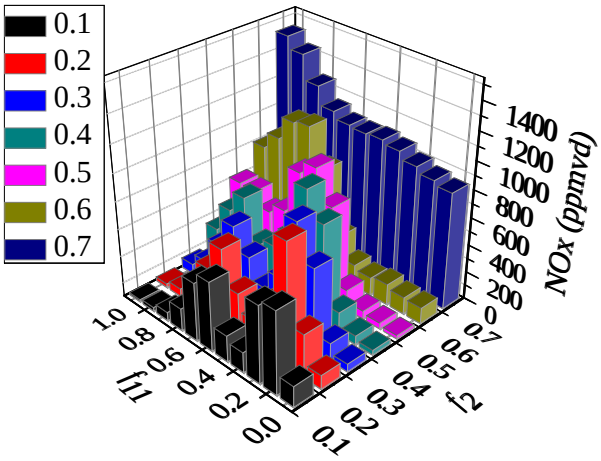


Fig.7: NOx emission of different air distribution scheme

Next step is confirming the cooling air flow and the dilution air flow. Define the ratio of dilution air flow to the last half combustor air flow as f_{21}. In Figure 8, temperature increases along with f_{21} increasing. When f_{21}=0 (the air of last half combustor all goes into cooling zone), the PSR4 has the lowest wall temperature. NOx formation of PSR4 is little at f_{21}=0~0.9 because temperature remains lower than 1800K. At f_{21}=1.0, temperature is 1949K, so NOx formation increases immediately.

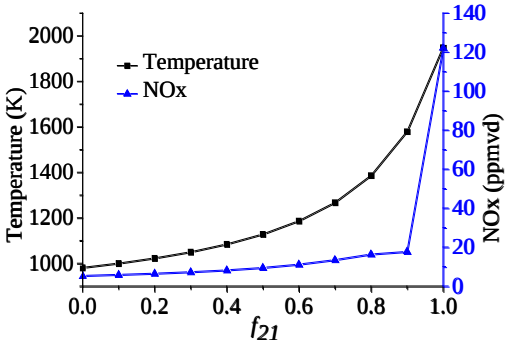


Fig.8: Temperature and NOx trend of PSR4

From Figure 9(a) it can be known that the variation of f_{21} does not affect temperature and NOx emission of combustor outlet. NOx emission keeps at 17.47ppmvd. Temperature keeps at 1949.5K. The UHC trend of Figure 9(b) also shows there are no unburned hydrocarbons at combustor outlet. The CO emission varies from 30.8ppmvd to 15.3ppmvd. Although the lowest CO emission is at f_{21}=1.0, this distribution scheme is not acceptable because temperature of the cooling zone is also an important parameter. Comprehensive consideration of various factors, the final result is f_{21}=0.

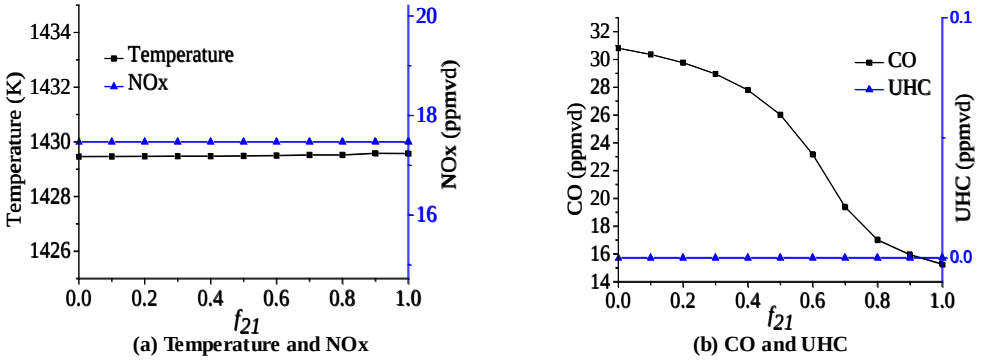


Fig.9: CO UHC temperature and NOx trend of combustor outlet

After analysis of the above data, based on the low NOx and CO emission and other factors, the optimum of air distribution scheme is shown in Table 1.

Table 1: Air distribution scheme

Zones	Swirler	Primary holes	Cooling holes	Dilution holes
Mas fraction	0.84	0.00	0.14	0.00

One-dimensional characteristic lengths

At the condition of optimum combustor air distribution scheme, the one-dimensional characteristic lengths of annular combustor are calculated based on Differential Element method. Take head combustion zone as an example. The DE method cuts PSR1 into infinitesimal elements, then taking CH_3 as the reference parameter, analyzes the reference parameter of every infinitesimal element to confirm the effective combustion volume of this zone. After the volume confirming, the characteristic length is easy to calculate.

There are 20 reactors in PSR1, which means the PSR1 is cut into 20 infinitesimal elements and the volume of each infinitesimal element is 40cm^3. In Figure 10, CH_3 starts to keep stable from the reactor number 14. So the effective volume of head combustion zone is 560cm^3. There are also 20 reactors in PSR2 and the reference parameter is CO. The volume of each infinitesimal element is 50cm^3. In Figure 11, CO starts to keep stable from the reactor number 15. So the effective volume of recirculation zone (central region) is 750cm^3.

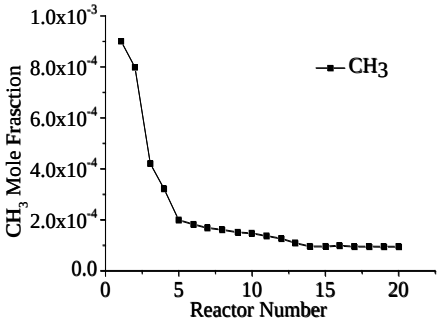


Fig.10: CH3 trend of PSR1

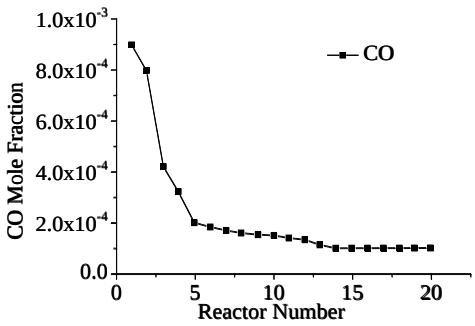


Fig.11: CO trend of PSR2

There are 20 reactors in PSR3 and the reference parameter is CH_3. The volume of each infinitesimal element is 50cm^3. In Figure 12, CH_3 starts to keep stable from the reactor number 15. So the effective volume of recirculation zone periphery (including upper layer and lower layer) is 750cm^3. The reactor number and reference parameter of PSR4 is the same with PSR3. The volume of each infinitesimal element is 40cm^3. CH_3 starts to keep stable from the reactor number 9. So the effective volume of wall cooling zone is 360cm^3.

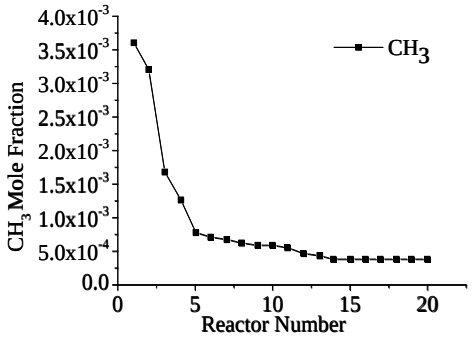


Fig.12: CH3 trend of PSR3

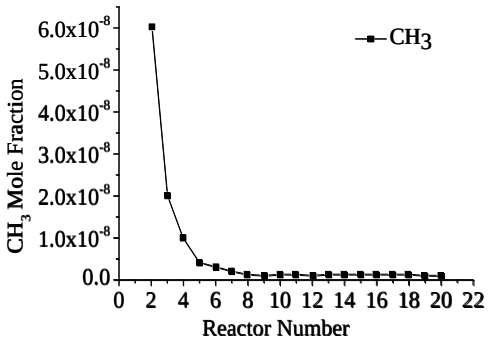


Fig.13: CH3 trend of PSR4

There are also 20 reactors in PSR5 and the reference parameter is CO. The volume of each infinitesimal element is 80cm^3. In Figure 14, CO starts to keep stable from the reactor number 16. So the effective volume of primary combustion zone is 1280cm^3.

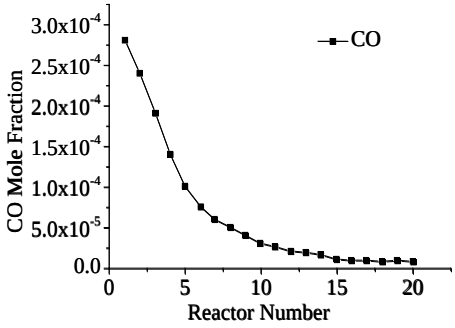


Fig.14: CO trend of PSR5

From the above analysis, it can be known that the effective volume except dilution zone is 3700 cm^3. The dilution stage isn't calculated because it usually does not have a regular shape or even nearly regular shape. The design area of other combustor stages is near 100.098cm^2, so the one-dimensional characteristic length of this combustor (except dilution stage) is 37cm. With this effective volume and air distribution scheme, NOx emission is 3.458ppmvd and CO emission is 61.96ppmvd at combustor outlet.

CONCLUSION

Comparing to other CFD numerical simulation methods, chemical reactor network (CRN) approach simplifies the combustion flow field. The design period shortens for several orders of magnitude. Moreover, the traditional simulation methods are limited by computational time, so these simulations usually use a simple chemical reaction mechanism. But the CRN approach is not restricted because it has simplified the combustor into multiple 0-dimensional reactors. It can use large detailed chemical reaction mechanism during calculation. So the calculation of NOx is more precise and credible.

The optimum air distribution scheme of annular combustor using CRN approach in this paper is: swirler accounts for 86% of the total air amount; primary holes account for 0% of the total air amount; cooling holes account for 14% of the total air amount; dilution holes account for 0% of the total air amount.

The effective volume of combustion flow field (except dilution zone) is 3700 cm^3. The one-dimensional characteristic length is 37cm. The lowest emission is NOx 3.458ppmvd and CO 61.96ppmvd at combustor outlet.

Although the CRN approach cannot simulate exact flow characteristics of the combustion field, it has great advantages at emission prediction and one-dimensional design, which also can guide the three-dimensional combustor design and shorten the design period.

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