A new surrogate of Fischer–Tropsch fuel and its pollution emission in gas turbine combustor

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Abstract
Based on the analysis of the combustion process of liquid fuel in the gas turbine combustor, we suggest that a comprehensive surrogate fuel should be developed according to the basic physical and chemical properties that affect the diffusion combustion process. The present study took the carbon–hydrogen mole ratio, molar weight, density, viscosity, surface tension, initial boiling point, and lower heating value, as the target properties. The optimal direction method was utilized to obtain the mixture composition ratio which has the minimum deviation on the basic physical and chemical properties compared with the Fischer–Tropsch (F–T) fuel. This mixture, taken as the comprehensive surrogate fuel of the F–T fuel, was composed of 15% n-decane, 67% n-tetradecane, 13% iso-octane, and 5% methylcyclohexane in mole fraction. Further experiments were conducted to investigate the pollutant emissions of the F–T fuel and the surrogate fuel in a gas turbine combustor. The experimental results showed that the surrogate fuel can well predict the EI(CO) and EI(NOx) of the F–T fuel in the turbine combustor, and the difference in EI(UHC) is mainly influenced by the fuel evaporation property.

KEYWORDS
comprehensive surrogate fuel, Fischer–Tropsch fuel, gas turbine combustor, pollutant emission

1 | INTRODUCTION

To solve the issue of energy shortage and environmental pollution, it is necessary to develop novel clean energy. As an available energy source, the coal-based Fischer–Tropsch (F–T) fuels have drawn more and more attention.

With the synthetic technology of the F–T fuels growing increasingly mature, the high-efficiency catalyst as a critical factor has been widely investigated.1–4 Present mature F–T synthetic technique has been able to avoid the production of CO2 during the synthetic process.5,6 The investigations on the synthetic mechanism of the F–T fuels are performed more and more deeply. Fischer and Tropsch initially proposed the surface carbide model.7 Although describing the production of straight-chain alkanes well, this model cannot explain the production of branched alkanes or oxygenated compounds. After nearly a century of development, several models8,9 were successively proposed where the relatively mature model, carbene insert model,10–12 has been widely accepted. These studies are the basis of the wide application of coal-based F–T fuels. Due to the
characteristics of sulfur-free and few aromatic hydrocarbons, the fundamental combustion characteristics and chemical reaction mechanism of coal-based F-T fuels have been widely investigated as potential clean energy.\textsuperscript{13,14} Sung et al.\textsuperscript{15,16} experimentally investigated the autoignition characteristics, laminar flame speeds, and extinction stretch rates of the F-T fuel S-8 and conventional aviation kerosene Jet-A. They found that the two fuels had similar autoignition characteristics (such as two-stage ignition characteristics and negative temperature coefficient [NTC] trend), very similar laminar flame speeds, but the ignition delay times of the S-8 were shorter than that of the Jet-A. Wang et al.\textsuperscript{17} compared the ignition delay times of three F-T fuels, namely, S-8, Shell GTL, and Sasol IPK with that of the conventional Jet-A. They reported that due to the difference in derived cetane number, four fuels had significantly different ignition delay times in the low-temperature regime and NTC regime, while little different ignition delay times in the high-temperature regime. Gokulakrishnan et al.\textsuperscript{18} experimentally measured the ignition delay times of the S-8 and JP-8 in an atmospheric flow reactor and found that shorter ignition delay times for S-8 fuel than for JP-8 due to the absence of aromatic components in S-8 fuel. They utilized the mixture composed of n-decane and iso-octane (80\% iso-octane and 20\% n-decane) as the surrogate of the S-8 to investigate the influence of the branched alkanes on the ignition delay time. Naik et al.\textsuperscript{19} developed two surrogate fuels (28\% iso-octane, 61\% n-decane, 11\% n-dodecane, and 32\% iso-octane, 25\% n-decane, 43\% n-dodecane by mol) for two F-T fuels, namely, Shell GTL and S-8, and assembled detailed chemical reaction mechanisms which have been experimentally validated by ignition delay time, autoignition temperature, laminar flame speed, extinction strain rate, and NOx emission.

The combustion performance of the F-T fuel in gas turbine combustors has also been widely investigated. Hermann et al.\textsuperscript{20} experimentally measured the combustion performance, such as emissions of NOx, CO, and UHC, ignition and extinction points, and soot levels, of the F-T fuel provided by the Oroboros AB Company in a single can-type combustor at a pressure of 4 bar, and compared with those of the conventional aviation kerosene Jet-A1. They reported that the F-T fuel provides fewer emissions of NOx and soot than Jet-A1. Keramiotis et al.\textsuperscript{14} experimentally measured the combustion products of four F-T fuels in a laboratory-scale combustor and analyzed the influence of the component class in the F-T fuel on the combustion product. Novick et al.\textsuperscript{21} investigated the combustion performance and emissions of the F-T fuel using the full-scale combustor, while Rollbuhler et al.\textsuperscript{22} utilized the flame tube combustors.

Developing surrogate fuel is an important method to investigate fuel, and the surrogate fuel can be divided into a physical surrogate, chemical surrogate, and comprehensive surrogate.\textsuperscript{23} Those surrogate fuels developed for simulating the fundamental combustion characteristics belonged to the chemical surrogate. However, to accurately predict the combustion performance of the practical fuel in gas turbine combustors, the physical properties of the surrogate fuel were also greatly important, while the related research was still lacking. To analyze the influence of physical properties and chemical reaction kinetics on liquid fuel combustion, the present study developed a comprehensive surrogate fuel for the coal-based F-T fuel,\textsuperscript{24} based on the diffusion combustion process which affects the pollutant emissions in gas turbine combustor, and experimentally investigated the pollutant emissions and combustion efficiencies of the F-T fuel and the surrogate fuel in a gas turbine combustor at two typical operating conditions of the aeroengine, namely, idle and cruise, to investigate whether the surrogate fuel can predict the pollutant emissions of the F-T fuel. Using the comprehensive surrogate fuel as the research means, the influences of the physical properties and chemical kinetics on pollutant emissions were analyzed in detail.

2  |  THE F-T FUEL AND ITS SURROGATE FUEL

2.1  |  The F-T fuel

The coal-based F-T fuel was produced by Tianjin University.\textsuperscript{24} Its basic physical and chemical properties were measured according to the China National Standards,\textsuperscript{25-28} as shown in Table 1. The Brook 456-GC gas chromatograph was utilized to analyze the composition of the F-T fuel which was composed of 32.9\% straight-chain alkanes, 64.8\% branched alkanes, and 2.3\% cycloalkanes in mass fraction. Figure 1 compares the carbon number distributions of the F-T fuel and conventional aviation kerosene RP-3. The carbon number distribution of the F-T fuel is much broader than that of conventional aviation kerosene RP-3. Through analysis, we calculated the average molecular formula of the F-T fuel as \( \text{C}_{12.16}\text{H}_{26.39} \).

2.2  |  Target properties of the surrogate fuel

The combustion process of liquid fuel in gas turbine combustors is typical diffusion combustion. The liquid fuel firstly becomes the fuel particles which are further
vaporized. The fuel vapor burns with the air and the flame is stabilized in the recirculation region. Consequently, the pollutant emissions in gas turbine combustors are driven by a combination of atomization, evaporation, and combustion which should be investigated simultaneously. The development of surrogate fuels needs to consider the basic physical and chemical properties which affect the atomization, evaporation, and combustion process.

The main physical properties affecting the fuel atomization include surface tension, viscosity, and density, which are taken as the important target parameters. Although the main physical property affecting the fuel vaporization is the fuel vapor pressure, it is more practical to measure the distillation curve of the F-T fuel as a complicated mixture. Furthermore, the temperature at which the fuel begins to vaporize has an important effect on the combustion characteristics of the liquid fuel, so the initial boiling point (IBP) is taken as the target parameter to judge the vaporization. To ensure the identical combustion temperature of two fuels that directly affect the NOx emissions, both the equivalence ratio and the lower heating value (LHV) should be kept consistent, respectively, and the equivalence ratio is determined by the carbon–hydrogen molar ratio (C/H), and fuel-to-air ratio. Consequently, the LHV of the fuel and the C/H are taken as important target parameters.

In summary, the present study takes C/H, molar weight (MW), LHV and density, surface tension, viscosity, and IBP as the target properties to judge whether the surrogate fuel matches the F-T fuel.

### 2.3 Composition selection of the surrogate fuel

The selected compositions of the surrogate fuel should not only cover the corresponding class in the F-T fuel.

| TABLE 1 Properties comparisons between the F-T fuel and the surrogate fuel |
|---------------------------------------------------------------|
| **The F-T fuel** | **Surrogate-TUFT model** |
| Composition | Straight-chain alkanes (32.9% mass) | n-Decane (15% mol) |
| | Branched alkanes (64.8% mass) | n-Tetradecane (67% mol) |
| | Cycloalkanes (2.3% mass) | iso-Octane (13% mol) |
| | | Methylcyclohexane (5% mol) |
| Number of carbon atoms | 12.16 | 12.27 |
| Number of hydrogen atoms | 26.39 | 26.44 |
| H/C | 2.1709 | 2.1548 |
| MW (g/mol) | 173.15 | 173.68 |
| LHV (MJ/kg) | 43.680 | 43.956 |
| Initial boiling point (K) | 442.45 | 437.63 |
| Final boiling point (K) | 533.35 | 526.73 |
| Density (20°C) (kg/m³) | 754.3 | 756.4 |
| Viscosity (20°C) (mPa s) | 1.66 | 1.79 |
| Viscosity (–20°C) (mPa s) | 4.65 | 5.70 |
| Surface tension (20°C) (mN/m) | 24.67 | 23.44 |

**Abbreviation:** F-T, Fischer–Tropsch.

**FIGURE 1** Carbon number distributions of RP-3 and the coal-based Fischer–Tropsch (F-T) fuel
but also be easier to obtain its chemical reaction mechanism. The iso-octane (i-C₈H₁₈) and methylcyclohexane (c-C₇H₁₄; MCH) whose reaction mechanisms are relatively mature are selected as the branched alkanes and cycloalkanes in the surrogate fuel, respectively. Due to much smaller carbon and hydrogen atomic numbers, the n-tetradeacne (n-C₁₄H₃₀) is added as the straight-chain alkane to match the MW of the F-T fuel. Because the boiling point of the n-tetradeacne (526.85 K) is much higher than those of the iso-octane (372.35 K) and MCH (373.55 K), an obvious turning point occurs on the distillation curve of the surrogate fuel with only these three components, which is inconsistent with the practical fuel. Consequently, it requires a kind of component whose boiling point is among those three components. As a candidate component, n-decane with a mature chemical reaction mechanism is widely applied in the development of surrogate fuels, and its boiling point (447.15 K) is between those of iso-octane, MCH, and n-tetradeacne. Consequently, we select the n-decane as the fourth component of the surrogate fuel.

The properties of the surrogate components can be obtained from the DIPPR property database. Figure 2 shows the density, surface tension, viscosity, and vapor pressure of the surrogate components as a function of temperature.

### 2.4 Computational method for the target properties of the surrogate fuel

The LHV was estimated using the mass fraction. \( y_i \) is the mass fraction.

\[
\text{LHV}_{\text{mix}} = \sum y_i \text{LHV}_i.
\]  

The multi-component system consisting of hydrocarbons in vapor–liquid equilibrium can be approximately seen as the ideal mixture except for the conditions close to the critical region. Consequently, the density was calculated using the volume fraction \( v_i \). Different from the mole fraction and mass fraction, the volume fraction is a function of temperature.

\[
\rho(T)_{\text{mix}} = \sum v(T)_i \rho(T)_i.
\]

The parachor equation was used to estimate the mixture surface tension, neglecting the vapor mixture density which is very small compared to the liquid mixture density. \( P \) is the parachor, \( \rho(T)_{L,\text{mix}} \) is the density of the liquid mixture, \( \rho(T)_{V,\text{mix}} \) is the density of the vapor mixture, \( M_{\text{mix}} \) is the MW of the liquid mixture, \( \rho(T)_{L,\text{mix, molar}} \) is the molar density of the liquid mixture, \( x_i \) is the molar fraction.

**Figure 2** Temperature-dependent (A) density, (B) surface tension, (C) viscosity of the Fischer–Tropsch (F-T) fuel and the surrogate components, and (D) vapor pressure of the surrogate components.
\[ \sigma(T)_{\text{mix}} = \{P_{L,\text{mix}}[\rho(T)_{L,\text{mix}} - \rho(T)_{V,\text{mix}}]/M_{\text{mix}}\}_{\text{molar}} \]

\[ \approx \{P_{L,\text{mix}}\rho(T)_{L,\text{mix, molar}}\}_{\text{molar}} \]

\[ \rho(T)_{L,\text{mix, molar}} = \rho(T)_{L,\text{mix}}/M_{\text{mix}} \]

\[ P_{L,\text{mix}} = 0.5 \sum_{i} \sum_{j} x_{i}x_{j}(P_{i} + P_{j}) \]

The viscosity of the mixture was estimated using the Grunberg–Nissan equation with the regression term set to zero, which applies to hydrocarbon mixtures as suggested by Poling et al. \(^{35}\) with expected errors of about 15%.

\[ \ln(\mu(T)_{\text{mix}}) = \sum x_{i} \ln(\mu(T)_{i}) + 0.5 \sum_{i} \sum_{j} x_{i}x_{j}G_{ij} \]

The relative volatility method was used to solve the simultaneous equations of Dalton’s law of partial pressures, Raoult’s law, and Antoine’s equation for obtaining the boiling point temperature and vapor composition of the mixture at an equilibrium state. Assuming that a constant volume (5% of the total volume) of liquid mixture leaves the liquid phase into the vapor phase at each calculation step to calculate the mixture components in the next state which acted as the initial components of the next calculation. This process was repeated until all liquid mixtures has evaporated into vapor. All boiling point temperatures at every state were fitted to obtain the distillation curve of the mixture.

\[ \log(P(T)_{\text{vap},i}) = A_{i} - B_{i}/(T + C_{i}) \]

\[ x_{\text{vapor},i} = \frac{P(T)_{\text{vap},i}}{P_{\text{tot}}} x_{\text{liquid},i} \]

This calculation method was validated against the experimental distillation curve of the mixture of n-decane and n-tetradecane, as shown in Figure 3. That this method can capture the distillation curves of these two mixtures well.

The quadratic sum of the difference between the calculated target properties of the mixture and the F-T fuel was taken as the final target function. The optimal direction method in Matlab was utilized to obtain the composition ratio which minimized the target function. Consequently, the designed surrogate fuel, named Surrogate-TUFT (Tianjin University’s F-T fuel), was composed of 15% n-decane, 67% n-tetradecane, 13% iso-octane, and 5% MCH in mole fraction.

**2.5 Verification of physical surrogate capability**

The measured basic physical and chemical properties of the F-T fuel were compared with the calculated and measured values of the Surrogate-TUFT, as shown in Table 1 and Figure 4. In the preparation of surrogate fuel, the molar fractions of the components were transferred to the volume fraction at 20°C, and the volume of each component was measured using the graduated cylinder with a minimum scale of 1 ml.

Based on Lefebvre’s atomization theory, as for airblast atomizers, the atomization SMD of the fuel is affected by the fuel density, surface tension, viscosity, air density, velocity, as shown

\[ \text{SMD}/L_{c} = [1 + (\text{ALR})^{-1}] \left\{ A \left[ \sigma / (\rho_{L} U_{d}^{2} D_{p}) \right]^{0.5} + B \left[ \mu_{L}^{2} / (\sigma \rho_{L} D_{p}) \right]^{0.5} \right\} \]

Where \( A \) and \( B \) are constants whose values depend on atomizer design. For plain-jet atomizers, \( L_{c} \) is the initial liquid jet diameter, \( d_{0} \). For prefilming atomizers, \( L_{c} \) is the initial thickness of the liquid sheet. ALR is the air–liquid ratio, \( D_{p} \) is the prefilmer diameter. As shown in Figure 4A–C, the Surrogate-TUFT has similar density, surface tension, and viscosity with the F-T fuel under identical conditions, resulting in close atomization SMD of two fuels. In addition, for the same fuel, the atomization of SMD at
high temperatures is mainly influenced by the surface tension, air density, and velocity, while the effects of the fuel density and viscosity can be neglected. It can be seen that the Surrogate-TUFT can well simulate the atomization properties of the F-T fuel.

By comparing the calculated distillation curve of the Surrogate-TUFT with that of the F-T fuel as shown in Figure 4D, we found that the IBP and final boiling point of the two fuels were very close at atmospheric pressure, while in other volume fraction ranges the distillation temperature of the Surrogate-TUFT was slightly higher than that of the F-T fuel. The two most important points on the distillation curve are the IBP and the final boiling point because they represent the boiling points of the most easily vaporized and the most difficult vaporized components in the fuel mixture, respectively, which are directly related to the initial evaporation temperature and the complete evaporation temperature of mixed fuel. It can be seen that the Surrogate-TUFT can better simulate the evaporation properties of the F-T fuel.

Because the experiments were conducted at high temperature and high-pressure conditions, it is necessary to investigate the effect of ambient pressure on the fuel distillation curve. Figure 5 shows the IBP of the Surrogate-TUFT as a function of ambient pressure. With the increase in the ambient pressure, the IBP gradually increased, while the growth rate gradually slowed down.

Because C/H and LHV of the Surrogate-TUFT were very close to those of the F-T fuel, under the identical fuel-to-air ratio, their combustion temperatures were quite close.

In summary, the Surrogate-TUFT can be used as a physical surrogate fuel for the F-T fuel.
3 | EXPERIMENTAL APPARATUS

3.1 | Combustor design

The schematic diagram of the gas turbine combustor used in the present study is shown in Figure 6. The whole flame chamber was 220.3 mm in length, and its cross-section was 84.5 mm × 85.0 mm at the dome. The air was injected into the flame chamber through the swirler, primary holes, dilution holes, and cooling holes, respectively. Their effective areas occupied 17.3%, 14.0%, 17.7%, and 51% of total effective area, respectively. Under the identical chamber pressure loss, the airflow rates of each component of the flame chamber were only proportional to their effective areas. The mass flow rate of the primary zone (PZ) (occupying 42.75%) was the sum of those of the swirler, dome cooling, half of the primary holes, and cooling holes; and the mass flow rate of the combustion zone (CZ) (occupying 61.54%) was the sum of those of the swirler, dome cooling, primary holes, the chamber cooling from dome to primary holes, and half of the chamber cooling from primary holes to dilution holes.

The fuel was atomized through an airblast atomizer, composed of a pressure-swirl atomizer, counter-rotating swirler, and venturi tube. The swirler was composed of inner and outer swirler, and its total effective area was experimentally calibrated to be 200 ± 0.9 mm$^2$. The inner swirler, consisting of oblique holes to induct a velocity containing an axial velocity component, had a swirl number of 0.91. Based on the flow direction, its rotation direction was right-handed; the outer swirler, utilizing radial blades to induct a velocity not containing an axial velocity component, had a swirl number of 0.93. Based on the flow direction, its rotation direction was left-handed. The pressure-swirl atomizer was supplied through the main stage and pilot stage to obtain a hollow spray cone with a cone angle of 67°. The flow numbers of the main stage and pilot stage were 13.423 and 2.837 (kg m$^3$/Pa s$^2$)$^{0.5}$, respectively. The flow number, $F_{N_{SI}}$, was calculated through the Formula (10).

The initially atomized fuel collided with the venturi tube, resulting in the liquid film on the internal surface of the venturi tube. The liquid film was further atomized by the shear flow between the inner and outer swirlers. The small liquid drops entered the recirculation region induced by the swirled and started burning. When less fuel was required, only the pilot stage was utilized.

$$F_{N_{SI}} = \frac{\text{flow rate, kg/s}}{(\text{pressure differential, Pa})^{0.3}(\text{liquid density, kg/m}^3)^{0.5}}.$$  \hspace{1cm} (10)

3.2 | Experimental system

Figure 7 shows the schematic diagram of the experimental system utilized in the present study, which was composed of an air supply system, fuel supply system, and signals acquisition system. High-pressure air with atmospheric temperature was heated to the required temperature through the heat exchanger, and the flow rate was measured using the orifice flowmeter with an accuracy of 1%. After the uniform flow plate, the clean air entered the combustor, and its total pressure, static pressure, and static temperature at the combustor entrance were experimentally measured. The fuel in the tank compressed by high-pressure air was injected into the combustor through the main and pilot stages of the pressure-swirl atomizer after the filter to ensure the stability of the fuel supply. The fuel flow rates were measured by the Coriolis-type flowmeter with an accuracy of 1%. The burned gas sampled by the sampling probe was transferred to the gas analyzer to analyze the product concentration.

The concentration of CO and CO$_2$ was measured by SIEMENS U6 analyzer with an accuracy of ±2%, which was based on the nondivergent infrared method. The concentration of NOx was measured by a CAI-600 analyzer with an accuracy of ±0.5%, which was based on the chemiluminescence method. The concentration of UHC was measured by the BASELINE 9000 series total hydrocarbon analyzer with an accuracy of ±1%, which is based on the hydrogen flame ion detection method.

3.3 | Experimental parameters

The present study was conducted under two experimental conditions to investigate the pollutant emissions of the F-T fuel and the Surrogate-TUFT in the gas turbine combustor. Table 2 lists the experimental parameters in detail, which are designed according to two typical operating conditions of the aeroengine, namely, idle and cruise.
4 RESULTS ANALYSIS AND DISCUSSIONS

4.1 Effect of chemical dynamics of the Surrogate-TUFT on the pollutant emissions

The single PSR model in Chemkin was utilized to calculate the pollutant emissions of the Surrogate-TUFT at different equivalence ratios to analyze the effect of chemical dynamics. Although the combustion process in the real combustor is different from the chemical reaction process in a single PSR, the results of a single PSR can provide a valuable reference for analyzing the pollutant emissions in the real combustor. Based on the analysis of Ichihashi et al.,\textsuperscript{38} lots of high-temperature combustion products appeared in the PZ, while a fraction of combustion reactions still occurred in the CZ. At low...
experimental parameters, the combustion mainly occurred in the PZ due to the lower fuel-to-air ratio. Consequently, the parameters of PSR were determined according to the combustor structure and experimental parameters used in the present study, as shown in Table 3. The chemical reaction mechanism adopted the model proposed by Ranzi et al. The calculation results are shown in Figure 8.

Corresponding to the actual experimental parameters (the equivalent ratio of 0.5234 at low experimental parameters, and the equivalent ratio of 0.6545 at high experimental parameters), the EI(CO) and UHC caused by the chemical kinetics at high experimental parameters is 29.0% and 26.2% of those at low experimental parameters, respectively. However, the EI(NOx) caused by chemical kinetics at low experimental parameters is 10.8% of that at high experimental parameters.

4.2 | Experimental pollutant emissions in gas turbine combustor

Under two designed experimental parameters, the pollutant emissions of the F-T fuel and the Surrogate-TUFT in the gas turbine combustor were experimentally measured, as shown in Figure 9 where L and H refer to low and high experimental parameters, respectively. At low and high parameters, the experimental stable state lasted for 20 and 10 s, respectively. All experimental results were the average value of the experimental data at this time.

Taking the F-T fuel as the reference, at low experimental parameter, the EI(CO), EI(NOx), and EI(UHC) of the Surrogate-TUFT are higher than those of the F-T fuel by 3.6%, 1.6%, and 27.5%, respectively, and the combustion efficiency of the Surrogate-TUFT is lower than that of the F-T fuel by 0.08%; at high experimental parameter, the CO emissions of two fuels are extremely low, and the EI(NOx) and EI(UHC) of the Surrogate-TUFT are higher than those of the F-T fuel by 3.1% and 30.1%, respectively, and the combustion efficiency of the Surrogate-TUFT is lower than that of the F-T fuel by 0.03%.

4.3 | Discussion

4.3.1 | Influencing factors on the pollutant emissions

In the turbine combustor, the pollutant emissions of the F-T fuel and the Surrogate-TUFT were affected not only by the fuel's basic physical and chemical properties but also by its chemical dynamics. Because the basic physical and chemical properties and chemical dynamics of

| TABLE 3 | List of PSR parameters |
| --- | --- | --- |
| State | Low experimental parameters | High experimental parameters |
| Volume (cm$^3$) | 256.796 | 654.645 |
| Inlet mass flow rate (g/s) | 216.8 | 1053.45 |
| Inlet temperature (K) | 520 | 600 |
| Operation pressure (MPa) | 0.5 | 2.0 |

FIGURE 8 Calculated pollutant emissions of the Surrogate-TUFT at two experimental parameters as a function of equivalence ratio in PSR.
the Surrogate-TUFT have been analyzed in detail, its pollutant emissions in the turbine combustor are firstly discussed in this section. Due to the turbulence/combustion interactions, the effects of the basic physical and chemical properties and chemical kinetics on the pollutant emissions in gas turbine combustors are very difficult to analyze. Yet, we can use the results of the single PSR as a reference to obtain some qualitative conclusions.

The EI(CO) in the turbine combustor at low and high experimental parameters was 23.14 g/kg and basically zero, respectively, as shown in Figure 9A, while the EI(CO) caused by chemical dynamics at high experimental parameter (ϕ = 0.6545) was approximately 29.0% of that at low experimental parameter (ϕ = 0.5234), as shown in Figure 8A. It can be seen that there was an obvious difference in the pollutant emission trend in the turbine combustor and PSR, demonstrating that the basic physical and chemical properties had an obvious influence on the emission of CO. The high ambient pressure inhibited the fuel evaporation because the IBP increased with the increase in the ambient pressure (as shown in Figure 5), while the high ambient temperature promoted the fuel evaporation. At the low experimental parameter, the IBP was 525.6 K, and the combustor inlet temperature was 520 K; at the high experimental parameter, the IBP was 626.8 K, and the combustor inlet temperature was 600 K. It can be concluded that the evaporation conditions at the two experimental parameters were similar, and the effect of the fuel evaporation on the emission of CO can be neglected. However, at high experimental parameters, the smaller atomization SMD caused by smaller surface tension and larger air density greatly reduced the fuel vaporization time, resulting in less emission of CO.40

Figure 9A shows the ratio of the EI(NOx) at the low experimental parameter to that at the high experimental parameter in the turbine combustor, which was higher than that in the PSR, as shown in Figure 8B. The EI(NOx) in PSR caused by chemical dynamics at high experimental parameters was much higher than that at low experimental parameters. This was mainly because the emission of the thermal NOx increased with the increase in pressure and temperature. However, the smaller atomization particle size at high experimental parameters had a negative effect on the production of NOx.40 In summary, the fuel chemical kinetics, and basic physical and chemical properties simultaneously affected the EI(NOx) in the turbine combustor.

Based on the research reported by Graham et al.,41 the EI(UHC) in the turbine combustor was mainly affected by the fuel’s physical properties. The experimental results showed that the EI(UHC) at high experimental parameter was approximately 44.0% of that at low experimental parameter as shown in Figure 9A which was mainly affected by the atomization particle size.

4.3.2 Pollutant emission comparisons between the F-T fuel and the Surrogate-TUFT

As for the turbine combustor, each emission index of the Surrogate-TUFT was slightly higher than that of the F-T fuel. This was because the Surrogate-TUFT provided a very close atomization particle size while slightly lower vaporization compared with the F-T fuel under identical conditions. Except for the UHC emission, the differences in other emission indexes were all limited to 4% between the two fuels. Consequently, the Surrogate-TUFT can predict the EI(CO) and EI(NOx) of the F-T fuel well, and the difference in the vaporization did not cause an obvious difference in the EI(CO) and EI(NOx).

The UHC emission of the Surrogate-TUFT was higher than that of the F-T fuel by approximately 30% in the turbine combustor, which may be caused by the
difference in the vaporization. At atmospheric pressure, the distillation temperature of the Surrogate-TUFT was higher than that of the F-T fuel by 30 K at maximum. To better predict the UHC emission of the F-T fuel in the turbine combustor, the surrogate fuel should provide a good prediction of not only the atomization process but also the distillation curve.

5 CONCLUSION

Based on analyzing the combustion processes of liquid fuel in gas turbine combustors, we propose that the comprehensive surrogate fuel should be developed according to the basic physical and chemical properties that affect the diffusion combustion process. The present study selects C/H, MW, density, viscosity, surface tension, IPB, and LHV as the target properties. The candidate components are n-decane, n-tetradecane, iso-octane, and MCH. The optimal direction method is utilized to obtain the mixture component ratio which minimizes the deviation in the basic physical and chemical properties compared with the F-T fuel. This mixture, taken as the comprehensive surrogate fuel in the present study named Surrogate-TUFT, was composed of 15% n-decane, 67% n-tetradecane, 13% iso-octane, and 5% MCH in mole fraction. Furthermore, the pollutant emissions of the two fuels in the turbine combustor are also experimentally investigated and some useful conclusions are obtained as follows:

1. The atomization particle size has an important effect on the emission of CO, and the EI(CO) decreased with the decrease in the atomization SMD.
2. The thermal EI(NOx) increased with the increase in the pressure and temperature, while the smaller atomization particle size decreases the EI(NOx).
3. In the turbine combustor, the Surrogate-TUFT can predict the EI(CO) and EI(NOx) of the F-T fuel well, and the difference in the vaporization does not cause an obvious difference in the EI(CO) and EI(NOx).
4. The difference in UHC emission of the Surrogate-TUFT and the F-T fuel in the turbine combustor is mainly influenced by the fuel evaporation property.

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