THE EFFECTS OF INLET AIR QUANTITY AND INLET OXYGEN MOLE FRACTION ON THE COMBUSTION AND FLUID FLOW IN A SULFUR RECOVERY UNIT THERMAL REACTOR

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ABSTRACT

Owing to the high temperature inside a sulfur recovery unit (SRU) thermal reactor, detailed experimental measurements are difficult. In the author's previous studies, several methods have been assessed to resolve the abnormality of the SRU thermal reactor under high temperature operation. This paper presents a new easier and more economical method. The effects of inlet air quantity and inlet O_2 mole fraction on the combustion and fluid flow in a SRU thermal reactor are investigated numerically. The flow field temperature, S_2 recovery, H_2S mole fraction, and SO_2 emissions are analyzed. This paper provides a guideline for adjusting the inlet air quantity and the inlet O_2 mole fraction to reduce the high temperature inside a thermal reactor and to ensure an acceptable sulfur recovery.

Keywords: SRU thermal reactor; inlet air quantity; inlet oxygen mole fraction; S_2 recovery; H_2S destruction; SO_2 emission; thermal reactor temperature.

EFFETS DE LA QUANTITÉ D'ENTRÉE D'AIR ET D'ENTRÉE DE LA FRACTION MOLAIRE D'OXYGÉNE SUR LA COMBUSTION ET L'ÉCOULEMENT DU FLUIDE DANS UN RÉACTEUR THERMIQUE À RÉCUPÉRATION DE SULFURE

RÉSUMÉ

En raison des températures élevées à l'intérieur d'une unité de récupération de sulfure d'un réacteur thermique, les mesures expérimentales détaillées sont difficiles à prendre. Dans des études précédentes de l'auteur, plusieurs méthodes ont été évaluées pour résoudre les anomalies d'un réacteur thermique soumis à des opérations à température élevée. Nous présentons une méthode nouvelle plus facile et plus économique. Les effets de la quantité d'air introduit et la fraction molaire O_2 sur la combustion et le débit du fluide dans le réacteur thermique sont étudiés d'un point de vue numérique. La température du champ d'écoulement, la récupération de S_2, la fraction molaire H_2S et les émissions de SO_2 sont analysées. Cet article apporte une ligne de conduite pour l'ajustement de la quantité d'air d'entrée, et l'entrée de la fraction molaire O_2 pour réduire l'élévation de la température à l'intérieur d'un réacteur thermique et assurer la récupération acceptable de sulfure.

Mots-clés : réaction thermique SRU; quantité d'entrée d'air; entrée de l'oxygène de fraction molaire; récupération; destruction de H_2S; émissions de SO_2; température d'un réacteur thermique.

NOMENCLATURE

C_f	skin friction coefficient
C_μ	turbulence model constant (= 0.09)
k	turbulence kinetic energy (m^2/s^2)
L	hydraulic diameter (m)
l	characteristic length (m)
T	temperature (K)
XYZ	Cartesian coordinates with origin at the centroid of the burner inlet (m)
Greek symbols	
ε	turbulence dissipation rate (m^2/s^3)

1. INTRODUCTION

A sulfur recovery unit (SRU) thermal reactor is perhaps the most important equipment in sulfur plant. It converts the ammonia, hydrogen sulfide and hydrocarbons in the reactants into sulfur. Most of the sulfur elements are recovered from the SRU thermal reactor.

Owing to the high temperature inside a SRU thermal reactor, detailed experimental measurements are difficult. Existent researches of the SRU thermal reactors have been reviewed in previous studies [1–5]. They are concentrated on the discussions of practical operation problems. On the other hand, numerical simulations can give detailed informations inside a power or an energy system. A recent application of the numerical simulation to a power system has been performed by Boretti [6], who investigated the operation of a liquefied petroleum gas (LPG) engine fitted with Direct Injection (DI) and Jet Ignition (JI). In the author's previous studies, several methods have been assessed to resolve the abnormality of the SRU thermal reactor under high temperature operation and to improve the recovery of sulfur, including (1) changing the choke ring dimensions [1], (2) changing the choke ring position [2], (3) modifying the geometry of the zone 1 corner to a streamlined geometry [3, 4] and (4) replacing the choke ring by a vector wall [5]. However, these methods are either expensive or require an overhaul of the SRU thermal reactor. This paper presents a new easier and more economical method. The effects of inlet air quantity and inlet O_2 mole fraction on the combustion and fluid flow in a SRU thermal reactor are investigated numerically. Practical operating conditions from a petrochemical corporation in Taiwan are used as the design conditions for the discussion. Configuration and dimensions of the first section of a sulfur recovery unit for a typical petroleum refinery have been shown in [1, 2].

The remaining sections of this paper are divided as follows: Section 2 discusses the numerical methods and physical models, in Section 3 results and discussion are presented, and Section 4 gives the conclusions.

2. NUMERICAL METHODS AND PHYSICAL MODELS

The main chemical reactions in a SRU thermal reactor include a thermal step and a catalytic step.

$$2H_2S + 3O_2 \rightarrow 2SO_2 + 2H_2O$$

$$2H_2S + SO_2 \rightarrow 3S + 2H_2O$$

In addition to the above reactions and the combustion of hydrocarbon fuels, other chemical reactions taking place in a SRU thermal reactor are

$$2NH_3 + 1.5O_2 \rightarrow N_2 + 3H_2O$$

$$2NH_3 + SO_2 \rightarrow N_2 + H_2S + 2H_2O$$

In this study, the FLUENT commercial code [7] is employed to simulate the reacting and fluid flow in a SRU thermal reactor. The SIMPLE algorithm by Patankar [8] is used to solve the governing equations. The discretizations of convection terms and diffusion terms are carried out by the power-law scheme and the central difference scheme, respectively. In respect of physical models, considering the accuracy and stability of the models and referring to the evaluation of other researchers, the standard k-ε model [9], P-1 radiation model [10] and non-premixed combustion model with β-type probability density function [11] are adopted for turbulence, radiation and combustion simulations, respectively. The standard wall functions [12] are used to resolve the flow quantities (velocity, temperature, and turbulence quantities) at the near-wall regions. Detailed governing equations and convergence criterion were described in [13].

In this study, the numerical model of a SRU thermal reactor is constructed using an unstructured grid. Five cell densities (10,826 cells, 187,354 cells, 342,856 cells, 683,672 cells and 1,124,627 cells) are tested to ensure a grid-independent solution. The computational results show that the sizes of the corner recirculation zone in zone 1 and zone 2 and the cross-sectional average temperature profiles obtained using the last two meshes almost coincide, with a deviation of less than 0.5%. Therefore, the mesh of 683,672 cells is used for the subsequent discussion. The numerical model for the SRU thermal reactor investigated and an illustration of the heat exchanger tubes have been shown in [1, 2].

The heat absorption rate for each heat exchanger tube is 40,000 W/m2 and the other walls are adiabatic. No slip condition is applied on any of the solid walls. The exit of the heat exchanger section is connected to other equipment at 300K and 1 atm by a pipe that is 1.372 m in diameter and 11.5 m in length.

3. RESULTS AND DISCUSSION

In this study, two types of oxygen supplies are investigated: an oxygen-normal supply and an oxygen-rich supply. The design conditions (including the species compositions, the temperature, the pressure and the velocity) at the acid gas inlet holes of zone 1 and zone 2 and at the air inlet hole have been tabulated in [1, 2]. These conditions are practical operating conditions that are used by a petrochemical corporation in Taiwan. The turbulence kinetic energy is 10% of the inlet mean flow kinetic energy and the turbulence dissipation rate is computed using

$$\varepsilon = C_\mu^{3/4} \frac{k^{3/2}}{l}, \tag{1}$$

where $l = 0.07L$ and L is the hydraulic diameter.

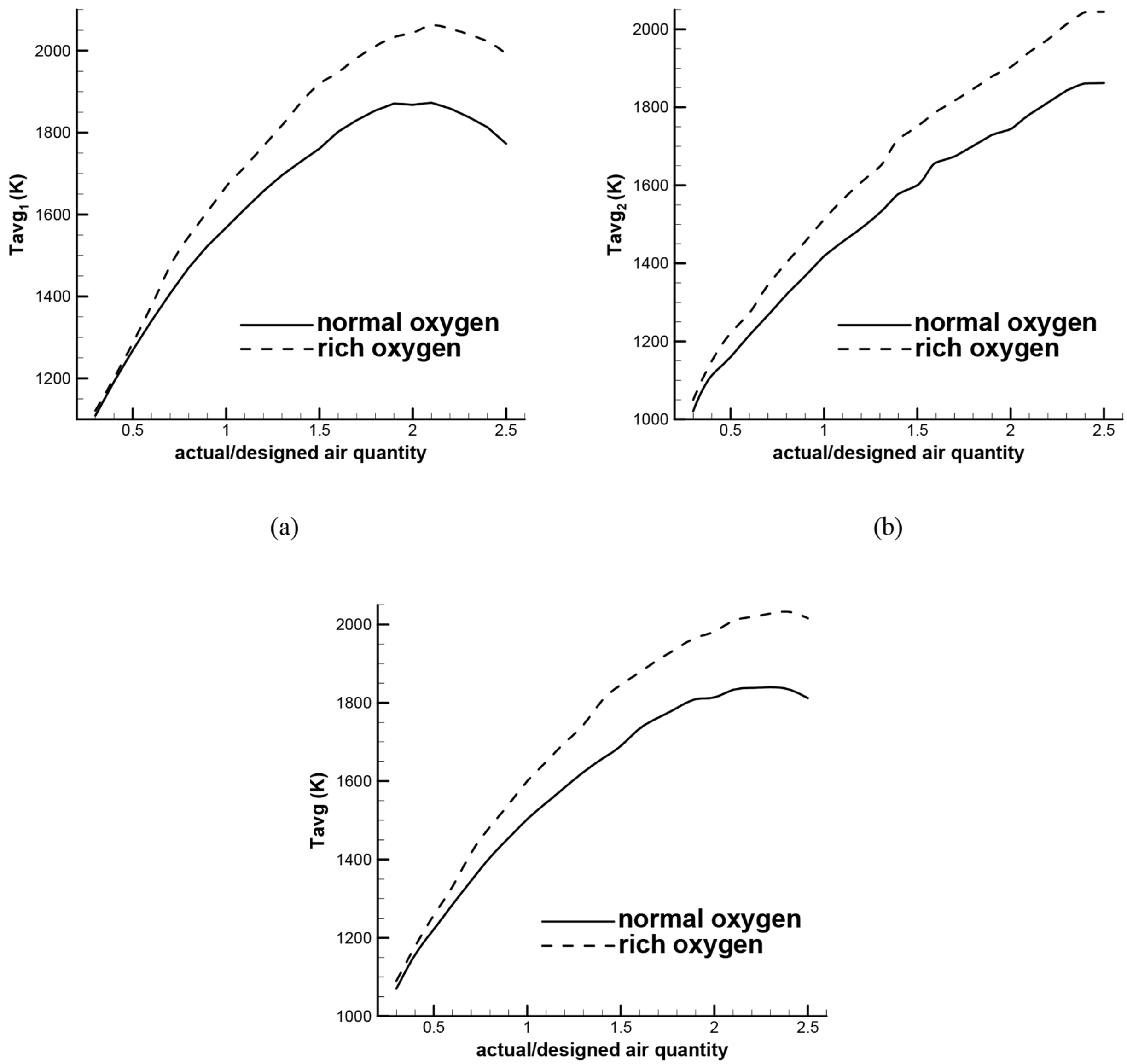
To validate the numerical methods used in this study, the simulation results were compared with available practical data. The exit S_2 mole fractions from the SRU thermal reactor of a petrochemical corporation in Taiwan were measured at the design conditions. It has been shown in [1, 2] that the respective deviations are 1.3% for an oxygen-normal supply and 8.3% for an oxygen-rich supply, which are acceptable from a viewpoint of engineering applications.

3.1. The Effect of the Inlet Air Quantity

Figures 1 and 2 show a comparison of the temperature and the species mole fraction for a SRU thermal reactor with different inlet air quantities. The inlet air quantities range from 0.3–2.5 times the design inlet air quantity, but the fuel (acid gas to zone 1 and zone 2) is maintained at the design conditions.

Figure 1 shows that the temperature increases as the inlet air quantity increases, until a maximum temperature is reached at about 2.2 times the design inlet air quantity. This demonstrates that the design conditions are fuel-rich (or air-lean) conditions.

Figure 2(a) shows that the H_2S mole fraction decreases as the inlet air quantity increases because more H_2S is converted to S_2 due to the higher temperature when the inlet air quantity increases. However, Fig. 2(b) shows that S_2 recovery reaches a maximum value at almost 0.9 times the design inlet air quantity. This is



(c)

Fig. 1. A comparison of the temperature for a SRU thermal reactor for different inlet air quantities: (a) the average temperature in zone 1; (b) the average temperature in zone 2; (c) the average temperature in the thermal reactor.

because S_2 can also react with air to form SOx at higher temperatures. This is seen in Fig. 2(c), which shows that SO_2 emissions increase as the inlet air quantity increases, because a larger inlet air quantity produces a higher temperature. The design conditions produce an almost optimal S_2 recovery. Figure 2(b) also shows that an oxygen-rich supply increases S_2 recovery because there is a more complete chemical reaction. SO_2 emissions are also greater for an oxygen-rich supply because the temperature is higher, as shown in Fig. 2(c).

It is seen that when the inlet air quantity increases by 10%, the temperature increases by about 50°C for an oxygen-normal operation, but for an oxygen-rich operation, the temperature increases by about 60°C because there is more oxygen. The current design conditions allow an almost optimal S_2 recovery.

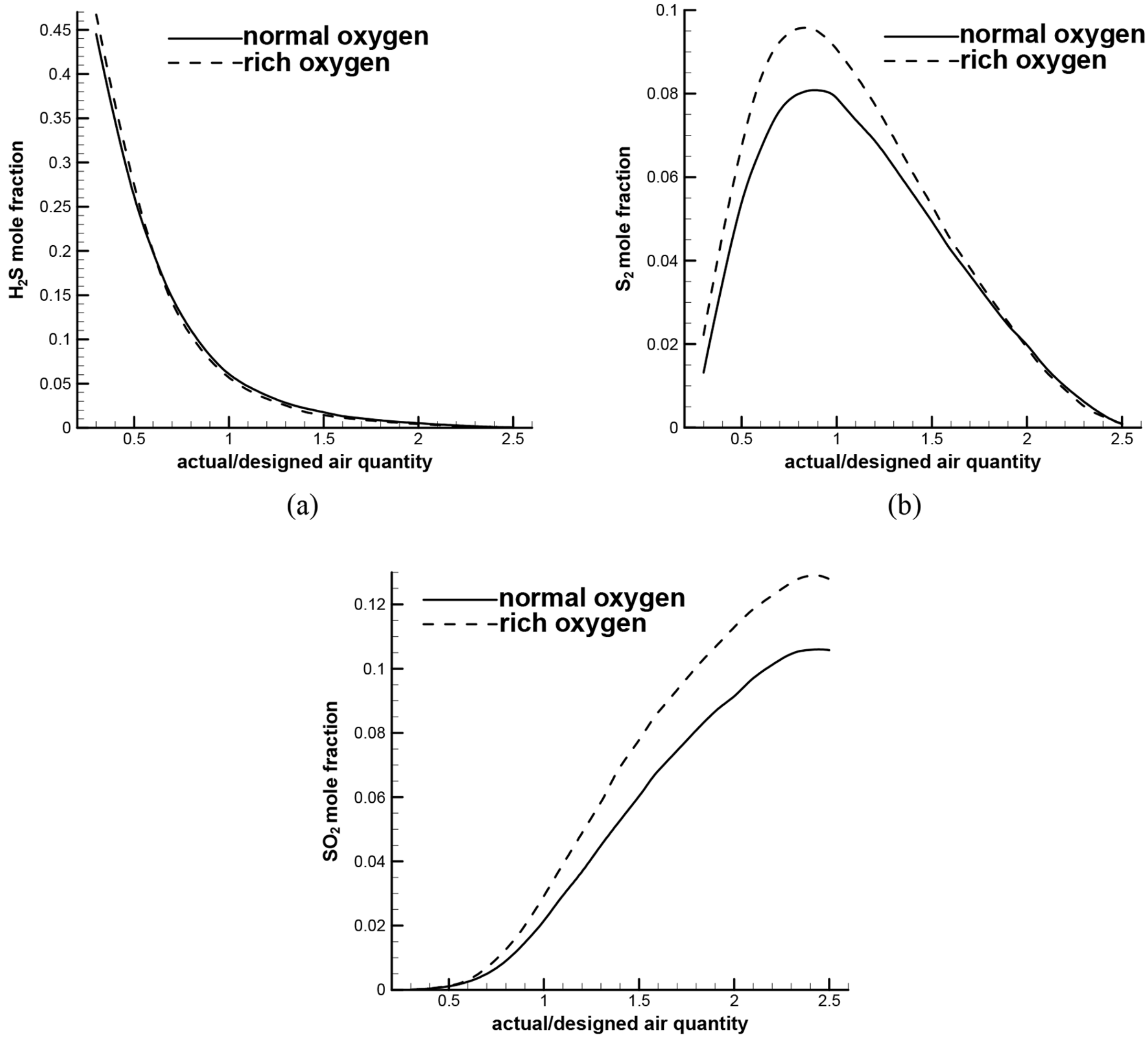


Fig. 2. A comparison of the species mole fraction for a SRU thermal reactor with different inlet air quantities: (a) the H_2S mole fraction at the exit; (b) the S_2 mole fraction at the exit; (c) the SO_2 mole fraction at the exit.

3.2. The Effect of the Inlet O_2 Mole Fraction

Figures 3 and 4 show a comparison of the temperature and the species mole fraction for a SRU thermal reactor with different inlet O_2 mole fractions. The inlet O_2 mole fractions range from 0.16–0.25. For inlet O_2 mole fractions less than or equal to 0.2 (lean oxygen), the inlet air quantity is equal to the oxygen-normal case. For inlet O_2 mole fractions greater than 0.2 (oxygen-rich), the inlet air quantity is equal to the oxygen-rich case. The fuel (acid gas to zone 1 and zone 2) conditions are maintained at the design conditions.

Figure 3 shows that the temperature increases monotonically as the inlet O_2 mole fraction increases because there is a more complete chemical reaction. Figures 3(b)–(d) show that the average temperature for an inlet O_2 mole fraction of 0.21 is lower than that for an inlet O_2 mole fraction of 0.2 because the inlet air quantity for the oxygen-rich case is less than that for the oxygen-normal case. As mentioned in [1, 2,

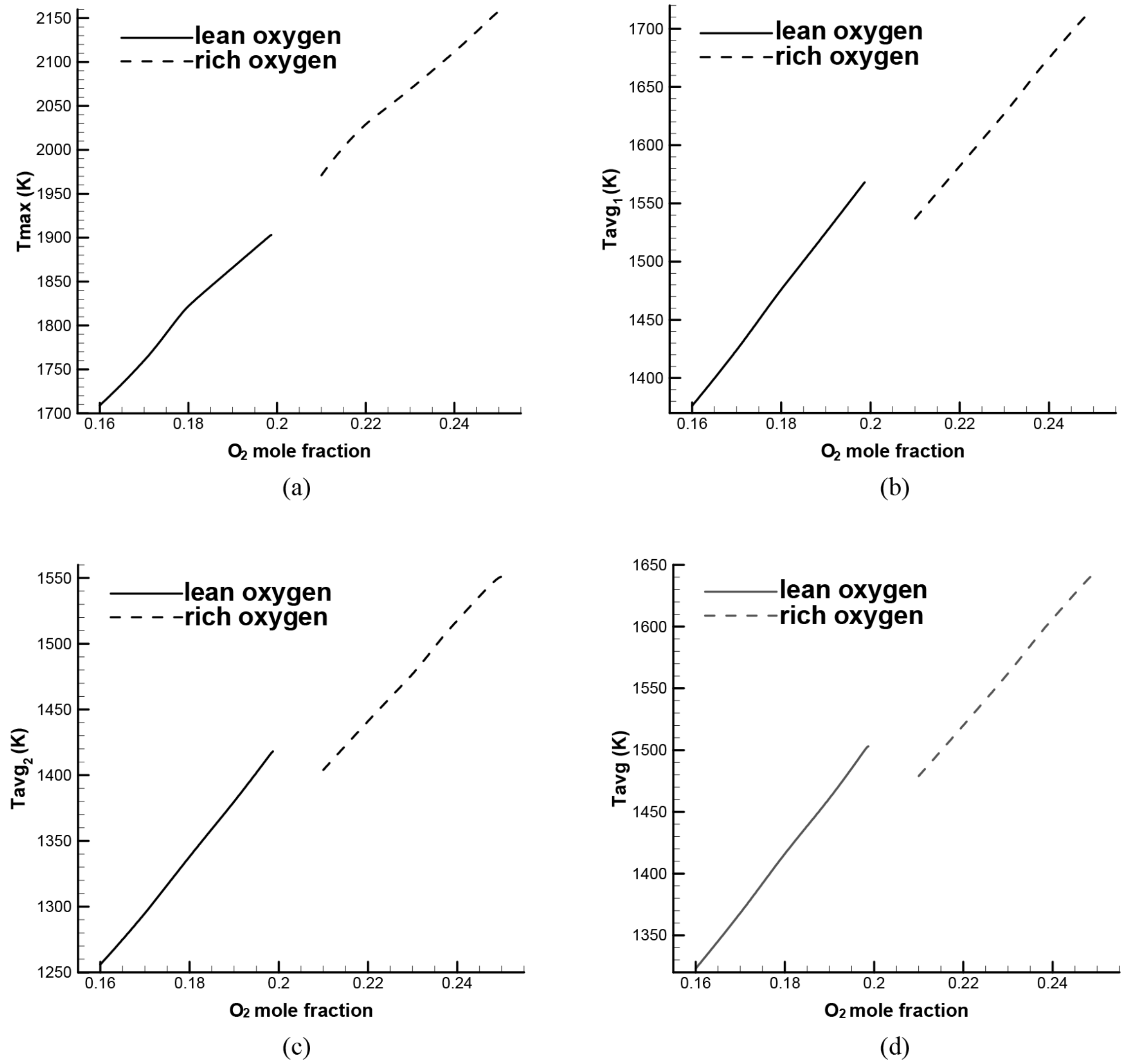
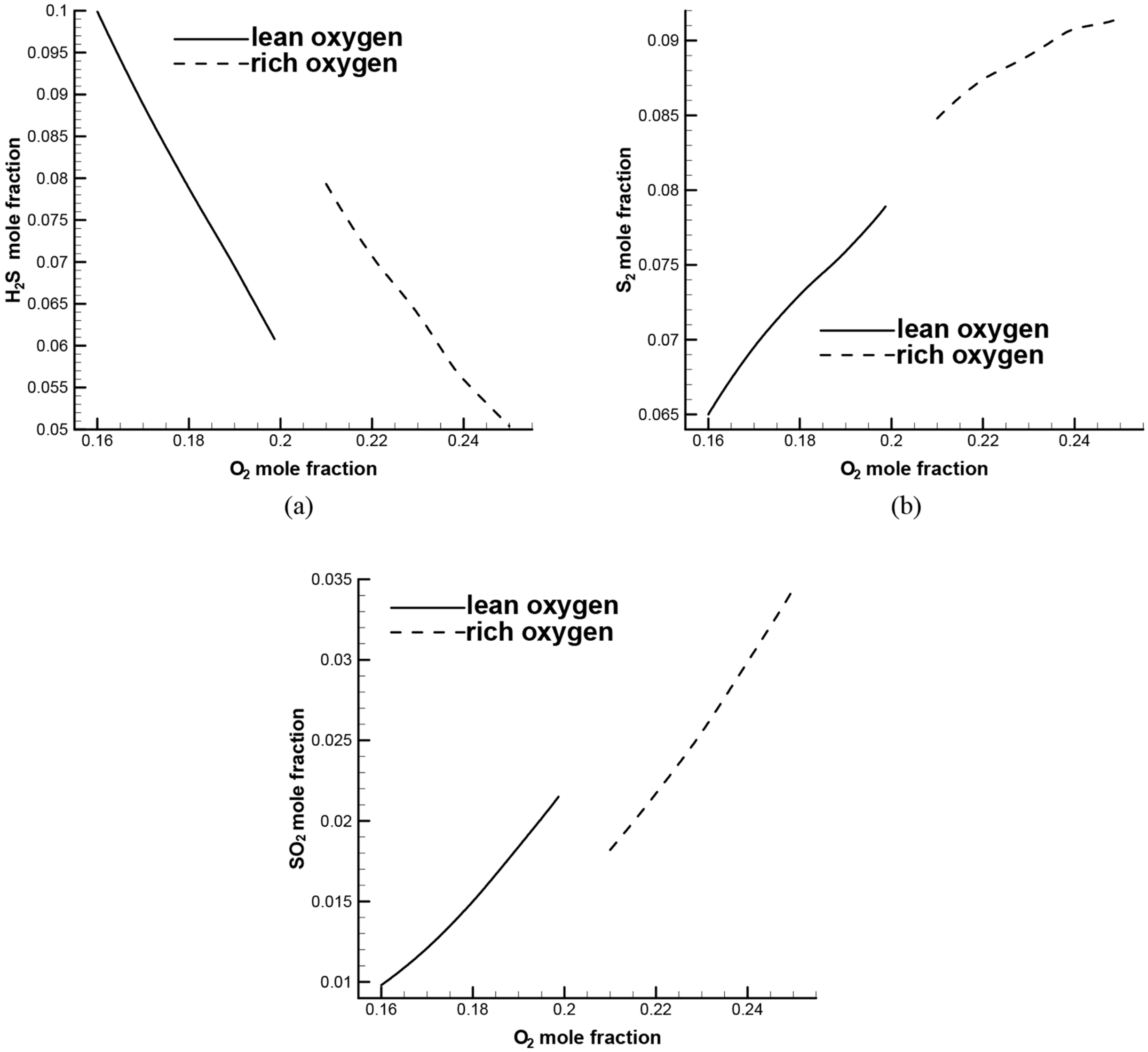


Fig. 3. A comparison of the temperature for a SRU thermal reactor with different inlet O_2 mole fractions: (a) maximum temperature; (b) the average temperature in zone 1; (c) the average temperature in zone 2; (d) the average temperature in the thermal reactor.

4], a typical value for the maximum service temperature of the refractory is 1700°C (≈1973K). Figure 3(a) shows that the local maximum temperature exceeds the suggested maximum service temperature for the oxygen-rich cases, although the average temperature is acceptable. Therefore, a high temperature region such as zone 1 corner must be inspected very carefully during the annual maintenance period if there is an oxygen-rich operation.

Figure 4(a) shows that the H_2S mole fraction decreases monotonically as the inlet O_2 mole fraction increases, but Fig. 4(b) shows that S_2 recovery increases as the inlet O_2 mole fraction increases. More H_2S is converted to S_2 when the inlet O_2 mole fraction increases because the temperature is higher and there is a more complete chemical reaction. However, Fig. 4(b) shows that S_2 recovery mitigates for larger inlet O_2 mole fractions because S_2 can also be converted to SOx at higher temperatures. Figure 4(c) shows that SO_2 emissions increase monotonically as the inlet O_2 mole fraction increases because the temperature is higher.



(c)

Fig. 4. A comparison of the species mole fraction for a SRU thermal reactor with different inlet O_2 mole fractions: (a) the H_2S mole fraction at the exit; (b) the S_2 mole fraction at the exit; (c) the SO_2 mole fraction at the exit.

In a practical SRU thermal reactor, high temperatures can damage the refractory. In this case, the temperature must be reduced. It is seen that when the inlet O_2 mole fraction decreases by 0.01, the temperature decreases by about 45°C and S_2 recovery and SO_2 emissions decrease by about 3 and 14%, respectively, relative to the design conditions.

4. CONCLUSIONS

This paper numerically investigates the effects of inlet air quantity and inlet O_2 mole fraction on the combustion and fluid flow in a SRU thermal reactor in order to provide a guideline for adjusting the operating conditions to reduce the temperature inside the thermal reactor and to allow an acceptable sulfur recovery.

From the simulation results, the following is concluded:

1. When the inlet air quantity increases by 10%, the flow field temperature increases by about 50°C for an oxygen-normal operation, but for an oxygen-rich operation, the temperature increases by about 60°C. The flow field temperature increases as the inlet air quantity increases, until a maximum temperature is reached at about 2.2 times the design inlet air quantity. The S_2 recovery reaches maximum efficiency at almost 0.9 times the design inlet air quantity. The current design conditions result in an almost optimal S_2 recovery. The H_2S mole fraction decreases as the inlet air quantity increases, but the SO_2 emissions increases as the inlet air quantity increases.

2. When the inlet O_2 mole fraction decreases by 0.01, the temperature decreases by about 45°C, but S_2 recovery and SO_2 emissions decrease by about 3 and 14%, respectively, relative to the design conditions. The flow field temperature, S_2 recovery and SO_2 emissions increase as the inlet O_2 mole fraction increases, but the H_2S mole fraction decreases as the inlet O_2 mole fraction increases. However, S_2 recovery mitigates for larger inlet O_2 mole fractions.

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