



## Full Length Article

# Prediction of hot coke oven gas reforming by LES coupled with the extended flamelet/progress variable approach

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## ABSTRACT

Large-eddy simulation (LES) coupled with the extended flamelet/progress variable approach (EFPV) has been performed to predict characteristics of reacting flows in a bench-scale hot coke oven gas (HCOG) reformer. In order to investigate the capability of capturing effects of operating conditions, simulations were carried out in two different cases in which the coke oven gas temperature and oxygen ratio were altered. Results showed that the LES coupled with the EFPV performed very well in terms of predicting temperature distribution as well as the temperature variation trend between the two cases. In addition, major species such as H<sub>2</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O and CH<sub>4</sub>, as well as minor species like benzene and some typical polycyclic aromatic hydrocarbons (PAH) were analyzed to illustrate their activities and dominant chemical events. With regards to the composition of the dry reformed gas, comparisons were made between the experimental data and the numerical simulation results, and reasonable results have been obtained. It has been confirmed that the general feature of the reacting flows in the HCOG reformer can be precisely captured by the present LES.

## 1. Introduction

Besides searching energy alternatives, it is of great significance to make the most of the available energy resource to cope with the energy challenge. According to the data from World Coal Association, nowadays, 70% of steel production all over the world uses coal [1]. In the coking process of steel mills, considerable coke oven gas as a by-product was generated [2], and various routes of its utilization were reported [3]. Recently, utilization of the HCOG attracts increasing attention. Many researchers devoted to exploring effective and efficient methods through considerable experiments [4–9]. Other than experimental study, researchers also made effort to get a deeper insight into the chemical mechanism and fluid dynamics by means of simulations [9–13].

Taking advantage of catalyst makes it possible to convert the HCOG at a relatively mild operating condition, as well as obtain a high conversion rate. However, the occurrence of the sulfur poisoning and carbon plugging makes the catalyst-bed vulnerable. Gradually deactivation results in a decrease of conversion efficiency, and thus put this method at a disadvantage. Although non-catalytic reforming of COG requires a more strict reaction condition compared with those who used catalyst, HCOG allows researchers to utilize the heat in the feedstock.

Onozaki et al. made the use of the heat from the hot gas, which was 1050K, to drive the reaction and reformed the HCOG partially oxidized without relying on any catalyst [7]. Higher than 98% carbon conversion rate was achieved, and three to five times more H<sub>2</sub> and CO than feedstock were obtained. Also, the technology was proved to be lower cost and higher efficiency than separating cold coke oven gas in the conventional method.

Jess explored the kinetics of the thermal conversion of modeled coke oven gas in a tubular flow reactor [8]. Hydrogen, steam, naphthalene, toluene, and benzene were used as model compounds. Based on his experimental data, Norinaga et al. performed a detailed chemical kinetic modeling approach to simulate the thermal conversion rate of this modeled coke oven gas and it was proved to be reliable [10]. They also attempted to use this detailed chemical kinetic model to predict non-catalytic partial oxidation of HCOG, and the influence of oxygen concentration in the inlet gas mixture was investigated [11]. In the meanwhile, Norinaga et al. developed a reforming technology of HCOG to obtain products which were suitable for methanol production [9]. They operated a tubular reactor with four oxygen injectors installed, which was also used in our present study, to partially oxidize the HCOG and had identified the most suitable reforming conditions. Based on their work, coupling with a detailed kinetic chemical model consisting

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2216 reactions with 257 species, a plug flow model and a one-dimensional axial diffusion model were employed by Appari et al. to simulate the reaction flow of partially oxidized HCOG reforming [12]. Both temperature along the axial length of the reactor and species concentration of the reactor outlet predicted by the models shared good agreement with the experimental data. However, this research was on the premise of one-dimensional simulation and some ideal assumptions. In order to capture the features of reacting flow under a more realistic flow condition, Li et al. implemented a three-dimensional CFD simulation [13]. A reduced chemical mechanism with 410 reactions and 47 species was employed. Although satisfactory prediction of major gas species composition was obtained, they treated tarry constituents only by benzene which cannot present features of tar very well. Therefore, events of tarry species were uncovered and are waiting to be excavated. When it comes to reproducing temperature distribution, they used an adiabatic thermal boundary condition which is not that realistic, and also they conceded that the Reynolds-average Navier–Stokes (RANS) model has its limitation.

Recently, large-eddy simulation has been significantly paid attention to capture the phenomenon which is essentially unsteady, such as combustion. Large-eddy simulation is capable to represent the instantaneous events and the fluctuation. Moreover, it uses fewer adjustable parameters compared with RANS model which brings out better applicability for different cases or systems.

In LES modeling of single-phase as well as spray combustion, a series of flamelet-based models have gained widespread popularity [14–18]. The flamelet models enable researchers to get access to the fully detailed chemical mechanism. In addition, optimized and efficient of tabulated techniques provide a mapping of flamelet library in turbulent flow simulations [19], which greatly reduces computational cost.

Pierce and Moin [20] originally extended diffusion flamelet model to FPV which can overcome the ambiguity of the classical steady diffusion flamelet model. The mixture fraction ( $Z$ ) along with the progress variable ( $C$ ) which is a substitute for the scalar dissipation rate ( $\chi$ ) in the classical steady flamelet model are used as tracking scalars to determine the values of variables in the physical space. And diffusion flamelet models are still being developed with great potential [21–24].

The purpose of this study is to investigate the detailed behaviors of the HCOG reforming reacting flow by means of LES coupled with the EFPV. In this paper, a three-dimensional numerical simulation for bench-scale HCOG reforming which is noncatalytic and partially oxidized is presented. Two cases are examined to ensure the reliability of the simulation executed in this work. Temperature and temperature variation trend between the two cases, as well as temperature deviation between the measured data and simulation results are represented. Behaviors of major species such as  $O_2$ ,  $H_2$ ,  $CO$ ,  $CO_2$ ,  $H_2O$  and  $CH_4$  in the reformer are discussed. Additionally, major chemical events are

analyzed. And concentrations of minor aromatic species like benzene and typical PAH species are displayed. Moreover, comparisons between numerical results and measured experimental data concerning the exit major species compositions are presented.

## 2. Computational setup and numerical methods

### 2.1. Governing equations

The governing equations considered for the partial oxidation reforming process are presented in the Eqs. (1)–(6) in the order of mass, momentum, energy, mixture fraction, progress variable and PAH species mass fraction conservation, respectively.

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}}) = 0 \tag{1}$$

$$\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) = -\nabla \bar{p} + \nabla \cdot \bar{\boldsymbol{\sigma}} + \nabla \cdot \bar{\boldsymbol{\tau}} \tag{2}$$

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{h}) = \nabla \cdot (\bar{\rho} \tilde{D}_h \nabla \tilde{h}) + \nabla \cdot \mathbf{q}_h \tag{3}$$

$$\frac{\partial \bar{\rho} \tilde{Z}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{Z}) = \nabla \cdot (\bar{\rho} \tilde{D}_Z \nabla \tilde{Z}) + \nabla \cdot \mathbf{q}_Z \tag{4}$$

$$\frac{\partial \bar{\rho} \tilde{C}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{C}) = \nabla \cdot (\bar{\rho} \tilde{D}_C \nabla \tilde{C}) + \nabla \cdot \mathbf{q}_C + \bar{\rho} \tilde{\omega}_C \tag{5}$$

$$\frac{\partial \bar{\rho} \tilde{Y}_{pi}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{Y}_{pi}) = \nabla \cdot (\bar{\rho} \tilde{D}_{Y_{pi}} \nabla \tilde{Y}_{pi}) + \nabla \cdot \mathbf{q}_{Y_{pi}} + \bar{\rho} \tilde{\omega}_{pi} \tag{6}$$

Here  $\rho$  is density,  $\mathbf{u}$  is velocity vector,  $p$  is pressure,  $\boldsymbol{\sigma}$  is stress tensor,  $\boldsymbol{\tau}$  is SGS stress,  $Z$  is mixture fraction, while  $h$  is specific total enthalpy.  $D$  and  $\mathbf{q}$  are diffusion coefficient and subgrid-scale term, respectively.  $\omega_C$  and  $\omega_{pi}$  are production rate for progress variable and PAH species  $i$ , respectively.  $C$  is progress variable. There are various definitions of  $C$  [25], and it is defined by the summation of product species  $CO_2$ ,  $CO$ ,  $H_2$  and  $H_2O$  in this study [26,27]. Moreover,  $\bar{\cdot}$  and  $\tilde{\cdot}$  denote the LES filtering and Favre averaging, respectively.

The source term for PAH species will be described in section 2.2.2, while the detailed expression for other source and turbulent transport terms can be found in the literature [28,20,29].

The LES solver used in this study is FFR-Comb (NuFD/FrontFlowRed extended by Kyushu University, Kyoto University, CRIEPI and NuFD) [30–33].

### 2.2. Computational details

#### 2.2.1. Computational domain

The computational domain for the HCOG reformer is designed to

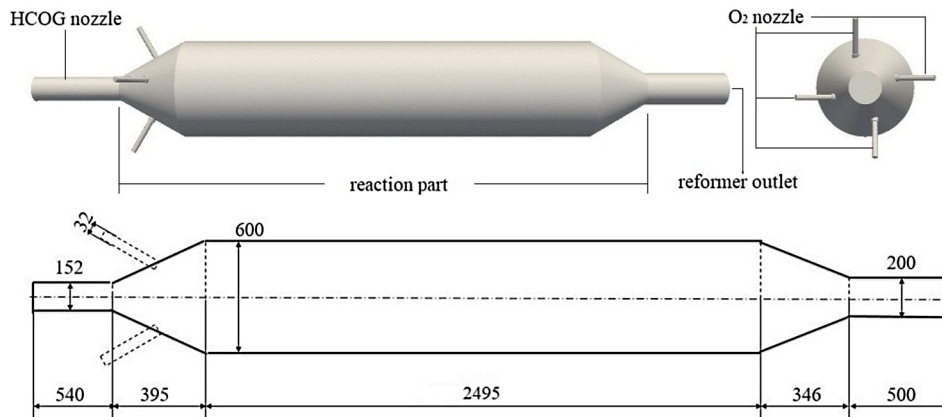


Fig. 1. Geometry of HCOG reforming reactor (unit: mm).

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