



Simulation of industrial-scale gas quenching process for partial oxidation of nature gas to acetylene



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HIGHLIGHTS

- Simulate the industrial-scale gas quenching reactor of jet-in-cross-flow by CFD coupled detailed chemical mechanism.
- Compare predicts of interaction of turbulence and reaction with PDF and EDC model.
- Evaluate the effect of mass flow ratio on mixing and quenching performance.
- Acetylene hydrogenation to ethylene is responsible for acetylene depletion.

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ABSTRACT

In the water quenching process for partial oxidation (POX) of nature gas to acetylene, the temperature of the product gas mixture directly decreases from about 1800 K to 360 K, thus the heat cannot be recovered. To overcome this problem, a new gas quenching process of jet-in-cross-flow (JICF) was proposed for the partial oxidation (POX) process to enhance the energy efficiency. The computational fluid dynamics (CFD) coupled with detailed chemistry was employed to simulate the mixing and quenching performance in an industrial-scale JICF reactor. Both the Probability Distribution Function (PDF) and Eddy Dissipation Concept (EDC) models were used to compute the chemical source term, and the PDF model predicted a higher acetylene loss. The uniform index (UI), temperature, species concentrations and acetylene loss were investigated during the quenching process. Using the PDF, the optimum main/jets flow mass ratio was determined as 2.59, at which the loss percent of acetylene was about 3 wt%. The simulation results show that the gas quenching process is very attractive because the heat can be effectively recovered after the quenching at a cost of slight loss of acetylene.

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1. Introduction

The shale gas production has developed fast, with the annual growth increasing from 2.7% in 1995–2000 to 47.9% in 2005–2011 [1]. Shale gas is estimated to provide up to 50% of the natural gas production in 2040 [2]. The abundant resource and low price make natural gas very attractive as petrochemical feedstock to produce basic chemicals [3,4]. The partial oxidation (POX) of natural gas is the major process for the production of acetylene and synthesis gas, which requires quick quenching to get the maximum yield of acetylene [5–7]. The water quenching [8,9] is used in most of the industrial POX process, and the oil quenching [8,10,11] has been tested in a demonstration scale. The water quenching process uses water as the quenching medium and the temperature of gas

mixture decreases rapidly from 1800 K to 360 K in milliseconds. Although a high yield of acetylene is achieved, the vast reaction heat is wasted, resulting in a high energy consumption. The oil quenching process uses aromatic oil with a high boiling point as the quenching medium and increases the terminal temperature to 470–520 K, which improves the energy efficiency [8] but results in a complicated composition of the product gas and needs more a complex separation process. In our previous work [12–14], a new technology has been proposed that the syngas produced in the process can be used as the direct quenching medium. By mixing the syngas of 50–100 °C with the hot reacting gas, the reacting gas can be cooled to 400–600 °C in a few milliseconds so that the acetylene consumption reactions are quickly quenched to give a high acetylene yield. The heat recovery efficiency will be much higher than that of the water quenching approach due to the higher termination temperature. Uebel et al. [15,16] developed a new quenching concept for entrained-flow gasifiers in order to increase the H₂/CO ratio within the quench vessel and thereby minimize

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efforts in the subsequent catalytic water-gas shift reaction (WGSR). To achieve this target, steam instead of water was injected into the quench chamber to realize CO conversion via homogeneous WGSR. They further performed a CFD-based multi-objective optimization of this quench conversion reactor.

In [14], the jet-in-cross-flow (JICF) and impinging flow configurations for the gas quenching process were studied by CFD simulations using detailed chemistry. The results showed that the gas quenching process was feasible for the POX process and the acetylene loss was slightly lower with the impinging flow configuration. To achieve fast mixing of fluids, the JICF configuration has been extensively studied by many researchers concerning the effect of size, shape, spacing and number of jets and the ratio of main and jetting flows on the mixing characteristics [17–22].

In the methane POX process, the most important and value-added product is acetylene, which is an intermediate species and will be consumed if the quenching is not quick enough. For a better evaluation of the gas quenching process, further works are needed to get reliable and quantitative results. Because the gas quenching process involves the complex interaction between turbulent mixing and millisecond reactions, accurate experiments are very challenging. Computational fluid dynamics (CFD) simulations using detailed chemistry are efficient to predict the fields of velocity, temperature and species concentrations, quantitatively analyze the quenching efficiency, and optimize the reactor design and operation parameters.

To calculate the finite-reaction rate in turbulent combustion flame, the PDF [23,24] and eddy dissipation concept (EDC) models [25–27] are both widely used in the literature. The PDF method provides an effective solution to the closure problem that arises from Reynolds averaging nonlinear chemical source terms in the instantaneous governing equations [28]. Xu and Pope [29] showed that the PDF model had a good ability of predicting the local extinction and reignition behaviors in piloted-jet flames of methane [29]. Liu et al. [7] and Zhang et al. [6] used the PDF model to simulate the temperature and major species concentrations in a three-burner POX reactor, and obtained a good agreement with the industrial data. Compared with the PDF, the EDC has the advantage of incorporating detailed chemistry at a much lower computational cost. Over the past 30 years, the EDC has been widely applied in the industry for the numerical simulations of turbulent combustion problems. Sefanidis et al. [25] simulated the steam cracking furnace with the EDC by CFD coupled with detailed chemistry. Rehm et al. [26] reported theoretical and numerical investigation on the EDC model for turbulence-chemistry interaction at gasification conditions, and found that the simulations could be improved by changing the model parameters. Xu et al. [30] studied the natural gas non-catalytic partial oxidation (NC-POX) reformer by CFD simulations with the GRI 3.0 mechanism. Both the modified EDC and PDFs model were applied to calculate the chemistry and turbulence interaction. They found that the EDC model agreed better with the operating data of an industrial reformer. Evans et al. [27] modeled the lifted jet flames in a heated co-flow using an optimized EDC model, and the simulation results agreed well with the measured temperature and concentrations of hydroxyl (OH) and formaldehyde (CH₂O). De et al. [31] investigated turbulence-chemistry interaction with the EDC model for the Delft-Jet-in-Hot-Coflow (DJHC) flames, with focus on assessing the performance in combination with two-equation turbulence models and chemical kinetic schemes. They found that the EDC model correctly predicted the experimentally observed variation trend of lift-off height with jet Reynolds number. Zhang et al. [32] applied the EDC model in CFD coupled with detailed chemistry to simulate the JICF reactor of a partially decoupled process (PDP) for methane conversion. The PDF and EDC models were compared in some literature, which mainly focused on the syngas production, or the

reduction of soot and NO_x emissions in combustion. For example, Xu et al. [30] studied the natural gas (NG) non-catalytic partial oxidation (NC-POX) reformer by CFD simulations with the PDF and EDC models. However, the studies of the gas quenching for the fuel-rich POX process for methane to acetylene are very limited.

The present work aimed to study the gas quenching process in an industrial-scale JICF reactor for POX of methane by CFD simulations using detailed chemistry. The model and detailed chemical mechanism were first validated by pilot-scale quenching experimental data, laminar flame data and industry POX data. Then the quenching process of POX was simulated by CFD coupled with detailed chemical mechanism. Both the PDF and EDC models were used to calculate the chemical source term, and their effects on the simulation results were discussed in detail. The predictions of the uniform index (UI), temperature, species concentrations were compared and analyzed. The effect of the mass flow ratio between main and jetting flows on the loss of acetylene was studied and the optimal mass flow ratio was determined based on acetylene loss and energy consumption.

2. Modeling methodology

2.1. Mathematical models

The mathematical models were based on Reynolds averaged Navier-Stokes (RANS) equations. The turbulence was described by the *k*- ϵ turbulence model. Both the PDF and EDC models were used to compute the chemical source term. The simulations were carried out using FLUENT 14.0.

When the PDF was used, the transport equation for the composition PDF was solved by the Lagrangian particle-based Monte Carlo method [33]. The modeling of the micromixing is crucial for the single-point PDF methods. The mixing model involves two parts: a model for the scalar time scale τ_ϕ that describes how fast the scalar PDF changes, and a scalar mixing model that describes how the scalar PDF changes [21–23]. A commonly used model for the scalar time scale is given by [34]

$$\tau_\phi = \frac{\tau_t}{C_\phi} \quad (1)$$

where τ_t is the dissipation time scale of turbulence and C_ϕ is a model parameter.

Three widely used mixing models, namely the interaction by exchange with the mean (IEM) model [34], the modified Curl's coalescence/dispersion (CD) model [34] and the Euclidean minimum spanning tree (EMST) model [35–37], are available in FLUENT. Among these models, only the EMST model has the desirable property [38] of being local in composition space, therefore it was used in this work with the default value $C_\phi = 2$.

The EDC model describes the chemical reactions in terms of both reaction rate and turbulence mixing [26,27]. This model is based on the energy cascade model and it divides the flow field into two parts, the “fine structures” and the surrounding flow. Reactions are considered to only occur in the “fine structures” where the reactants are mixed at molecular level. The length fraction of the fine scale is modeled as [39]

$$\zeta^* = C_\zeta \left(\frac{v\epsilon}{k^2} \right)^{1/4} \quad (2)$$

where * denotes fine-scale quantities. The volume fraction of the fine structure is calculated as ζ^{*3} , and the species are assumed to react in the fine structures over a time scale τ^* , which is expressed as

$$\tau^* = C_\tau \left(\frac{\nu}{\epsilon} \right)^{1/2} \quad (3)$$

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