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Evaluation, development, and validation of a new reduced mechanism for methane oxy-fuel combustion

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ABSTRACT

The chemical kinetics under oxy-fuel combustion is significantly different from that of conventional air-combustion due to the effect of the high CO_2 concentration. Although previous studies have made substantial achievement in reaction mechanisms for air-combustion, their performance under oxy-fuel conditions is still unknown. This study proposes a new 22-species, 19-step reduced mechanism for methane oxy-fuel combustion, developed using comprehensive mechanism evaluation, reduction, and validation methods. First, through quantitative error evaluation against a large experimental data set, for the first time we find that USC-Mech II obtains the best overall predictions among seven detailed combustion mechanisms in oxy-fuel conditions, particularly for the prediction of CO concentration. This detailed mechanism is then thoroughly simplified (including both skeletal and time-scale reduction) with error control under both atmospheric and pressurized oxy-fuel conditions. The obtained reduced mechanism is systematically validated using the detailed mechanism and the relative errors are found to be less than 10%. Relative to other mechanisms, this specially developed reduced mechanism for oxy-fuel combustion not only has minimal species, but also significantly improves the prediction of CO formation. The chemical influence of CO_2 under oxy-fuel conditions is further discussed to identify dominant elementary reactions for CO formation, which is important for future development of methane oxy-fuel combustion.

1. Introduction

The issue of climate change has become increasingly prominent, and there has been a growing emphasis on carbon capture (Fei et al., 2015; Stanger et al., 2015). Oxy-fuel combustion (Scheffknecht et al., 2011; Zheng and Liu, 2017) is being extensively investigated as a promising approach for large-scale carbon capture. By removing N_2 from air, the CO_2 level in the exhaust gas can be significantly increased (Chen et al., 2012). This combustion technology has recently been extended to pressurized conditions to further increase system efficiency (Gopan et al., 2015).

Importantly, many investigators have found that reaction mechanisms originally developed for air-combustion may produce questionable results under oxy-fuel conditions (Andersen et al., 2009; Bibrzycki and Poinsot, 2010). Unlike N_2, a very large amount of CO_2 directly participates in fuel oxidation reactions, and thus the chemical kinetics of oxy-fuel combustion is strongly affected (Liu et al., 2003, 2001; Wang et al., 2013). Glarborg and Bentzen (2008) found that, relative to combustion in air, more CO is produced during oxy-fuel combustion via reactions of CO_2 with H_2 and CH_x radicals. Andersen et al. (2009) discovered that the CO formation during oxy-fuel combustion is overestimated by the global reaction mechanisms originally developed for traditional methane air-combustion. Leiser et al. (2007); Bibrzycki and Poinsot (2010); Hjärtstam et al. (2012); Yin et al. (2011) and Hu et al. (2018) also pointed out that the reaction mechanisms for air-combustion may not accurately predict results of oxy-fuel combustion. Therefore, it is highly necessary to evaluate the performance of reaction mechanisms under oxy-fuel conditions.

To the best of our knowledge, no detailed mechanisms have been comprehensively tested in oxy-fuel combustion. For instance, the well-

Abbreviations: CSP, computational singular perturbation; *JLA*, the modified JL mechanism for oxy-fuel combustion of Andersen et al; *JLB*, the refined JL mechanism for oxy-fuel combustion of Bibrzycki et al; *JLH*, the refined JL mechanism for MILD oxy-combustion of Hu et al; *JLL*, the optimized JL mechanism for oxy-fuel combustion of Leiser et al; *LQSSA*, linearized quasi-steady-state approximation; *DRG*, directed relation graph; *DRGASA*, DRG-aided sensitivity analysis; *DRGEP*, DRG with error propagation; *DRGEPSA*, DRGEP with sensitivity analysis; *PCA*, principle component analysis; *OFD*, the detailed mechanism developed for oxy-fuel by Peter Glarborg's group; *QSSA*, quasi-steady-state approximation; *WDA*, the modified WD mechanism for oxy-fuel combustion of Andersen et al

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Nomenclature

Symbols

a_{fast}/a_{slow}	set of basis vectors for the fast / slow subspace
b^{fast}/b^{slow}	set of row basis vectors for the dual space of the fast / slow subspace
D	the effect of the fast time-scales on the i-th species of the mechanism
E	error function value
g	chemical source term
J	Jacobian of the source term g
K	number of species
L	spatial differential operator for convection and diffusion
M	number of fast time-scale
N	number of datasets
N_i	number of data points in the i-th dataset
P	pressure (atm)
P_{avg}	average pressure (atm)
$\lvert q_i \rvert$	net production rate of the i-th species
$\lvert q_i \rvert_{\max}$	the maximum net production rate over the domain
r_{AB}	dependence of species A on species B
T	temperature (K)
$\nu_{A,I}$	stoichiometric coefficient of species A in the i-th reaction
X_i	mole fraction of the i-th species
X_{O2}	ratio of O_2 in the oxidant by volume
$y_{ij}^{\exp}$	j-th data point in the i-th dataset
$\overline{Y_{ij}^{\exp}}$	average value of the j-th data point in the i-th dataset
Y_{ij}^{sim}	corresponding simulated value

Greek letters

$\sigma(y_{ij}^{\exp})$	standard deviation of the j-th data point in the i-th dataset
ε_{EP}	threshold
δ_B	induced error
Φ	equivalence ratio
ω_i	overall reaction rate of the i-th reaction

known GRI-Mech 3.0 (Smith et al., 1999) and USC-Mech II (Wang et al., 2007) mechanisms were originally developed for combustion in air, and their performance for oxy-fuel combustion is still unknown. Moreover, although the detailed mechanism of Peter Glarborg's group (Mendiara and Glarborg, 2009b) was specifically developed for oxy-fuel conditions (their mechanism is termed OFD in the present study), this mechanism has not been systematically validated with a large set of oxy-fuel experiments.

The present study will first evaluate the predictions of several detailed mechanisms under oxy-fuel conditions. However, just evaluating a mechanism does not guarantee its suitability for practical use. The use of computational fluid dynamics modeling with detailed mechanisms to model realistic combustor requires significant computing resources (Edge et al., 2011; Hu et al., 2018), especially for large eddy simulation (LES) (Pitsch, 2006) and direct numerical simulation (DNS). Although the computational cost can be significantly reduced by using a two-step or four-step global mechanism, the global mechanism cannot precisely capture transient processes and limit behaviors such as ignition and extinction because of the failure for build-up of the radical pool (Andersen et al., 2009; Hu et al., 2018). To maintain the accuracy of a mechanism while simultaneously decreasing the calculation cost, it is essential to develop simplified mechanisms based on a well-evaluated detailed mechanism. Therefore, after mechanism evaluation, the present study will then develop a new reduced mechanism for oxy-fuel combustion that involves minimal species and reactions, and more importantly, does not significantly decrease the accuracy.

For small hydrocarbon fuels, the mechanism reduction process involves two main steps: skeletal simplification and time-scale analysis (Lu and Law, 2009). For the first step, unimportant species and reactions are eliminated (Niemeyer et al., 2010). These unimportant species and reactions are identified and removed by a variety of systematic methods, including sensitivity analysis, Jacobian analysis (Turányi and Tomlin, 2014), CSP (Lam, 1993; Valorani et al., 2006), the directed relation graph (DRG) approach (Lu and Law, 2005), and other various DRG-based methods (Pepiot-Desjardins and Pitsch, 2008; Sun et al., 2010). These DRG-based methods remove unimportant species and reactions according to their relative contributions to the reaction rates, and coupled species are also considered. Additionally, skeletal mechanisms can be obtained by the CSP method with fast and slow importance indices (Lam, 1993; Lu and Law, 2006b; Valorani et al., 2006). For time-scale reduction, a further-reduced mechanism is obtained from skeletal mechanism through time-scale analysis methods such as CSP (Massias et al., 1999) or quasi-steady-state approximation (Lu and Law, 2006c). The present study will thoroughly develop new skeletal and reduced mechanisms through both skeletal and time-scale reduction methods.

This work first comprehensively evaluates the performance of seven detailed mechanisms for methane oxy-fuel combustion under both atmospheric and pressurized conditions, and then systematically develops and validates a new reduced mechanism for methane oxy-fuel combustion. To the best of our knowledge, this is the first investigation to evaluate the performance of reaction mechanisms in oxy-fuel conditions.

2. Methodology

2.1. Detailed mechanisms evaluated

Table 1 lists the seven well-known detailed combustion mechanisms evaluated in this work. The OFD mechanism (Mendiara and Glarborg, 2009a, b) is a detailed mechanism for the combustion of C1-C2 hydrocarbons and ammonia chemistry. This mechanism has been used in oxy-fuel conditions (Andersen et al., 2009; Barbas et al., 2015). GRI-Mech 3.0 (Smith et al., 1999) is widely adopted in predictions of ignition, flame structure, and NO chemistry for natural gas air-combustion. USC Mech II (Wang et al., 2007) is a well-known reaction model for the combustion of C1-C4 hydrocarbons. The UCSD 2016 mechanism (Williams, 2016) is a detailed reaction model for ignition, combustion, and detonations. It was developed by beginning with simple chemistry, and then proceeded gradually to more complex systems, and thus involves fewer species and reactions than mechanisms that attempt to include all potentially relevant elementary steps. The NUI NG II mechanism (Bourque et al., 2008) is used for the combustion of C1-C5 hydrocarbons. The AramcoMech 2 mechanism (Curran, 2016) was

Table 1
Detailed combustion mechanisms.

Mechanism	Species	Reactions	Scope	References
OFD	97	778	C1-C2 and ammonia	Mendiara and Glarborg (2009a, b)
GRI-Mech 3.0	53	325	Natural gas and NO	Smith et al. (1999)
USC Mech II	111	784	H_2/CO/C1-C4	Wang et al. (2007)
UCSD 2016	50	235	C1-C4	Williams (2016)
NUI NG II	132	821	Natural gas, up to C5	Bourque et al. (2008)
AramcoMech 2	493	2716	C1-C4	Curran (2016)
CRECK 2014	107	2642	C1-C3	Ranzi et al., (2014)

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