Modeling of large-scale oxy-fuel combustion processes

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Advanced modeling of large-scale oxy-fuel combustion processes

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Introduction

Oxy-fuel combustion is a promising carbon capture and storage technology and has gained increasing concerns worldwide. Combustion under oxy-fuel conditions is inherently different from conventional air-fuel combustion, among which radiative heat transfer and combustion chemistry are two of the fundamental issues. Efforts are made in both the aspects in this paper.

Methodology

Model development and verification;

Model implementation into CFD simulations of various oxy-fuel combustion processes and experimental validation.

Result

- **A new weighted-sum-of-gray-gases model (WSGGM) applicable to oxy-fuel combustion derived, validated and demonstrated: extending applicability to oxy-fuel, introducing a scaling temperature for an improved WSGGM data-fitting, and covering more representative conditions to better account for the variations in H_2O/CO_2 molar ratio in oxy-fuel flames (Yin et al., 2010).**
- **Various combustion mechanisms implemented in CFD of oxy-fuel combustion & recommendations made in the light of experimental validation (Yin et al., 2011).**

Table 1. **The three global mechanisms: "WD", "WD_refined", "JL_refined".**

No	Reactions	Rate equations [kmol/(m³·s)]	*A*	*b*	*E*
WD: Westbrook & Dryer 2-step mechanism					
1	$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$	$\frac{d[CH_4]}{dt} = AT^b e^{-E/(RT)} \cdot [CH_4]^{0.7}[O_2]^{0.8}$	5.01×10¹¹	0	2.0×10⁸
2	$CO + 0.5O_2 \rightarrow CO_2$	$\frac{d[CO]}{dt} = AT^b e^{-E/(RT)} \cdot [CO][O_2]^{0.25}$	2.24×10¹²	0	1.7×10⁸
WD_refined: refined Westbrook & Dryer 2-step mechanism for oxy-fuel combustion					
1	$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$	$\frac{d[CH_4]}{dt} = AT^b e^{-E/(RT)} \cdot [CH_4]^{0.7}[O_2]^{0.8}$	5.03×10¹¹	0	2.0×10⁸
2	$CO + 0.5O_2 \rightarrow CO_2$	$\frac{d[CO]}{dt} = AT^b e^{-E/(RT)} \cdot [CO][O_2]^{0.25}[H_2O]^{0.5}$	2.24×10⁶	0	4.2×10⁷
3	$CO_2 \rightarrow CO + 0.5O_2$	$\frac{d[CO_2]}{dt} = AT^b e^{-E/(RT)} \cdot [CO_2][H_2O]^{0.5}[O_2]^{-0.25}$	1.10×10¹³	-1	3.3×10⁸
JL_refined: refined Jones & Lindstedt 4-step mechanism					
1	$CH_4 + 0.5O_2 \rightarrow CO + 2H_2$	$\frac{d[CH_4]}{dt} = AT^b e^{-E/(RT)} \cdot [CH_4]^{0.5}[O_2]^{1.25}$	4.4×10¹¹	0	1.3×10⁸
2	$CH_4 + H_2O \rightarrow CO + 3H_2$	$\frac{d[CH_4]}{dt} = AT^b e^{-E/(RT)} \cdot [CH_4][H_2O]$	3.0×10⁸	0	1.3×10⁸
3	$H_2 + 0.5O_2 \leftrightarrow H_2O$	$\frac{d[H_2]}{dt} = AT^b e^{-E/(RT)} \cdot [H_2][O_2]^{0.5}$	5.7×10¹¹	0	1.5×10⁸
4	$CO + H_2O \leftrightarrow CO_2 + H_2$	$\frac{d[CO]}{dt} = AT^b e^{-E/(RT)} \cdot [CO][H_2O]$	2.8×10⁹	0	8.4×10⁷

- **Non-gray *vs.* Gray calculation of the Yin et al. (2010) oxy-fuel WSGGM *vs.* Gray calculation of the Smith et al. (1982) WSGGM in oxy-fuel combustion (Yin, 2012).**

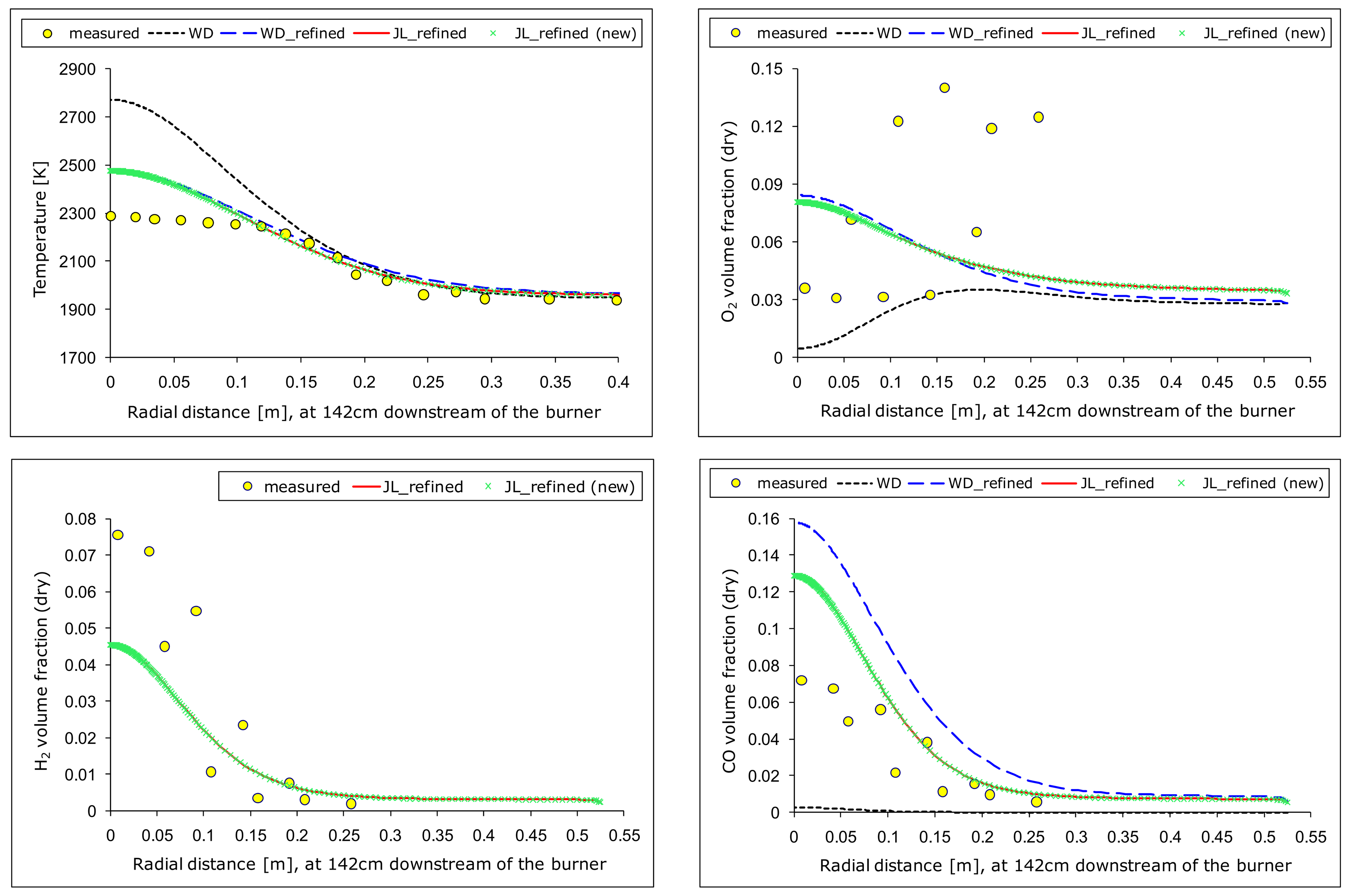

Figure 1. CFD of IFRF 0.8MW oxy-NG furnace, using different mechanisms & gaseous radiative property models [Smith et al. (1982) WSGGM by default, Yin et al. (2010) WSGGM as "new"; both gray calculations].

Case	Model for radiative properties	Sub-models in common
Case-0	The Smith et al. (1982) WSGGM, gray cal.	Fine structured mesh, standard k-ε, DO (2×2×8 directions), refined WD 2-step / EDC.
Case-1	The Yin et al. (2010) WSGGM, gray calculation	
Case-2	The Yin et al. (2010) WSGGM, non-gray cal.	

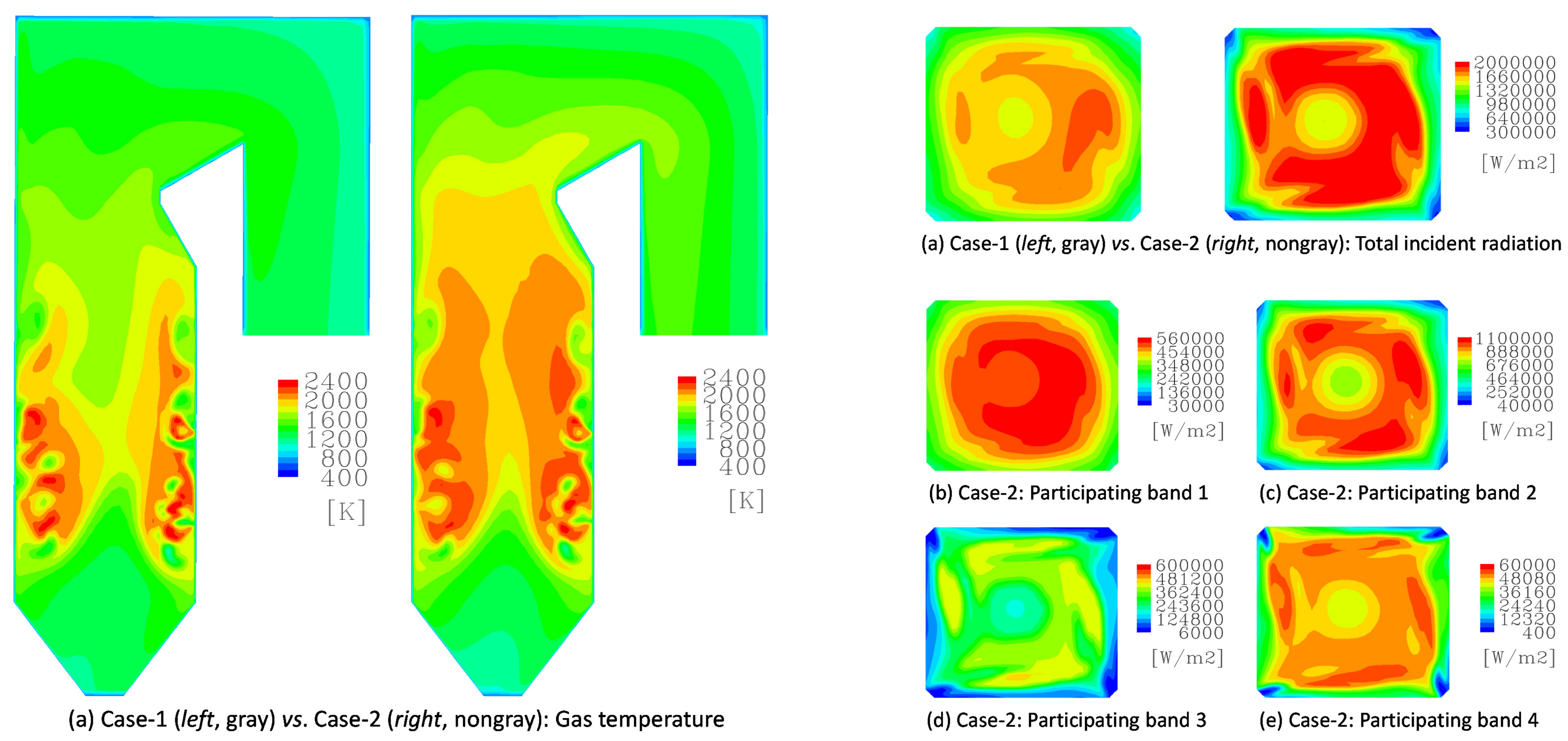

Figure 2. CFD results of a 1500MW (thermal input) utility boiler assumed to be operating under oxy-fuel condition with dry flue gas recycle.

Conclusions

1. **The original WD 2-step over-predicts flame temperature & largely under-predicts CO level;**
2. **The *refined* WD 2-step & JL 4-step reasonably predict the high CO level in oxy-fuel. The refined JL 4-step also reasonably predicts H_2 & flame temperature;**
3. **Applied to small-scale oxy-fuel combustion modeling *(L < a few meters)*, different WSGGMs make negligible difference.**
4. **Gray/non-gray of the same WSGGM make distinct difference, more remarkable than that between gray calculation of different WSGGMs;**
5. **Gray calculation over-predicts radiative HT to furnace walls, under-predicts gas temperature in furnace, and results in a higher CO prediction;**
6. **The demonstrated nongray-gas effects also apply for air-fuel conditions; may be compromised in solid-fuel combustion.**

Reference

[1] Yin, C.; Johansen, L.C.R.; Rosendahl, L.; Kær, S.K. "A new weighted sum of gray gases model applicable to CFD modeling of oxy-fuel combustion: Derivation, validation and implementation". *Energy & Fuels* 2010; 24(12): 6275-82.

[2] Yin, C.; Rosendahl, L.; Kær, S.K. "Chemistry and radiation in oxy-fuel combustion: A computational dynamics modeling study". *Fuel* 2011; 90(7): 2519-29.

[3] Yin, C. "Nongray-gas effects in modeling of large-scale oxy-fuel combustion processes". *Energy & Fuels* 2012, 26(6): 3349-56.

[4] Yin, C. "Modeling of large-scale oxy-fuel combustion processes". in *Proc. of the 4th Int. Conf. on Applied Energy*, ICAE2012, July 5-8, 2012, Suzhou, China, p. 3685-92.

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