A new air-fuel WSGGM for better utility boiler simulation, design and optimization

Yin, Chungen

Publication date:
2013

Document Version
Early version, also known as pre-print

International Conference on Power Engineering,
Oct 23-27, 2013, Wuhan, China

A new air-fuel WSGGM

(weighted sum of gray gas model) **for better utility boiler simulation, design & optimization**

Chungen Yin, Ph.D.

Associate Prof, Aalborg University, Denmark

(+45) 9940 9279; chy@et.aau.dk

Oct 24, 2013

Outline

- Intro: Why is WSGGM important
- Why need a new model
- The new air-fuel WSGGM
- Demo: Implementation & impacts
- Conclusions

Intro: Why is WSGGM important

- Energy eq. $$\frac{\partial(\rho h)}{\partial t} + div(\rho \vec{u}\, h) = div(k_{eff} \nabla T) \ + (S_{h,\,\mathrm{rad}} + S_{h,\,\mathrm{react}} + S_{h,\,\mathrm{DPM}})$$

$$\begin{cases} S_{h,\,\mathrm{rad}} = f_1(I(\vec{r},\hat{s}), T_g) \\ \dfrac{dI(\vec{r},\hat{s})}{ds} = \alpha(\vec{r})\left[I_b(\vec{r}) - I(\vec{r},\hat{s})\right] + \sigma_s(\vec{r})\left[\dfrac{1}{4\pi}\int_{4\pi} I(\vec{r},\hat{s}')\, \phi(\hat{s}' \Rightarrow \hat{s})\, d\omega' - I(\vec{r},\hat{s})\right] \\ \alpha(\vec{r}) = f_2(P, T, L, X_i) \end{cases}$$

- WSGGM: $$\varepsilon = \sum_{i=0}^{N} a_{\varepsilon,i}(T_g) \cdot \left(1 - e^{-k_i \cdot P \cdot L}\right) \qquad a_{\varepsilon,i}(T) = \sum_{j=1}^{J} b_{\varepsilon,i,j} \left(T_g\right)^{j-1}$$

  A multiple gray gas model – Good compromise between the most comprehensive approach (*fully addressing wavelength-dependency by dividing the entire spectrum into high-resolution intervals*) and the simplest gray assumption (*constant properties over the entire spectrum*); computationally effective; applicable to CFD.

DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

Why need new model (1/6): *the existing*

- The Smith et al. (1982) WSGGM – most widely used
- 5 tables for 5 partial pressures of CO_2 and H_2O vapor:
  - (1) $P_c \rightarrow 0$ atm;
  - (2) $P_w/P_c=1$ ($P_c=0.1$ atm);
  - (3) $P_w/P_c=2$ ($P_c=0.1$ atm);
  - (4) $P_w \rightarrow 0$ atm;
  - (5) $P_w=1$ atm;
- used for T_g up to 2400K; supplemented by the Coppalle and Vervisch (1983) WSGGM for higher temperatures till 3000K.

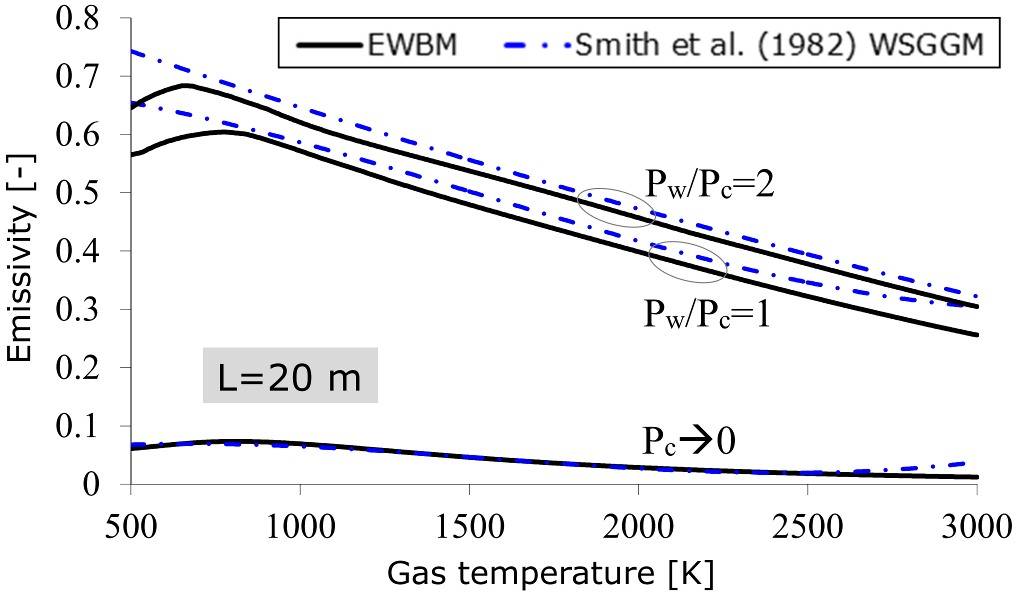
DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

Why need new model (2/6): *the existing*

- To account for variations in CO_2 and H_2O vapor concentrations in a flame

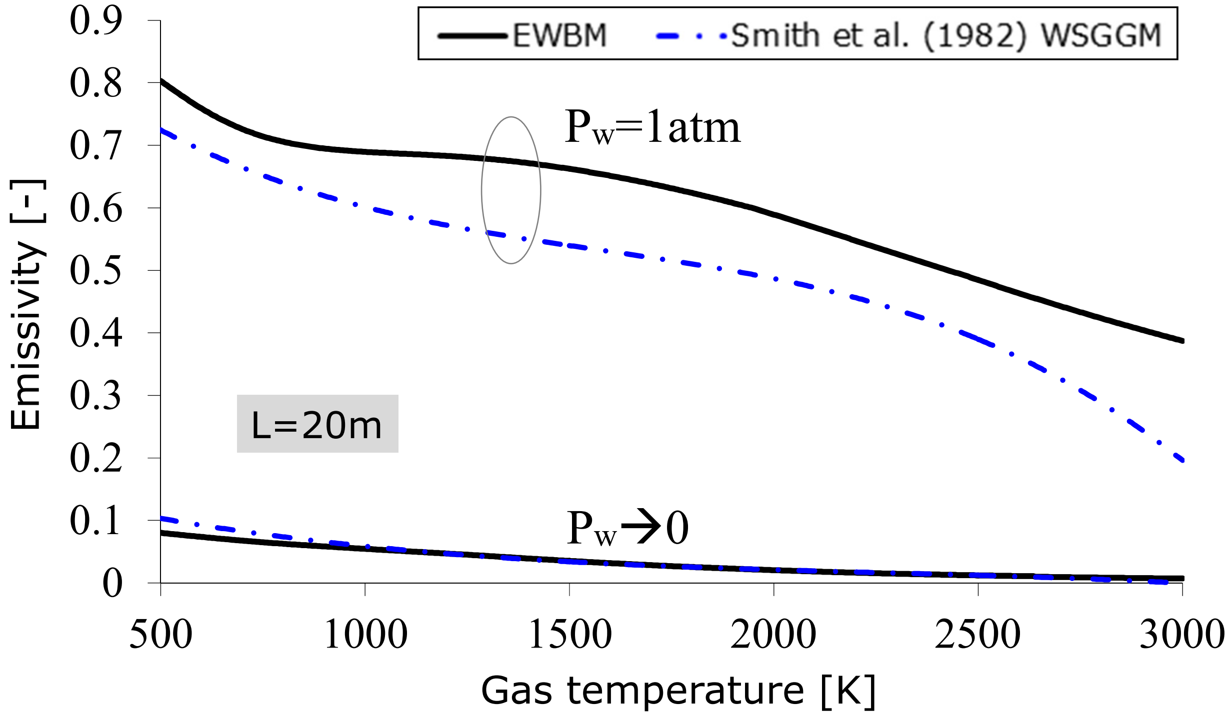
$$
\begin{aligned}
&\text{if } (P_w \le 0.5P_c), \text{ use } P_c \to 0 \text{ atm table}\\
&\text{else if } (P_w \le 1.5P_c), \text{ use } (P_w/P_c) = 1 \text{ table}\\
&\text{else if } (P_w \le 2.5P_c), \text{ use } (P_w/P_c) = 2 \text{ table}\\
&\text{else if } (P_w \le 0.5), \text{ use } P_w \to 0 \text{ atm table}\\
&\text{else, use } P_w = 1 \text{ atm table}
\end{aligned}
$$

Why need new model (3/6): *problems*



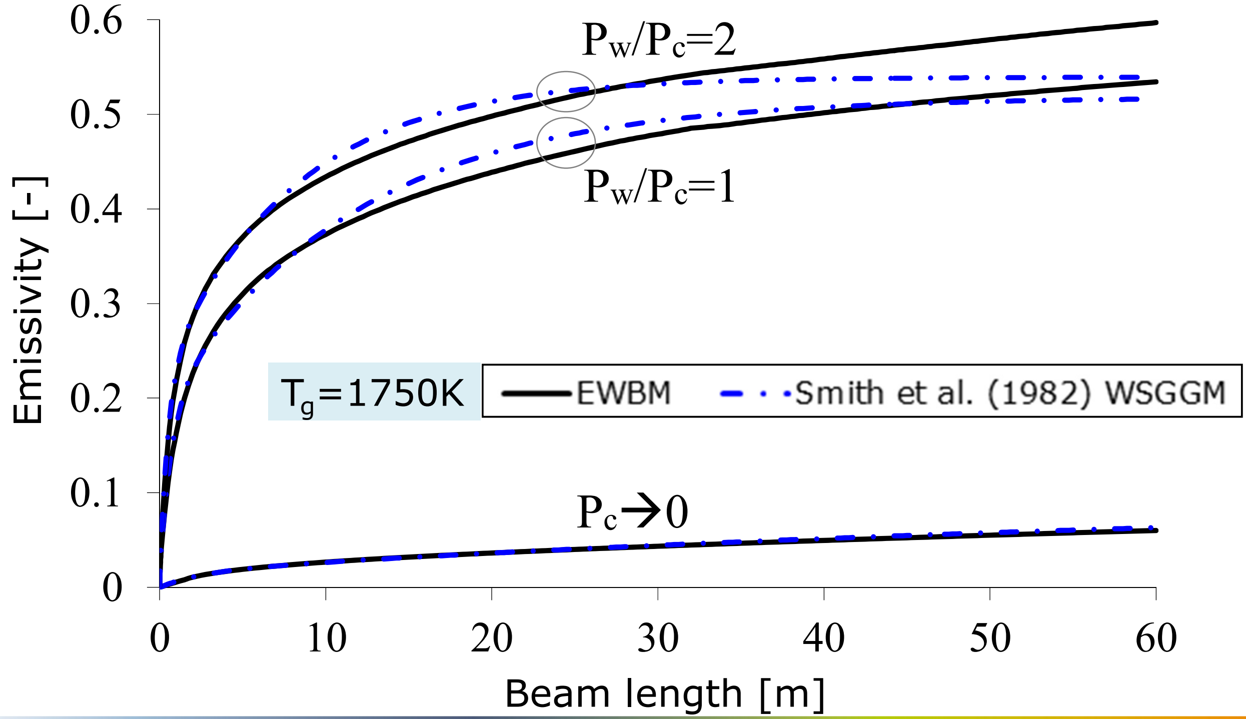
- **Inaccurate.** Relatively large error comparing the validated reference model, Exponential Wide Band Model (EWBM) – $f(T_g, P, L, X_i)$ – accurate but computationally prohibitive for CFD;
- **Incomplete.** (1) In representative conditions, e.g., when (P_w=0.499 P_c) → (P_w=0.501 P_c) which corresponds to a negligible change in composition, but the table to calculate the emissivity switched from P_c→0 to P_w/P_c=1 (a big change in ε); (2) incomplete in parameter ranges

Why need new model (4/6): *problems*



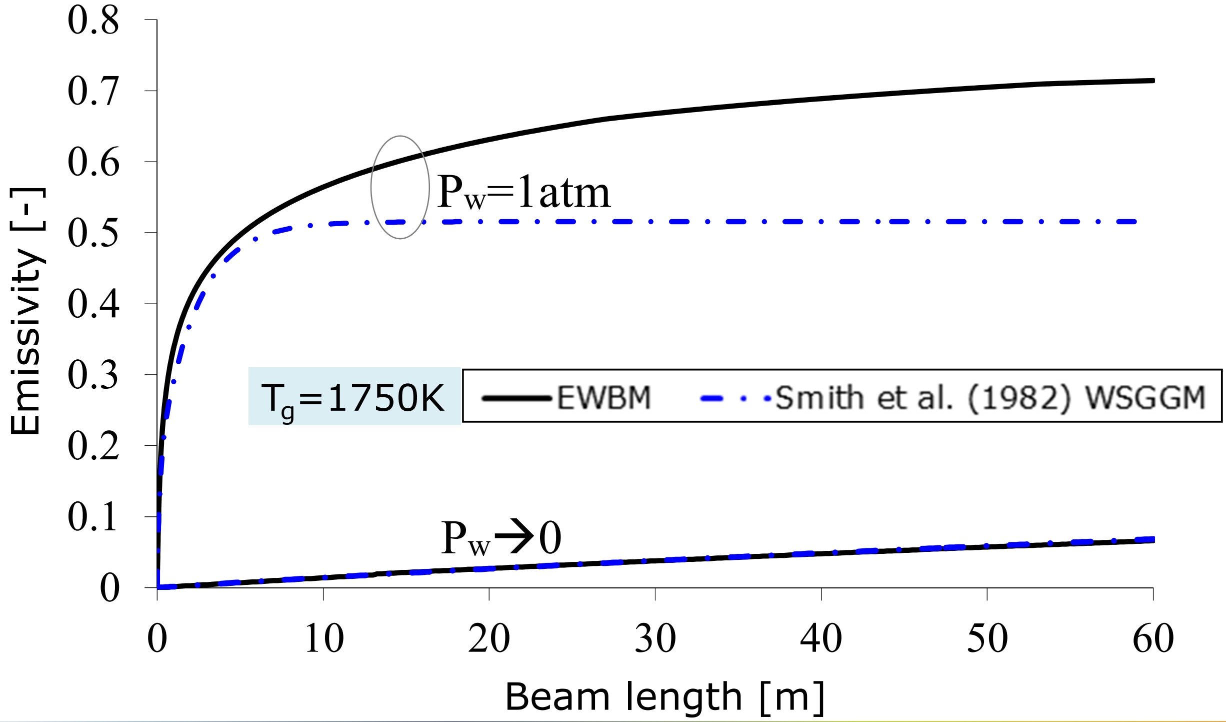
DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

Why need new model (5/6): *problems*



DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

Why need new model (6/6): *problems*



DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

The new WSGGM (1/7): *How to derive*

- Determine 7 representative air-fuel conditions in terms of P_c, P_w – *to effectively smoothen the effects of in-flame gas composition variations on the calculated gaseous radiative properties.*
- <u>For each condition</u>: use the validated EWBM to generate emissivity database, spanning a larger T_g-range (T_g=500-3000K, with a smaller interval of 25K) and also a larger P·L range (P·L=0.001-60 atm·m). Large emissivity database matrix: 146 discrete values for P·L times 101 data points for T_g.
- <u>For each condition</u>: use data-fitting optimization technique to derive new coefficients for a 4-gray gas plus 1-clear gas WSGGM from the emissivity database. T_{ref}=1200 [K] used to simplify the optimization and improve the data-fitting accuracy.

DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

The new WSGGM (2/7): *Formulation*

$$\varepsilon = \sum_{i=0}^{N} a_{\varepsilon,i}(T_g)(1 - e^{-k_i PL})$$

$$a_{\varepsilon,i}(T) = \sum_{j=1}^{J} b_{\varepsilon,i,j}\left(\frac{T_g}{T_{ref}}\right)^{j-1}$$

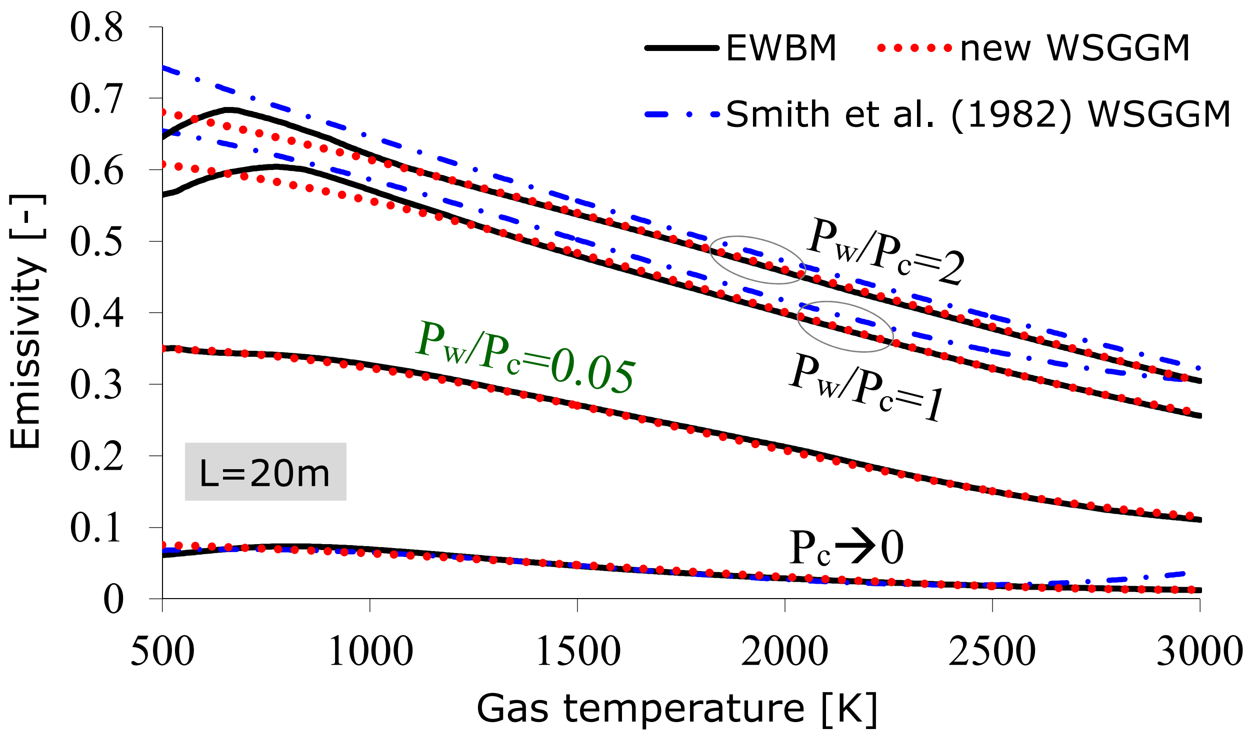
$$i = 1, ..., N$$

$$a_{\varepsilon,i} > 0$$

band i	k_i	$b_{\varepsilon,i,1}$	$b_{\varepsilon,i,2}$	$b_{\varepsilon,i,3}$	$b_{\varepsilon,i,4}$
Carbon Dioxide, $P_c \to 0$ atm					
1	0.163233	0.204623	−0.378060	0.666639	−0.203453
2	13.096584	−0.020227	0.256006	−0.195201	0.040493
3	175.474735	0.044221	0.003850	−0.020175	0.004919
4	1310.847307	0.039311	−0.054832	0.025370	−0.003891
Mixture, $P_w/P_c = 0.05$ ($P_c = 0.1$ atm)					
1	0.352505	0.315106	0.023475	−0.057930	0.008408
2	8.210621	0.092474	0.109146	−0.121000	0.027145
3	137.410012	0.031702	0.037396	−0.040731	0.008742
4	1269.710976	0.046138	−0.061392	0.027164	−0.003996
Mixture, $P_w/P_c = 1$ ($P_c = 0.1$ atm)					
1	0.261021	0.500119	−0.447068	0.286878	−0.059165
2	3.147817	0.071592	0.508252	−0.384253	0.073477
3	54.265868	0.155320	−0.104294	0.014096	0.001643
4	482.900353	0.072615	−0.100601	0.046681	−0.007224
Mixture, $P_w/P_c = 2$ ($P_c = 0.1$ atm)					
1	0.179160	0.542458	−0.658411	0.466444	−0.100186
2	2.388971	0.101734	0.518429	−0.386151	0.073453
3	28.415805	0.146066	−0.008745	−0.058325	0.015984
4	253.059089	0.129511	−0.187993	0.090709	−0.014493
Water Vapor, $P_w \to 0$ atm					
1	0.085523	0.966357	−0.790165	−0.050144	0.115202
2	0.475777	0.662059	−2.262877	2.309473	−0.572895
3	8.549733	0.060870	0.436788	−0.395493	0.085146
4	201.906503	0.103568	−0.153135	0.074910	−0.012091
Water Vapor, $P_w = 0.05$ atm					
1	0.232724	0.340618	−0.105469	0.068051	−0.017828
2	2.134299	0.175818	−0.063466	0.086631	−0.026581
3	9.266065	0.044325	0.288376	−0.258205	0.054333
4	134.988332	0.126628	−0.186480	0.090755	−0.014569
Water Vapor, $P_w = 1$ atm					
1	0.065411	−0.077336	0.661776	−0.362515	0.053534
2	0.696552	0.506777	−0.758948	0.516146	−0.102909
3	4.862610	−0.079989	0.851078	−0.604264	0.113500
4	60.255980	0.373898	−0.540887	0.258923	−0.040957

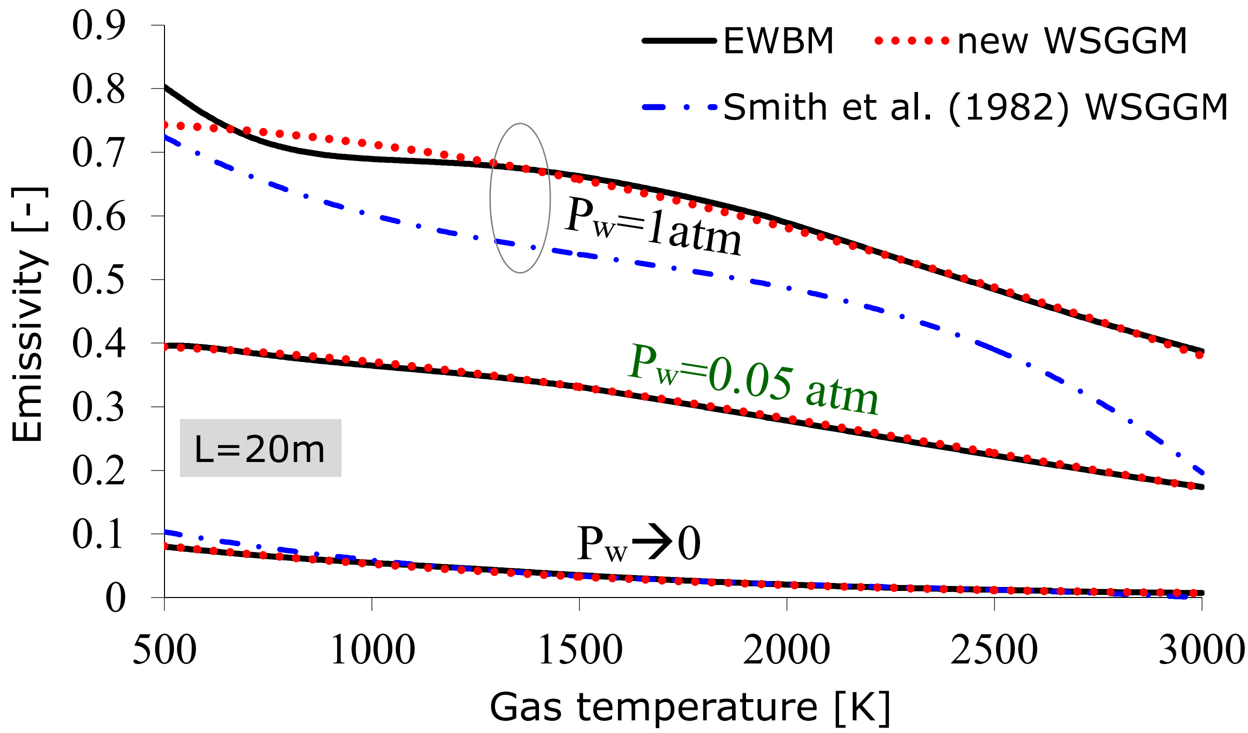
[a] $P_T = 1$ atm; $0.001 \le L \le 60$ m; $0.001 \le PL \equiv (P_w + P_c)L \le 60$ atm m; and $500 \le T_g \le 3000$ K.

The new WSGGM (3/7): *Comparison*



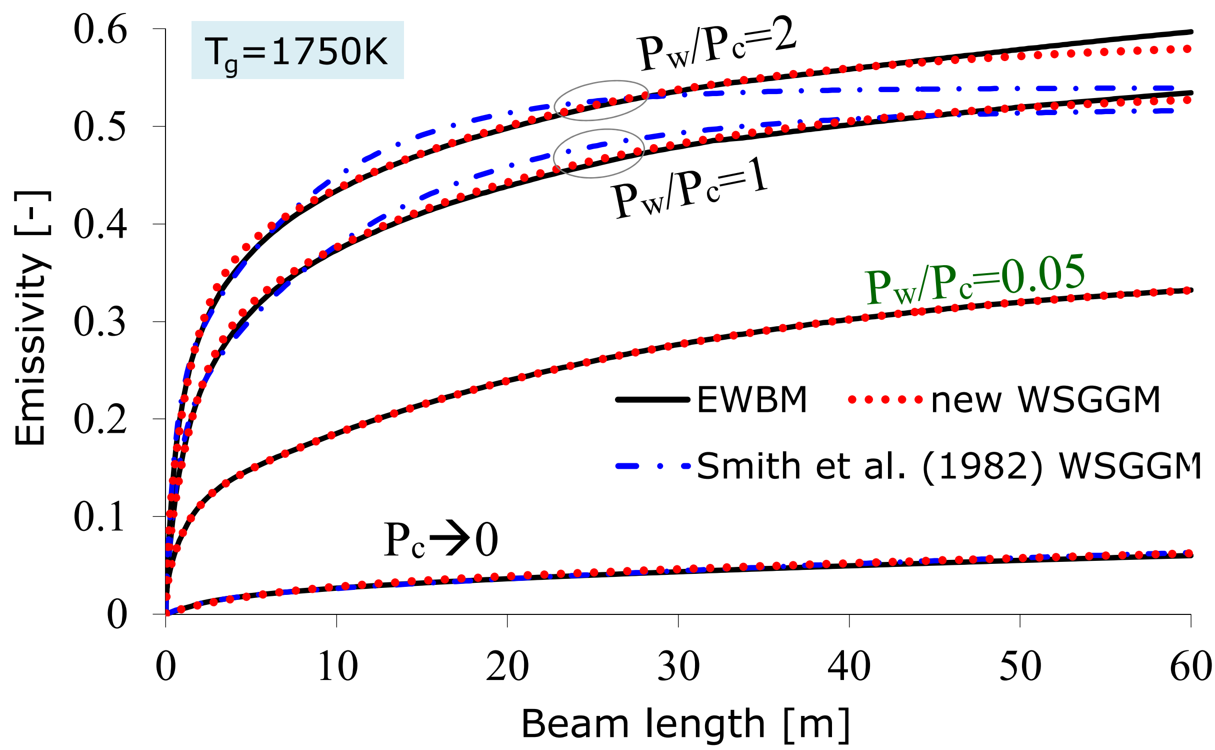
DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

The new WSGGM (4/7): *Comparison*



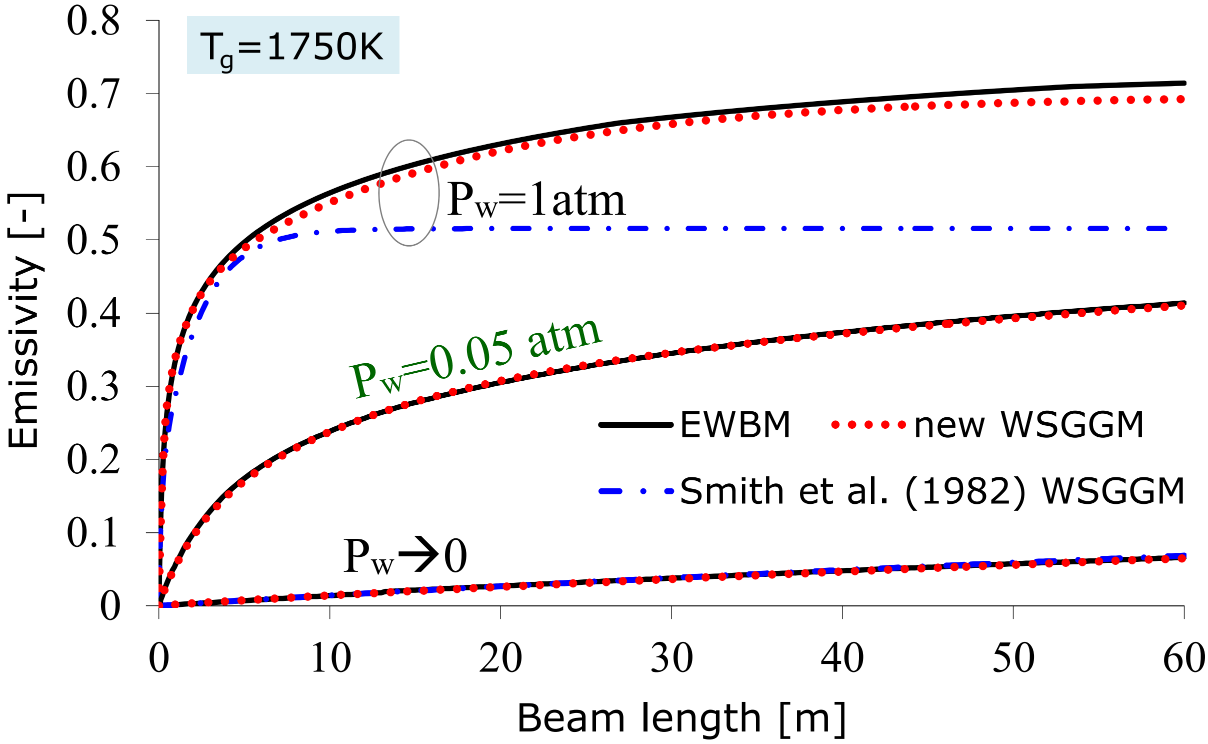
DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

The new WSGGM (5/7): *Comparison*



DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

The new WSGGM (6/7): *Comparison*



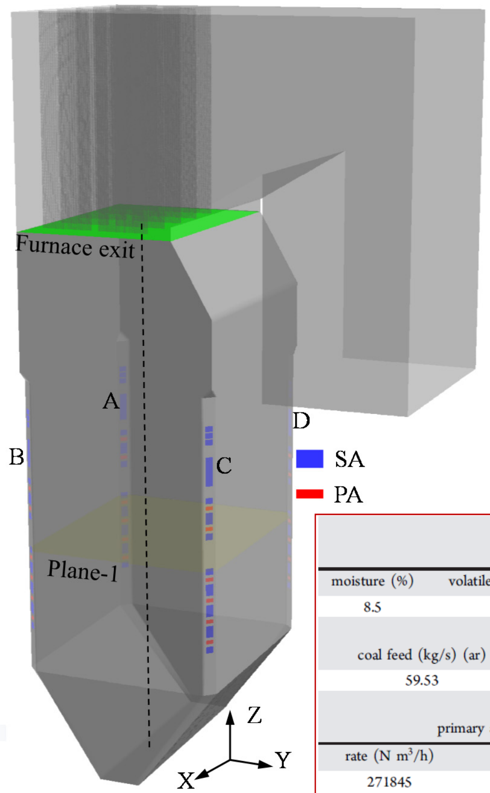
DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

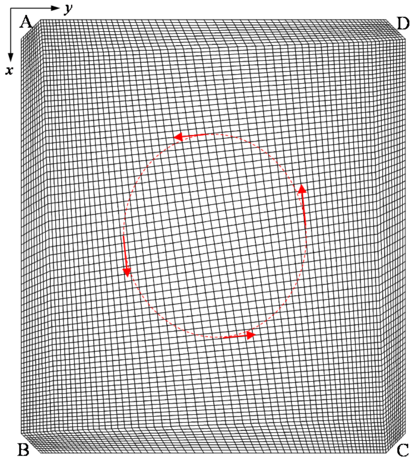
The new WSGGM (7/7): *How to use*

$$
\begin{aligned}
&\text{if } (P_w \le 0.01P_c),\ \text{use } P_c \rightarrow 0 \text{ atm table}\\
&\text{else if } (P_w \le 0.5P_c),\ \text{use } (P_w/P_c) = 0.005 \text{ table}\\
&\text{else if } (P_w \le 1.5P_c),\ \text{use } (P_w/P_c) = 1 \text{ table}\\
&\text{else if } (P_w \le 2.5P_c),\ \text{use } (P_w/P_c) = 2 \text{ table}\\
&\text{else if } (P_w \le 0.01),\ \text{use } P_w \rightarrow 0 \text{ atm table}\\
&\text{else if } (P_w \le 0.2),\ \text{use } P_w = 0.05 \text{ atm table}\\
&\text{else, use } P_w = 1 \text{ atm table}
\end{aligned}
$$

DEPARTMENT OF ENERGY TECHNOLOGY
AALBORG UNIVERSITY

Demo (1/5): *Problem description*





(1) Coal Analysis Data

proximate analysis [as received (ar)]					ultimate analysis [dry and ash free (daf)]				
moisture (%)	volatile matter (%)	fixed carbon (%)	ash (%)	LHV (kJ/kg) (ar)	C (%)	H (%)	O (%)	N (%)	S (%)
8.5	16.0	52.5	23.0	24965	85.01	4.79	7.18	1.70	1.32

(2) Coal Feeding Rate and Coal Particle Size (Rosin–Rammler Size Distribution)

coal feed (kg/s) (ar)	minimum size (μm)	mean size (μm)	maximum size (μm)	spread parameter
59.53	15	57	132	1.3

(3) Combustion Air

primary air		secondary air (including OFA)		air composition		
rate (N m^3/h)	temperature (K)	rate (Nm^3/h)	temperature (K)	O_2 (wt %)	N_2 (wt %)	H_2O (wt %)
271845	358	1458415	640	22.6	75.3	2.1

[a] ar, as received; LHV, lower heating value; and OFA, over-fire air.

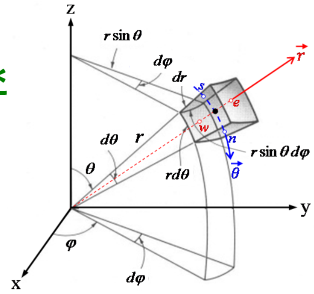
Demo (2/5): *Cases & sub-models*

	Gaseous Radiative Prop.	**Part-Rad. Inter.**	**Purpose**
case-1	Smith et al. (1982) WSGGM	Not included	case-**1** vs. **A**: to conclude effects of the refined WSGGM on gas combustion;
case-2	Smith et al. (1982) WSGGM	Included	case-**2** vs. **B**: to conclude effects of the refined WSGGM on solid fuel combust.
case-A	Refined WSGGM (via UDF)	Not included	
case-B	Refined WSGGM (via UDF)	Included	

Mesh of the boiler	**Structured mesh: 3,191,580 high-quality hexahedral cells**
Gaseous radiative property	Smith et al. (1982) air-fuel WSGGM vs. the new air-fuel WSGGM
Coal and feeding rate	Real coal fed into the furnace (with 8.5% moisture) used and moisture release appropriately addressed
Coal particle trajectories	432,000 coal particle streams tracked
Furnace wall: T_w & ε_w	The same wall emissivity (ε_w=0.7) used. The same rule for wall temperature estimation used. (the purpose is to check if the two WSGGMs make big difference in CFD results)
Other sub-models	RNG k-ε; 2-step global mechanism for gas-phase combustion, Eddy dissipation for turbulence-chemistry interaction; Kinetics/diffusion-limited char oxidation (into CO); DO for radiation; ………

Demo (3/5): *Novel for BW release*

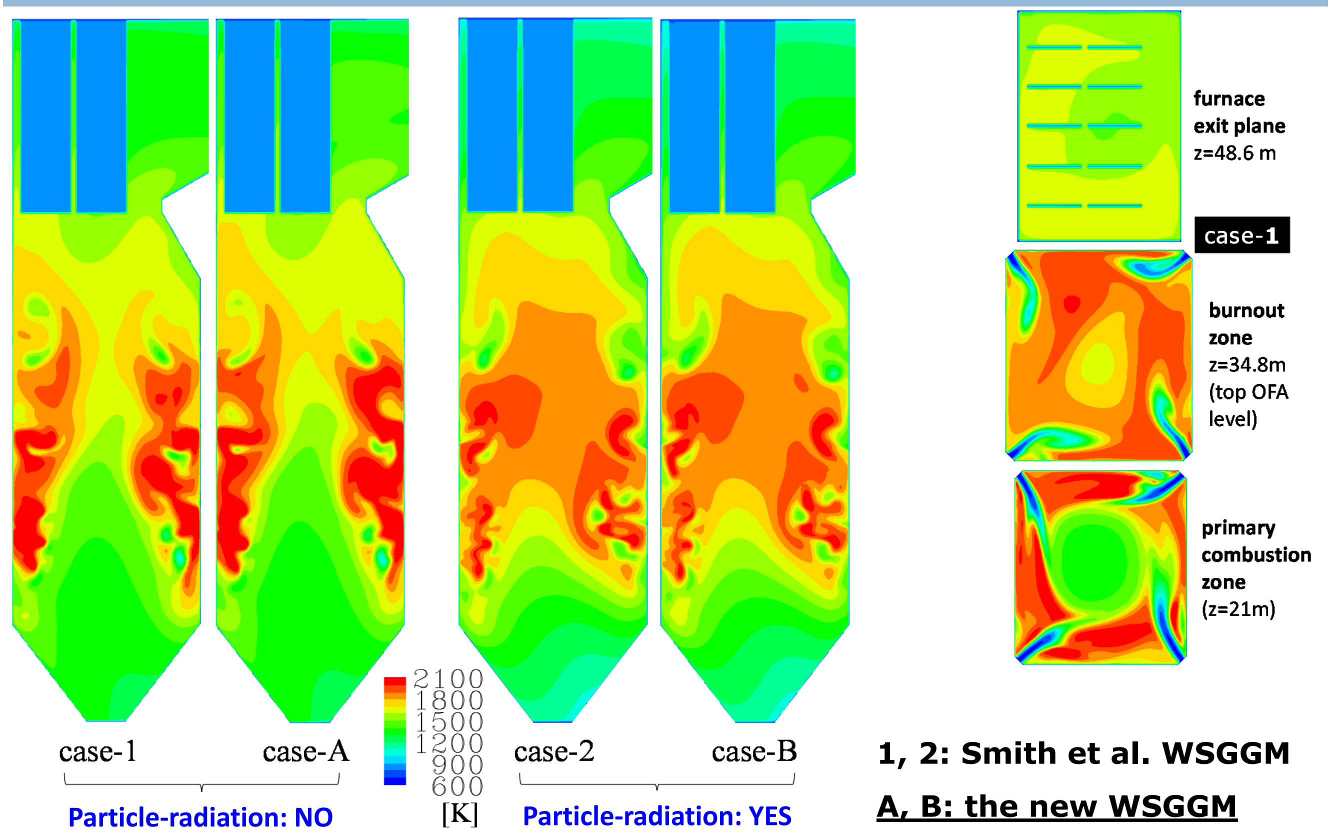
- ~~Wet combustion model (e.g., drying in FLUENT)~~
- ~~Complicated particle model using FVM*~~
- NOVEL compromise for BW release
  - Bound water (BW) in fuel released with volatiles
  - Modified "lumped" volatiles to include BW content, with modified formulation enthalpy
  - Modified latent heat of devolatilization to include evaporation heat



$$CH_{3.6992}O_{0.3494}N_{0.0944}S_{0.032}\cdot 0.4857\,H_2O + 1.2821\,O_2$$
$$\rightarrow CO + 2.3353\,H_2O\,(g) + 0.032\,SO_2 + 0.0472\,N_2$$

*: e.g., **C. Yin**, et al. (2010). "Co-firing straw with coal in a swirl-stabilized dual-feed burner: modeling and experimental validation". *Bioresource Technology* 2010; 101(11): 4169-4178.

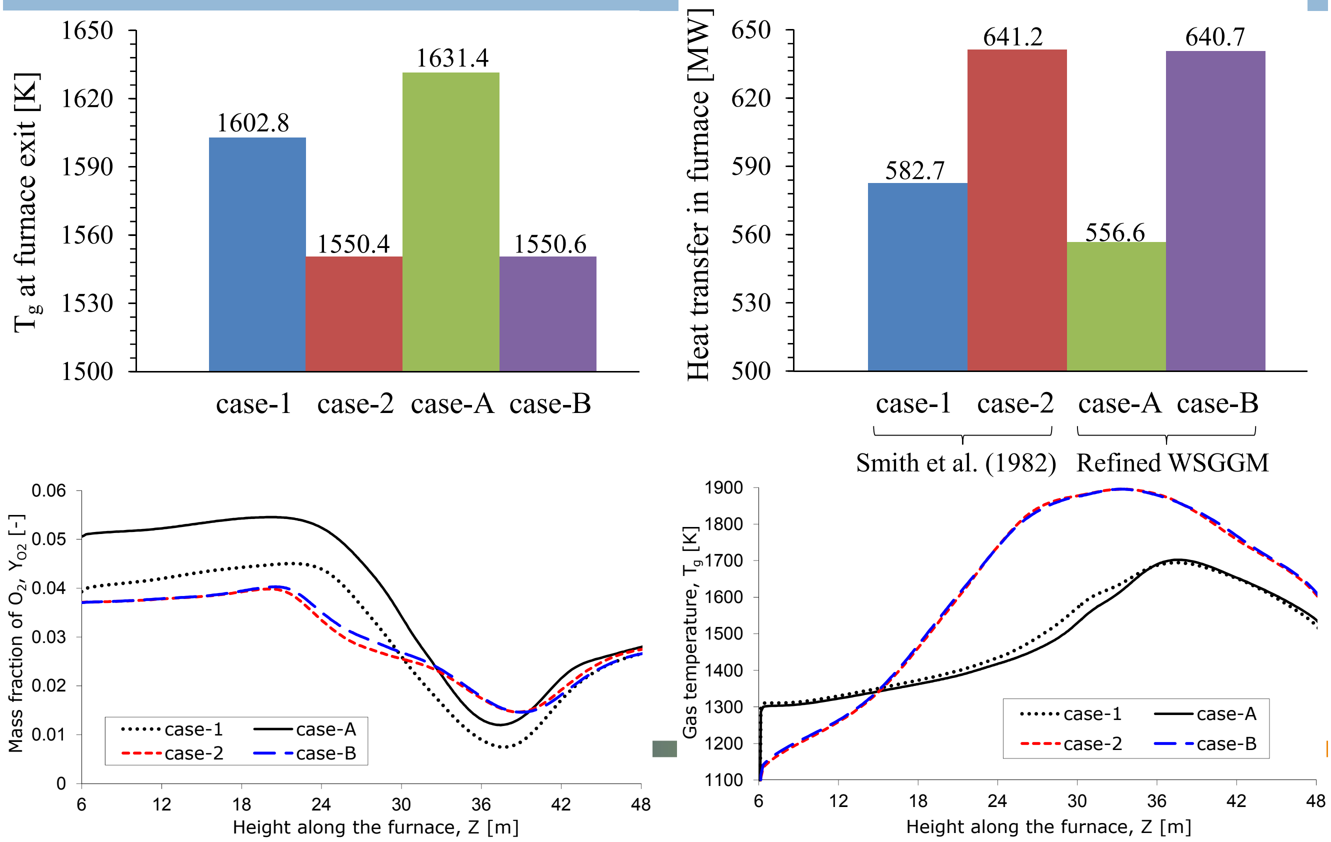
Demo (4/5): *Results*



1, 2: Smith et al. WSGGM

A, B: the new WSGGM

Demo (5/5): *Results*



Conclusions

- The new air-fuel WSGGM is much more accurate & complete; can be used alone; applicable to both non-gray and gray calculations.
- The new WSGGM makes distinct difference with the existing WSGGMs for gaseous fuel comb. processes.
- Such impacts are greatly compromised under solid-fuel combustion scenario because of the important role of particle-radiation interaction.
- The new air-fuel WSGGM is expected to replace all the existing for better CFD in future ☺!

Key references

C. Yin. "Refined weighted sum of gray gases model for air-fuel combustion and its impacts". *Energy & Fuels* 2013; 27(10): 6287-94 [a]

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

C. Yin, L.C.R. Johansen, L. Rosendahl, S.K. Kær. "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.

[a]: an extended version of the ICOPE conference paper

Thank you for your attention!

Any questions?