



A new model for gas radiative properties applicable to oxy-fuel combustion modelling

Yin, Chungen; Johansen, Lars Christian Riis; Rosendahl, Lasse; Kær, Søren Knudsen

Publication date:
2010

Document Version
Publisher's PDF, also known as Version of record

[Link to publication from Aalborg University](#)

Citation for published version (APA):
Yin, C., Johansen, L. C. R., Rosendahl, L., & Kær, S. K. (2010). *A new model for gas radiative properties applicable to oxy-fuel combustion modelling*. Poster presented at 33rd International Symposium on Combustion, Beijing, China.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal -

Take down policy

If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

A new model for gas radiative properties applicable to oxy-fuel combustion modelling

Chungen Yin, Lars C.R. Johansen, Lasse A. Rosendahl, Søren K. Kær



Department of Energy Technology, Aalborg University, Denmark

Introduction

Radiation is the principal mode of heat transfer in furnaces. Modeling of radiation heat transfer in combustion systems is very complicated. There are two key issues, i.e., how to calculate radiation intensity at different locations along different directions from radiative transfer equations and how to evaluate radiation properties at different locations. Different combustion environments (air-fuel or oxy-fuel) make no difference to the 1st key issue; they will only affect the gaseous radiative properties.

Models for gaseous radiative properties have been well established for air combustion. However, there is uncertainty regarding their applicability to oxy-fuel conditions. In this paper, a new and complete set of models for gaseous radiative properties is derived, which is applicable to CFD modeling of both air-fuel and oxy-fuel conditions. The derivation, calibration and implementation of the new model are given.

Method

- First, a computer code is developed to evaluate the emissivity of any gas mixture at any condition by using the exponential wide band model (EWBM), and the calculated results are calibrated in very details by data in literature.
- Then, the calibrated code is used to generate emissivity databases for representative air-firing and oxy-firing conditions, for each of which a new weighted-sum-of-gray-gases model (WSGGM) with new parameters is derived. The way to implement the new models into CFD simulations of combustion systems is given.
- Finally, as a demonstration, the new models are applied to CFD modeling of a 0.8MW oxy-natural gas flame furnace. The CFD results are compared with those based on the widely used WSGGMs in literature. Based on that, some useful guidelines on oxy-fuel modeling are recommended.

Result 1: Calibration of EWBM code

Based on "almost exact analytical expressions", a computer code in c++ is developed to evaluate the emissivity of any gas mixture that may consist of H₂O, CO₂, CO, CH₄, NO and SO₂ at any condition using the EWBM. The application of this code to a gas mixture is shown below, with almost all the values here calibrated with a reference example.

```
[0] Input Conditions: Gas temperature, T_g [K] = 1500.00
Total pressure, P [Pa] = 101325.00
Path length, S [m] = 0.500000
Mole fraction: (i=0) x_H2O=0.160; (i=1) x_CO2=0.085; (i=2) x_CO=0.020; (i=3) x_CH4=0.005

The detailed calculation results *****
[1] Calculate the lower and upper band limits (n_L, n_U) for j-th band of i-th participating species
n_L [cm^-1] n_U [cm^-1]
H2O (i=0) 11.7090 1.2753 268.398 4327.750522
CO2 (i=1) 11.7090 1.2753 232.379 24.995037
CO (i=2) 11.7090 1.2753 166.926 3.812881
CH4 (i=3) 11.7090 1.2753 123.935 2.647639
... (many more lines) ...

[2] Calculate band transmittances (tau_L, tau_U, tau_B), Planck blackbody fractional participation (f_L, f_U), and total emissivity
n_L [cm^-1] n_U [cm^-1] over_lap Band (i, j)
0.0000 560.391 (0, 0) (1, 0)
0.0000 772.850 (0, 0) (1, 1)
0.0000 773.609 (0, 0) (1, 2)
... (many more lines) ...

The total emissivity of the mixture at the above condition: epsilon = 0.167256724
The equivalent (gray) absorption coefficient: -(1/S)*log(1-epsilon) = 0.366059752
```

The detailed results of the EWBM code applied to calculate the total emissivity of an arbitrary gas mixture.

Result 2: The new models

The complete set of the new models consists of the following equations and new parameters for a number of representative air-fuel and oxy-fuel conditions, and the way to implement them into CFD modeling. Here, only the new WSGGM parameters for the representative oxy-fuel conditions are listed, as seen in Table 1.

$$\epsilon = \sum_{i=0}^I a_{\epsilon,i}(T_g) \cdot (1 - e^{-k_i \cdot P \cdot L})$$

$$a_{\epsilon,i}(T) = \sum_{j=1}^J b_{\epsilon,i,j} \left(\frac{T_g}{T_{ref}} \right)^{j-1} \quad i=1, \dots, I \quad a_{\epsilon,i} > 0$$

$I = 4, \quad J = 4, \quad T_{ref} = 1200$ (in the unit of K) for a better estimate

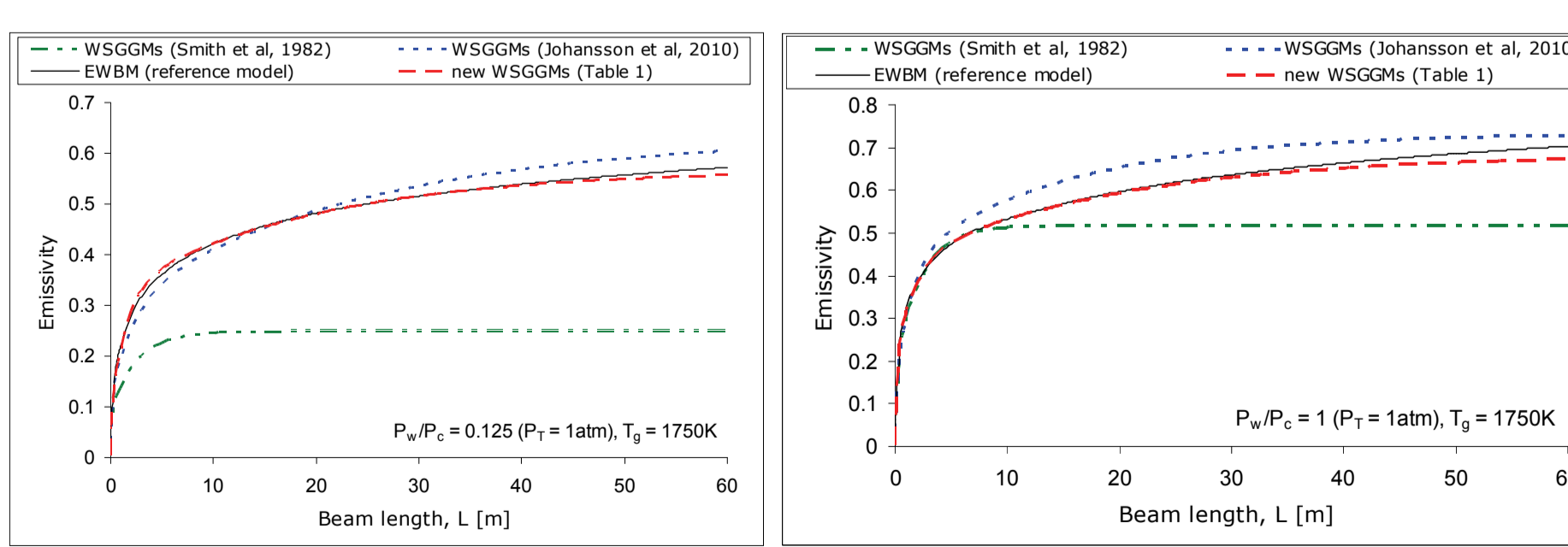
$k_0 = 0$: represent 'windows' in the spectrum; $a_{\epsilon,0} = 1 - \sum_{i=1}^I a_{\epsilon,i} > 0$

P : the sum of the partial pressures of all the participating gases, atm

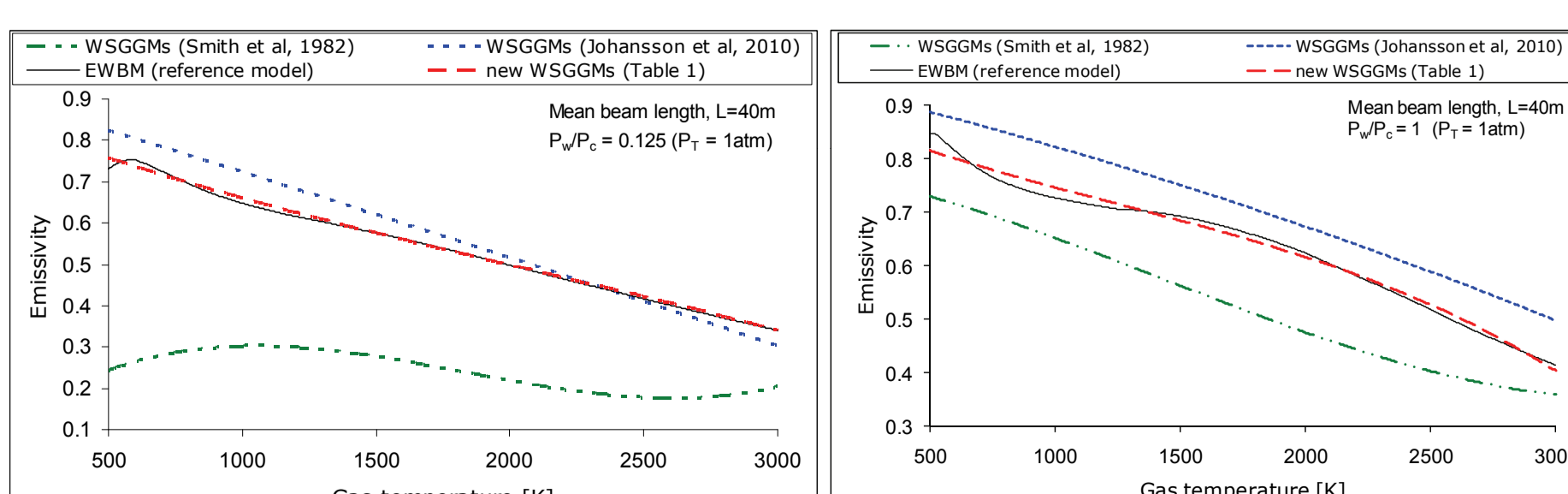
Table 1. New parameters for the WSGGMs, applicable to oxy-fuel flames.

i	k_i	$b_{\epsilon,i,1}$	$b_{\epsilon,i,2}$	$b_{\epsilon,i,3}$	$b_{\epsilon,i,4}$
$P_w/P_c \rightarrow 0$ atm, $P_c \rightarrow 0$ atm					
1	0.009422	0.778969	-1.342848	0.964858	-0.195747
2	0.115446	-0.011449	0.343754	-0.234886	0.044008
3	11.617018	-0.007627	0.242253	-0.173738	0.033868
4	319.911168	0.080082	-0.049280	0.001861	0.002232
$P_w/P_c = 0.1$ atm, $P_c = 0.1$ atm					
1	0.256738	0.492304	-0.483789	0.279329	-0.057770
2	3.108023	0.082656	0.486294	-0.360752	0.070509
3	52.585782	0.141385	-0.083662	0.002003	0.003902
4	440.845718	0.079515	-0.110361	0.051379	-0.007983
$P_w/P_c = 0.3$ atm, $P_c = 0.1$ atm					
1	0.132242	0.478371	-0.698643	0.430921	-0.109044
2	14.660767	0.101065	0.204118	-0.202202	0.042771
3	1.750654	0.185155	0.299794	-0.240346	0.046968
4	165.763926	0.191665	-0.277448	0.135514	-0.021280
$P_w/P_c = 1/8, P_w + P_c = 1$ atm (corresponding to dry flue gas recycling, FGR)					
1	0.051237	0.515415	-0.618162	0.430921	-0.092082
2	0.688383	0.199807	0.298581	-0.265758	0.052910
3	13.763205	0.138767	-0.001851	-0.049353	0.013012
4	289.841885	0.087511	-0.067295	0.013489	-5.54E-06
$P_w/P_c = 1/4, P_w + P_c = 1$ atm					
1	0.052594	0.486247	-0.644137	0.485654	-0.107808
2	0.752776	0.213959	0.306543	-0.264417	0.051889
3	11.543306	0.181991	-0.020460	-0.053791	0.015058
4	252.938841	0.106180	-0.096088	0.028114	-0.002443
$P_w/P_c = 1/2, P_w + P_c = 1$ atm					
1	0.052378	0.383225	-0.510937	0.442201	-0.106398
2	0.712283	0.251481	0.161562	-0.150405	0.028982
3	8.067637	0.208239	0.070697	-0.135668	0.032090
4	195.892573	0.147259	-0.156339	0.057698	-0.007266
$P_w/P_c = 3/4, P_w + P_c = 1$ atm					
1	0.051639	0.255953	-0.276222	0.311285	-0.084903
2	0.617759	0.340592	-0.126902	0.051357	-0.010259
3	6.051770	0.160253	0.289548	-0.284144	0.003444
4	150.875915	0.201452	-0.233937	0.095159	-0.013302
$P_w/P_c = 1/1, P_w + P_c = 1$ atm (corresponding to wet FGR)					
1	0.051487	0.164048	-0.087793	0.195253	-0.063573
2	0.571797	0.412652	-0.339810	0.197886	-0.038963
3	5.398936	0.112364	0.450929	-0.388486	0.079862
4	130.622859	0.238339	-0.288619	0.121962	-0.017651
$P_w/P_c = 2/1, P_w + P_c = 1$ atm (corresponding to, e.g., oxy-fuel combustion of natural gas, without FGR)					
1	0.054480	-0.002188	0.286129	-0.048594	-0.016243
2	0.555304	0.546857	-0.714799	0.452812	-0.088841
3	5.040174	-0.001911	0.761177	-0.581819	0.115069
4	100.372663	0.317219	-0.415470	0.186570	-0.028335
$P_w/P_c = 4/1, P_w + P_c = 1$ atm					
1	0.060800	-0.053959	0.434975	-0.152413	0.005094
2	5.608331	-0.094953	0.952010	-0.696161	0.136316
3	0.676040	0.606525	-0.853216	0.545562	-0.107328
4	84.540632	0.369661	-0.517493	0.244011	-0.038451

P_w/P_c and P_w/P_c are never constant throughout any real combustion system. The parameters of different representative conditions will be used based on local gas conditions in the combustion system under modeling.



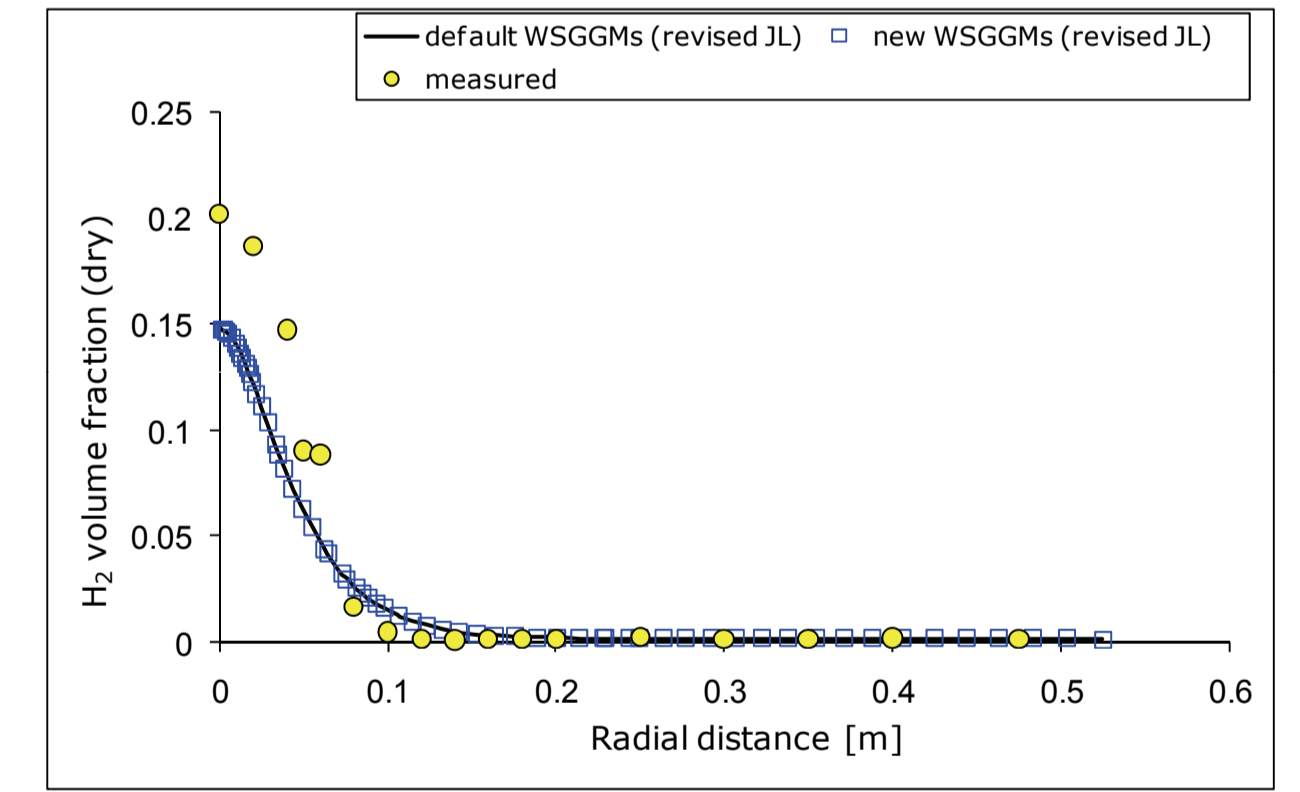
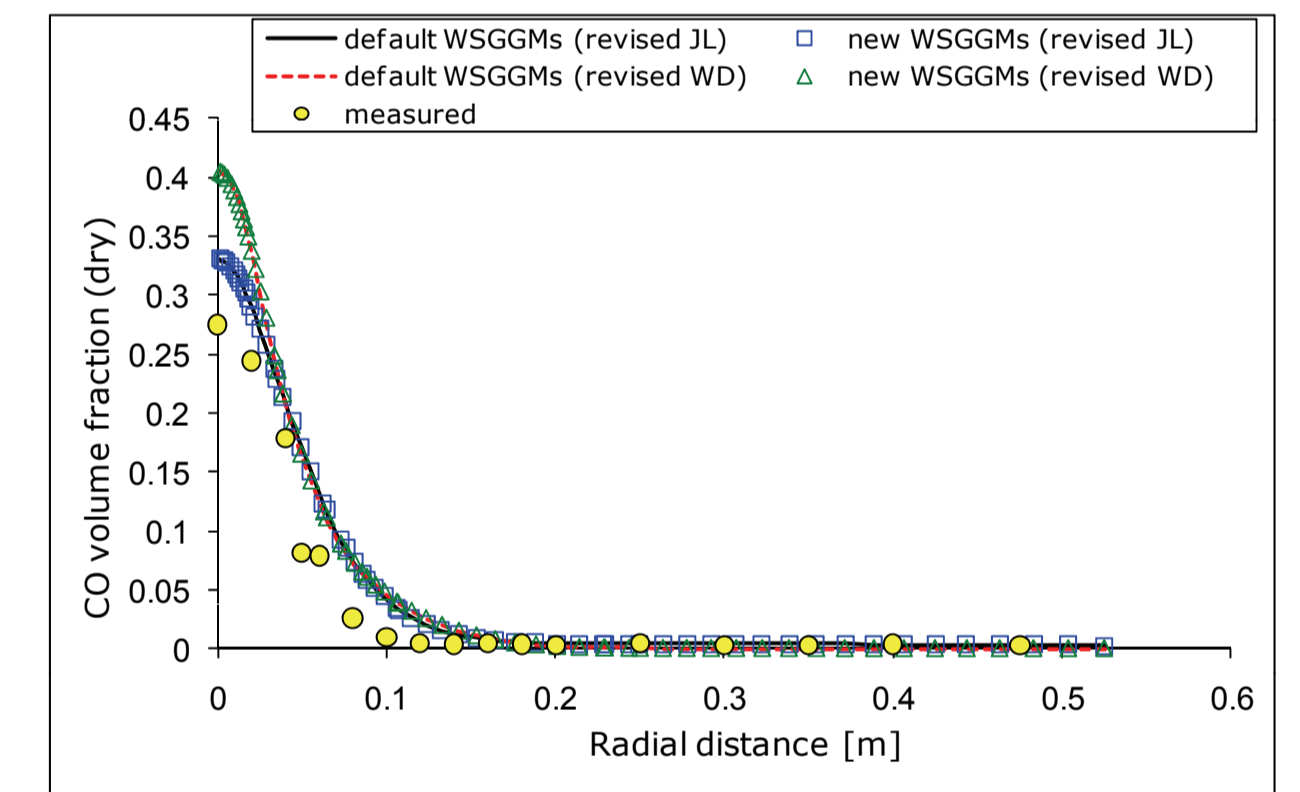
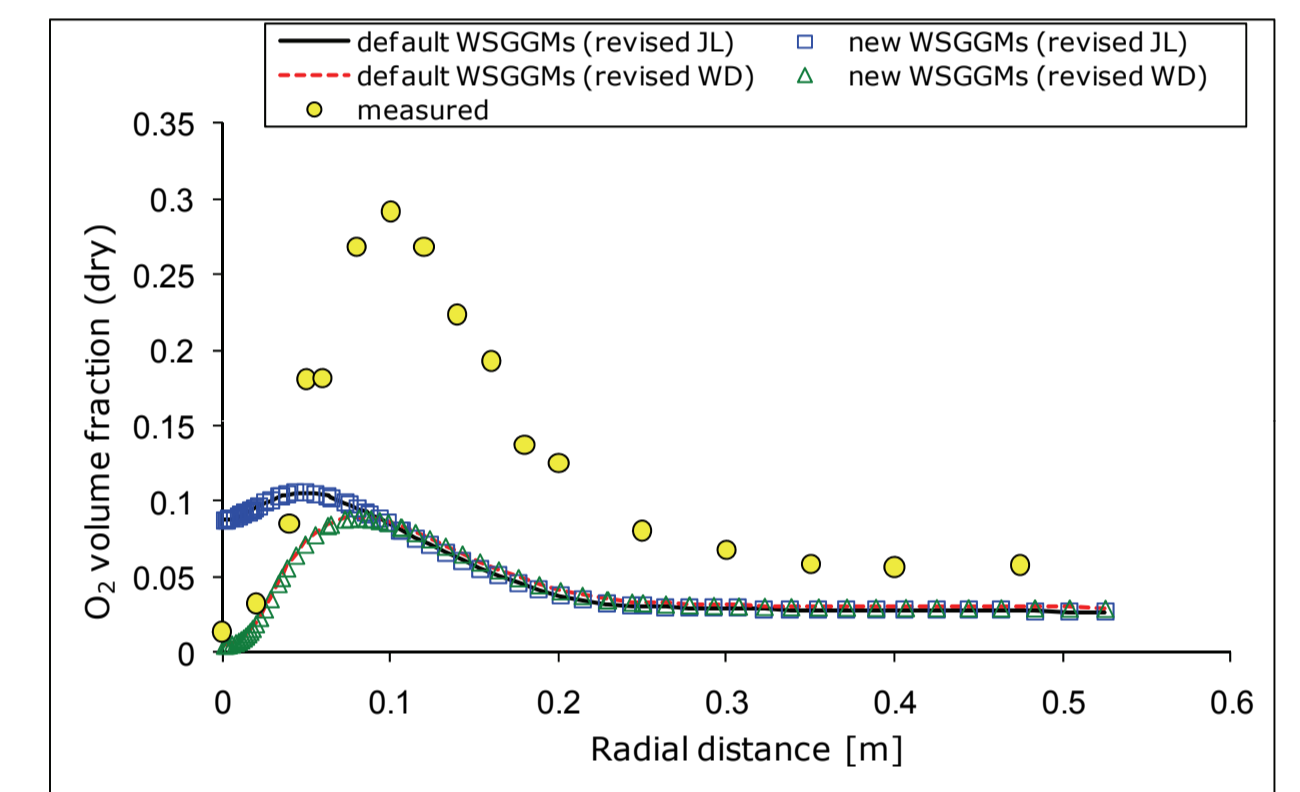
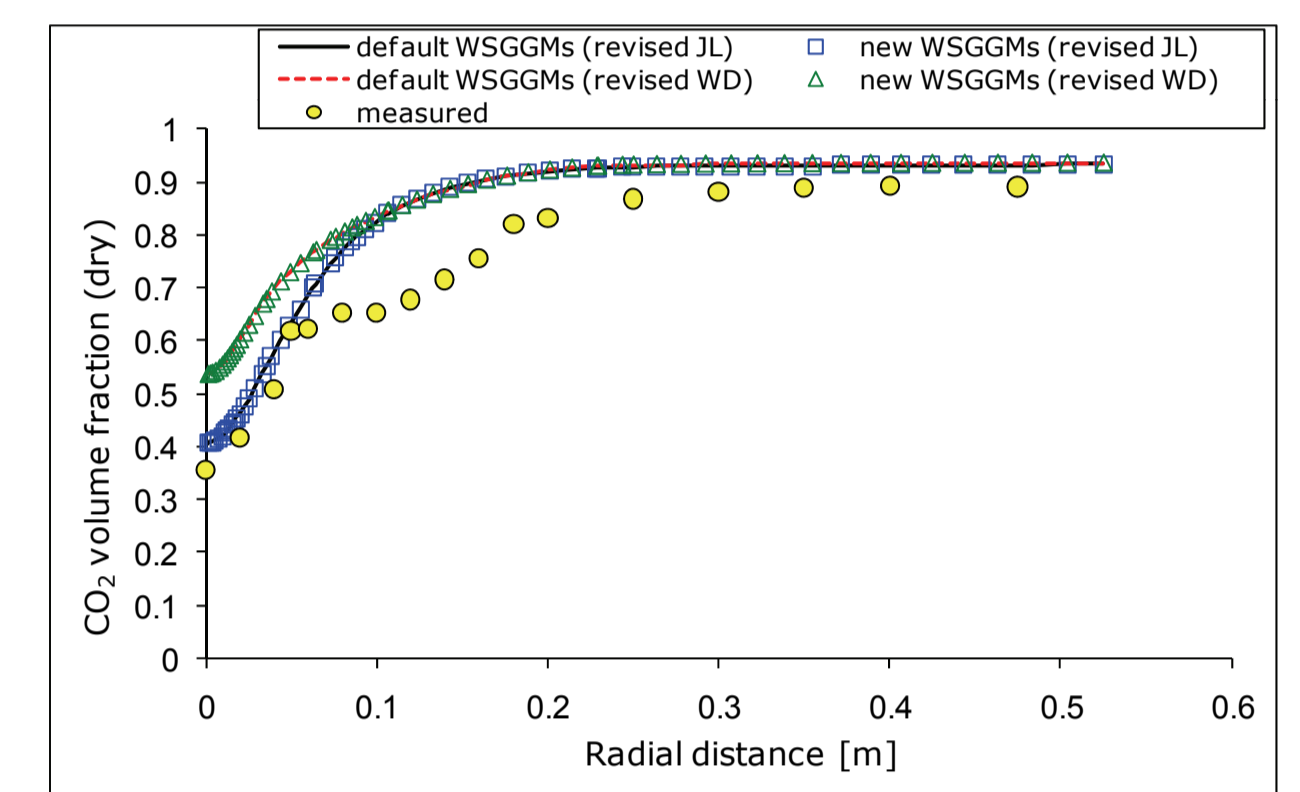
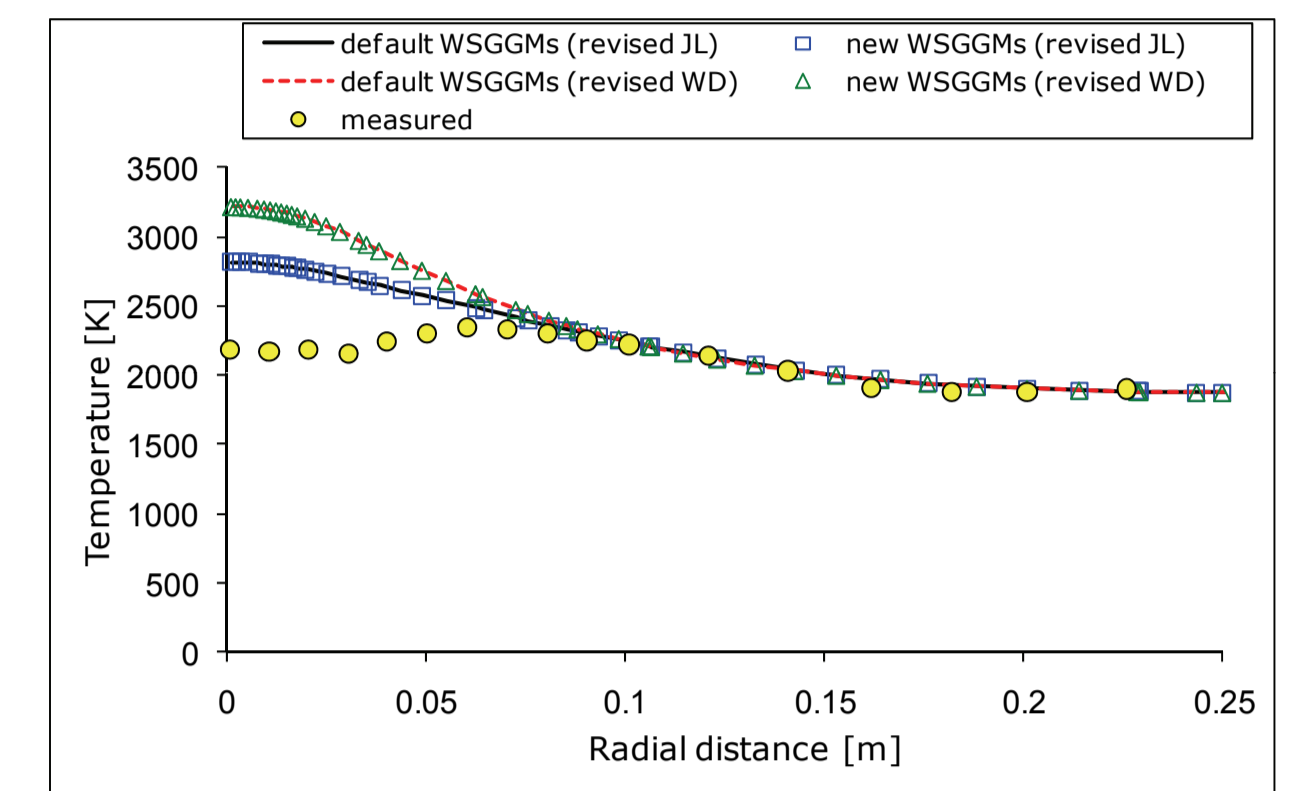
Emissivity vs. beam length at different P_w/P_c for constant temperature 1750K.



Emissivity vs. gas temperature at different P_w/P_c for constant beam length 40m.

Result 3: Demonstration

The new models have been applied to CFD of a 0.8MW IFRF oxy-natural gas flame furnace.



Conclusions

The new WSGGMs need to be used in CFD modeling of large-scale oxy-fuel furnaces. For small-scale facilities, they do not make remarkable difference. Combustion chemistry also plays a key role in oxy-firing modelling.

Contact:

Aalborg University, Dept. of Energy Technology

Chungen Yin

Ph: +45 30622577

Email: chy@et.aau.dk

Web: <http://www.iet.aau.dk>

Acknowledgements

This work was financially supported by Grant ForskEL 2009-1-0256, "Advanced modelling of oxy-fuel combustion of natural gas".