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

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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 H_2O, CO_2, CO, CH_4, NO and SO_2 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_T [Pa] = 101325.00
                               Path length,      S   [m]  =    0.50000
                               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 (η_L, η_U) for j-th band of i-th participating species ----------------------
   λ[μm]        χ[g/m2]    Pe      ω[1/cm]   α[m2/(g*cm)]     β        A[1/cm]     τ    Δη=A/(1-τ)[1/cm]  η_L[1/cm]  η_U[1/cm]
  H2O (i=0)
  71.43 (j=0)   11.7090  1.2753   268.398   4327.750522   0.03695   879.403   0.3052   1265.701          0.000    772.850
   6.25 (j=1)   11.7090  1.2753   218.436     41.200000   0.17712   259.220   0.5952    640.322       1279.839   1920.161
   2.66 (j=2)   11.7090  1.2753   232.379     24.995037   0.40010   253.996   0.7334    952.754       3283.623   4236.377
   1.87 (j=3)   11.7090  1.2753   166.926      3.913281   0.17365    45.346   0.9000    453.455       5123.272   5576.728
   1.38 (j=4)   11.7090  1.2753   123.935      2.647639   0.20987    31.001   0.9000    310.011       7094.995   7405.005
  CO2 (i=1)
  14.99 (j=0)   15.1962  1.0178    49.187     19.000000   1.12948   136.241   0.3610    213.219        560.391    773.609
  10.42 (j=1)   15.1962  1.0203    51.898      0.156331   0.90051     2.376   0.9000     23.756        948.122    971.878
   9.43 (j=2)   15.1962  1.0203    39.117      0.158436   2.66500     2.408   0.9000     24.076       1047.962   1072.038
   4.15 (j=3)   15.1962  1.0203    43.377    110.000000   4.15962   201.774   0.2150    257.030       2152.970   2410.000
   2.73 (j=4)   15.1962  1.0165    91.015      5.953672   3.30914    90.473   0.9000    904.730       3207.635   4112.365
   1.92 (j=5)   15.1962  1.0165   133.618      0.138024  12.02135     2.097   0.9000     20.974       5189.513   5210.487
  CO  (i=2)
   4.67 (j=0)    2.2757  1.0016    98.761     20.900000   0.05205    26.148   0.5984     65.118       2110.441   2175.559
   2.35 (j=1)    2.2757  1.0000    77.460      0.181109   0.13722     0.412   0.9000      4.122       4257.939   4262.061
  CH4 (i=3)
   7.63 (j=0)    0.3259  1.0012    81.333     28.000000   2.03872     9.124   0.9000     91.238       1264.381   1355.619
   3.31 (j=1)    0.3259  1.0012   216.887     46.000000   1.53867    14.989   0.9000    149.892       2945.054   3094.946
   2.37 (j=2)    0.3259  1.0012   232.379      4.248850   9.90290     1.384   0.9000     13.845       4213.078   4226.922
   1.71 (j=3)    0.3259  1.0012   174.284      0.811520  23.42482     0.264   0.9000      2.644       5859.678   5862.322

[2] Calculate band transmittances (τ_1, τ_2, τ_b), Planck blackbody fractional function (f_U, f_L), and total emissivity
  η_L[1/cm]   η_U[1/cm]   Overlapped_Bands(i, j)    τ_1      τ_2    τ_b=τ_1*τ_2    f_U       f_L      (1-τ_b)*(f_U-f_L)
    0.000      560.391      ( 0, 0) ( -, -)       0.3052   1.0000    0.3052     1.00000   0.99352      0.004500
  560.391      772.850      ( 0, 0) ( 1, 0)       0.3052   0.3610    0.1102     0.99352   0.98433      0.008176
  772.850      773.609      ( 1, 0) ( -, -)       0.3610   1.0000    0.3610     0.98433   0.98429      0.000027
  773.609      948.122      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.98429   0.97298      0.000000
  948.122      971.878      ( 1, 1) ( -, -)       0.9000   1.0000    0.9000     0.97298   0.97116      0.000181
  971.878     1047.962      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.97116   0.96491      0.000000
 1047.962     1072.038      ( 1, 2) ( -, -)       0.9000   1.0000    0.9000     0.96491   0.96280      0.000212
 1072.038     1264.381      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.96280   0.94346      0.000000
 1264.381     1279.839      ( 3, 0) ( -, -)       0.9000   1.0000    0.9000     0.94346   0.94172      0.000174
 1279.839     1355.619      ( 0, 1) ( 3, 0)       0.5952   0.9000    0.5357     0.94172   0.93282      0.004133
 1355.619     1920.161      ( 0, 1) ( -, -)       0.5952   1.0000    0.5952     0.93282   0.84847      0.034147
 1920.161     2110.441      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.84847   0.81415      0.000000
 2110.441     2152.970      ( 2, 0) ( -, -)       0.5984   1.0000    0.5984     0.81415   0.80616      0.003205
 2152.970     2175.559      ( 1, 3) ( 2, 0)       0.2150   0.5984    0.1287     0.80616   0.80188      0.003730
 2175.559     2410.000      ( 1, 3) ( -, -)       0.2150   1.0000    0.2150     0.80188   0.75599      0.036030
 2410.000     2945.054      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.75599   0.64526      0.000000
 2945.054     3094.946      ( 3, 1) ( -, -)       0.9000   1.0000    0.9000     0.64526   0.61382      0.003144
 3094.946     3207.635      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.61382   0.59031      0.000000
 3207.635     3283.623      ( 1, 4) ( -, -)       0.9000   1.0000    0.9000     0.59031   0.57455      0.001576
 3283.623     4112.365      ( 0, 2) ( 1, 4)       0.7334   0.9000    0.6601     0.57455   0.41325      0.054833
 4112.365     4213.078      ( 0, 2) ( -, -)       0.7334   1.0000    0.7334     0.41325   0.39545      0.004744
 4213.078     4226.922      ( 0, 2) ( 3, 2)       0.7334   0.9000    0.6601     0.39545   0.39304      0.000819
 4226.922     4236.377      ( 0, 2) ( -, -)       0.7334   1.0000    0.7334     0.39304   0.39140      0.000437
 4236.377     4257.939      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.39140   0.38767      0.000000
 4257.939     4262.061      ( 2, 1) ( -, -)       0.9000   1.0000    0.9000     0.38767   0.38696      0.000071
 4262.061     5123.272      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.38696   0.25687      0.000000
 5123.272     5189.513      ( 0, 3) ( -, -)       0.9000   1.0000    0.9000     0.25687   0.24839      0.000848
 5189.513     5210.487      ( 0, 3) ( 1, 5)       0.9000   0.9000    0.8100     0.24839   0.24575      0.000502
 5210.487     5576.728      ( 0, 3) ( -, -)       0.9000   1.0000    0.9000     0.24575   0.20306      0.004269
 5576.728     5859.678      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.20306   0.17432      0.000000
 5859.678     5862.322      ( 3, 3) ( -, -)       0.9000   1.0000    0.9000     0.17432   0.17406      0.000025
 5862.322     7094.995      ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.17406   0.08549      0.000000
 7094.995     7405.005      ( 0, 4) ( -, -)       0.9000   1.0000    0.9000     0.08549   0.07076      0.001473
 7405.005   100000.00       ( -, -) ( -, -)       1.0000   1.0000    1.0000     0.07076   0.00000      0.000000
                          ----------------------                                                  -----------------
                          ( -, -) means "no band"                                                 sum = 0.167256724

   The total emissivity of the mixture at the above condition,   ϵ = 0.167256724
   The equivalent (gray) absorption coefficient, -(1/S)*log(1-ϵ)  = 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.

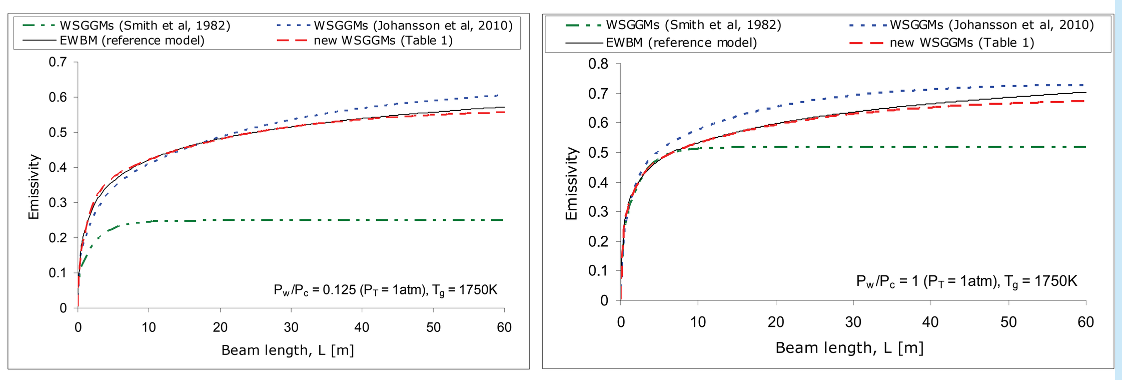
$$\varepsilon = \sum_{i=0}^{I} a_{\varepsilon,i}(T_g)\cdot\left(1-e^{-k_i\cdot P\cdot L}\right)$$

$$\begin{cases} a_{\varepsilon,i}(T) = \displaystyle\sum_{j=1}^{J} b_{\varepsilon,i,j}\left(\frac{T_g}{T_{\text{ref}}}\right)^{j-1} \quad i=1,\cdots,I \quad a_{\varepsilon,i}>0 \\ I=4,\quad J=4,\quad T_{\text{ref}}=1200 \text{ (in the unit of K) for a better estimate} \\ k_0=0 : \text{represent 'windows' in the spectrum;} \quad a_{\varepsilon,0}=1-\displaystyle\sum_{i=1}^{I} a_{\varepsilon,i}>0 \\ P: \text{ the sum of the partial pressures of all the participating gases, atm} \end{cases}$$

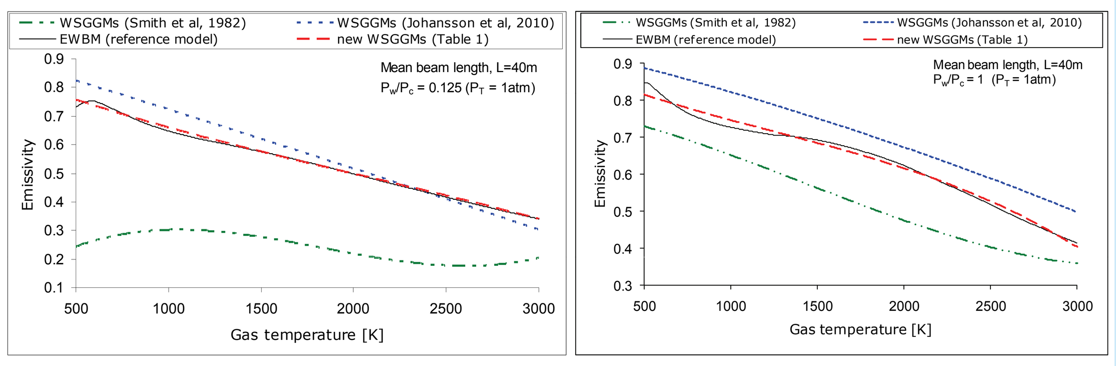
Table 1. New parameters for the WSGGMs, applicable to oxy-fuel flames.

i	k_i	$b_{\varepsilon,i,1}$	$b_{\varepsilon,i,2}$	$b_{\varepsilon,i,3}$	$b_{\varepsilon,i,4}$
$P_w \to 0$ atm, $P_c \to 0$ atm					
1	0.009422	0.778969	-1.342848	0.964858	-0.195747
2	0.415646	-0.011449	0.343754	-0.234886	0.044008
3	11.617018	-0.007627	0.242233	-0.173738	0.033868
4	319.911168	0.080082	-0.049280	0.001861	0.002232
$P_w = 0.1$ atm, $P_c = 0.1$ atm					
1	0.256738	0.492304	-0.433789	0.279329	-0.057770
2	3.108033	0.082686	0.486294	-0.369752	0.070509
3	52.585782	0.144385	-0.083662	0.002003	0.003902
4	440.845718	0.079515	-0.110361	0.051379	-0.007983
$P_w = 0.3$ atm, $P_c = 0.1$ atm					
1	0.132242	0.478371	-0.608643	0.475098	-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	0.133514	-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	0.052694	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	0.617739	0.340392	-0.126902	0.051357	-0.010259
3	6.051770	0.160253	0.289548	-0.284144	0.060344
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	0.764177	-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	-0.053999	0.434975	-0.152413	0.005094
2	5.608831	-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.



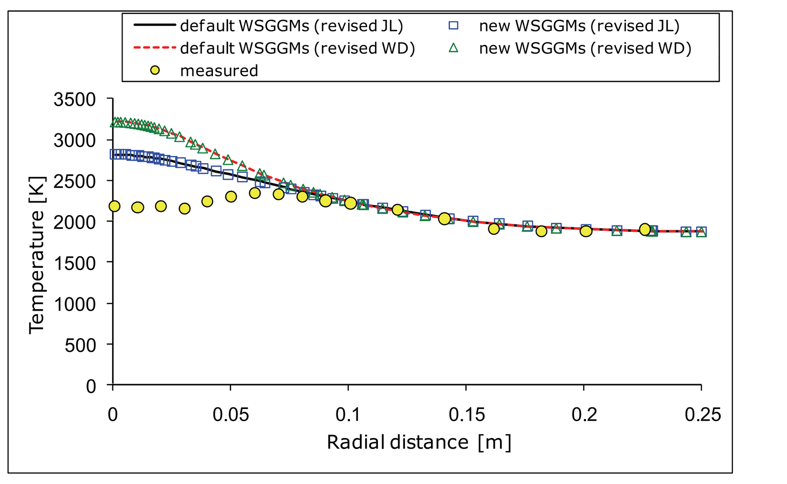
Emissivity vs. beam length at different P_w/P_c, for constant temperature 1750K.

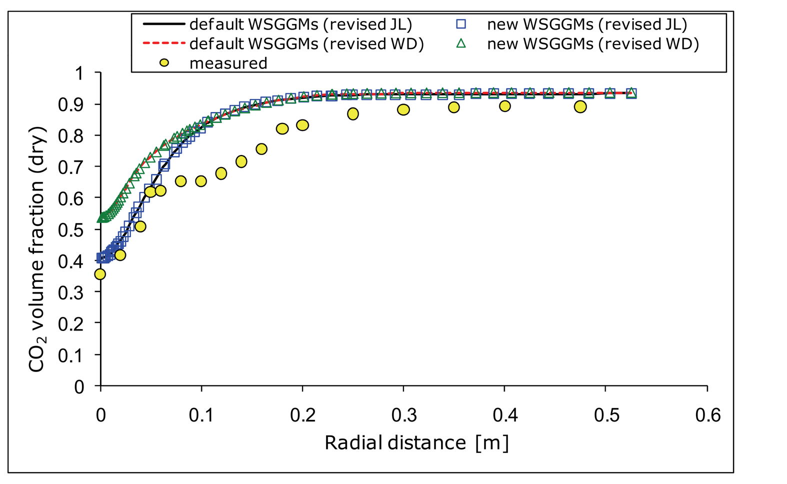


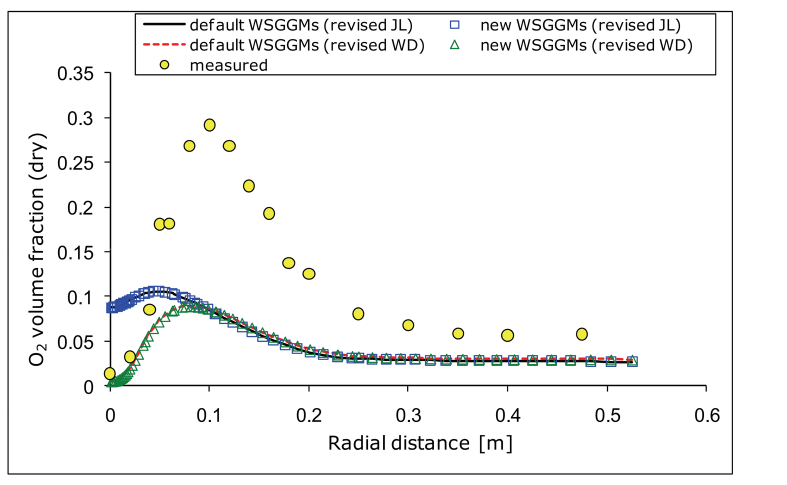
Emissivity vs. gas temperature at different P_w/P_c, for constant beam length 40m.

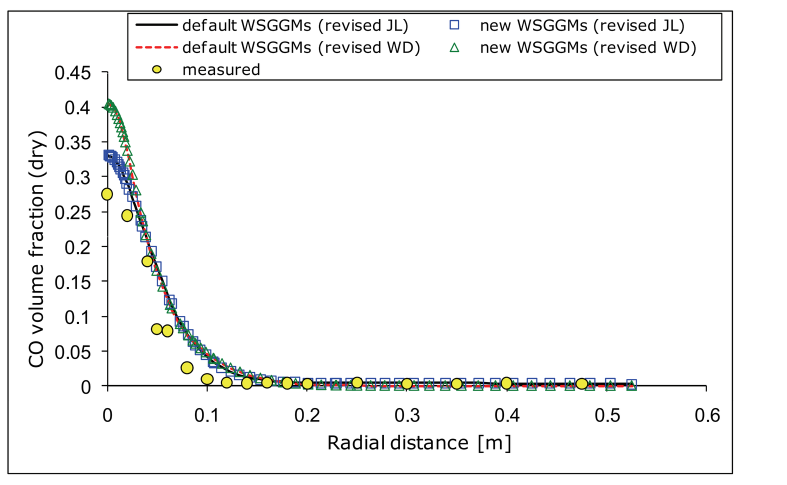
Result 3: Demonstration

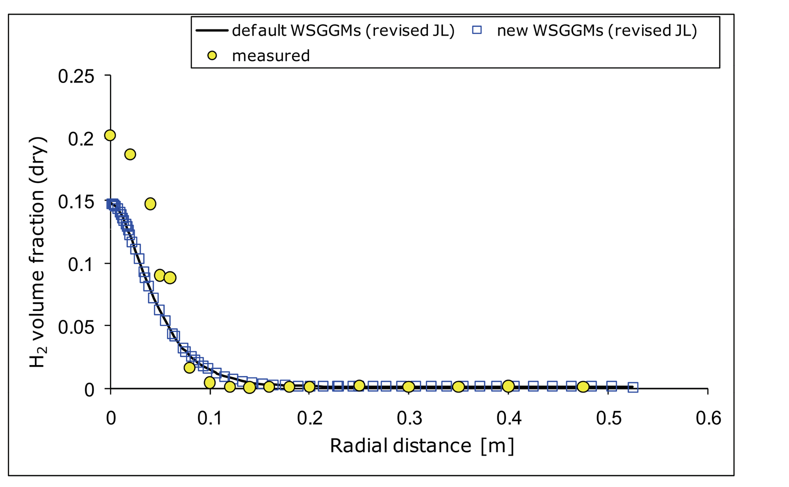
The new models have been applied to CFD of a 0.8MW IFRF oxy-natural gas flame furnace.











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.

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