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AN ASSESSMENT OF WSGG MODEL FOR CALCULATION OF RADIATIVE HEAT FLUX IN FDS

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Abstract. *In the present work, the performance of the Weighted-sum-of-gray-gases model for modeling radiative heat transfer for fire simulations in FDS is investigated. Here, the experiments of Hamins gas burners are simulated in Fire Dynamics Simulator (FDS) code and the calculated radiative heat flux is compared with the experimental measurements at different radial and vertical locations for two fuels of Methane and Acetylene. The fuels are different in terms of soot production where Methane is lightly and Acetylene is heavily sooting fuels. While the CO_2-H_2O mixture is modeled as a non-gray medium using the WSGG, soot is considered as a gray medium with a continuously active absorbing spectrum. The results showed that for the studied test cases, the WSGG model of FDS code properly predict the radiative heat flux with an acceptable accuracy. However, the increased computational cost of the code, due to larger number of RTE solution needed, may limit the benefit of the WSGG and non-gray gas modeling in general in fire calculations especially when the flame is soot-dominant.*

Keywords: *Spectral thermal radiation, non-Gray modeling, WSGG model, Fires, FDS*

1. INTRODUCTION

Radiative heat transfer is the dominant heat transfer mechanism in high-temperature systems (Bordbar and Hyppänen (2013), Bordbar and Hyppänen (2015)). Accordingly, an accurate prediction of this mechanism can affect the whole numerical modeling. In combustion and fire systems, radiative heat transfer is mainly due the participating species, namely H_2O, CO_2 and soot. The spectral absorption spectra of these species consist of thousands of hundereds lines over the spectrum. To predict radiative absorption and emission of the components, the line-by-line calculation is the most accurate approach but, due to the very high computational costs, its usage is limited to providing data for development and benchmarking of other simpler non-gray models. To provide a fast and accurate way to include non-grayness of the gases, many different models have been proposed during the last decades. Gray assumption is the very primary appproach which considers only one average value as absorption coefficient. This method enjoys the very low computational cost but its accuracy is questioned by several works (Darbandi *et al.* (2020); Bordbar *et al.* (2019)). Another approaches work based on implementing a few absorption coefficients based on deviding the spectrum into several portions or replacing the real spectra by smoother functions. Global models are a group of models that interpret the LBL spectra by alternative functions. Weighted-sum-of-gray-gases (WSGG) (Modest (1991)), spectral line based WSGG (SLW) (Denison and Webb (1993)), absorption distribution function (ADF) (Riviere *et al.* (1996)) and full spectrum correlated-k (Modest and Zhang (2002)) models are the most well-known global models .

The WSGG model is commonly known as the most widely used model in in modeling spectral radiation heat transfer in practical applications (Bordbar *et al.* (2014), Bordbar *et al.* (2020)). The reason is that WSGG model is computationally efficient and accurate and also its implementation is easier compared to the other models. This model was first proposed by Hottel and Sarofim (1965) in the framework of their zonal method and then was applied to any RTE solution methods by Modest (1991). In this method, instead of solving RTE for the spectral intervals over the entire spectrum, the spectrally integrated RTE is approximated with RTE solutions of only a few gray gases each with a certain weigth in the final summation. Traditionally, the WSGG model is used for H_2O-CO_2 mixtures as the main radiatively active combustion pruducts where the molar ratios can be considered constant. Yin *et al.* (2010) reported a WSGG model for the mixtures of H_2O-CO_2 in various combustion conditions. For oxy-fuel and air-fuel combustion scenarios, Bordbar *et al.* (2014), Johansson *et al.* (2011) and Kangwanpongpan *et al.* (2012) proposed WSGG models by including the molar ratios of H_2O and CO_2 of the mixture in the formulations of the model. In those works, Bordbar *et al.* (2014) and Kangwanpongpan *et al.* (2012) used LBL spectral database and Johansson *et al.* (2011) calculated the WSGG coefficients based on statistical narrow band model. Dorigon *et al.* (2013) reported two WSGG models for the H_2O-CO_2 mixures with molar ratios (Y_{H_2O}/Y_{CO_2}) of 1 and 2. Among the reviewed works, Bordbar's model is not limited to constant molar ratios but can be used for a wide range of thermal conditions with a high accuracy.

To date, performance of WSGG has been assessed in several researches. Kez *et al.* (2016) evaluated the statistical narrow band (SNB), the statistical narrow-band correlated-k (SNBCK), the wide-band correlated-k (WBCK) and the full spectrum correlated-k (FSCK) and several WSGG models in oxy-fuel combustion cases. Comparing the results obtained from the different models, they reported that Bordbar *et al.* (2014)'s WSGG model could predict SNB model as the benchmark solution at a satisfactory level however, the solution can be continued by FSCK model to achieve more accurate results. Later on, they studied different models for oxy-fuel furnace under coal-fired conditions and reported that the WSGG models of Bordbar *et al.* (2014) and Kangwanpongpan *et al.* (2012) were the most accurate WSGG models (Kez *et al.* (2017)). Fraga *et al.* (2017) employed gray gas and WSGG models to investigate turbulence-radiation interaction (TRI) effects in a non-reactive channel flow of a high temperature homogeneous participating gas. They reported that for high resolution LES of turbulent flames, the WSGG model could approximate the mean radiative heat flux accurately. Gronarz *et al.* (2017) studied radiative heat transfer in an oxy-fuel operated boiler using WSGG and SNBM models and reprted that the WSGG model had the sufficient accuracy. Centeno *et al.* (2018) employed WSGG model for calculation of thermal radiation in a non-gray sooting medium representing an axisymmetric laminar jet flame and compared it with LBL calculations. Their results showed that WSGG model was able to provide satisfactory solutions. Yang *et al.* (2019) evaluated WSGG model for radiative heat transfer calculation in realistic non-isothermal and homogeneous flames using decoupled and coupled calculations. Their research showed that using WSGG model improved the simulation accuracy of thermal radiation transfer. Using FDS code, Fraga *et al.* (2019b) and Fernandes *et al.* (2020) evaluated different gray gas formulations and reported the most accurate approach for the studied cases. In another research, Fraga *et al.* (2019a) employed FDS code and WSGG model to study Turbulence-Radiation Interaction in pool fires with low sooting fuels.

In this work, non-gray modeling of thermal radiation using the WSGG model for H_2O-CO_2 mixture and gray gas assumption for soot is studied using FDS code. The WSGG model of Bordbar is used for the mixture of H_2O and CO_2 and Sazhin's correlation is employed for gray modeling of soot. Here, Hamins gas burner experiments are the benchmark cases and the results of WSGG model are compared with experimantally measured values of heavily and lightly sooting fuels.

2. THEORY AND STATEMENT OF THE PROBLEM

Instead of solving hundreds of thousands RTEs in LBL calculations, the WSGG model approximates the entire absorption spectrum with a few gray gases. In WSGG model, the RTE is written as,

$$\frac{dI_j}{dx} = \kappa_j(x)(a_j(x)I_b(x) - I_j(x)) \tag{1}$$

where κ_j is the j-th gray gas absorption coefficient, $a_j(x)$ is the weight factor expressing the fraction of blackbody energy at the temperature of the medium corresponds to the spectral regions whose absorption is approximated by κ_j and $I_b(x)$ is Planck function. In Eq. (1), x is the position in the domain where gas specifications such as temperature are given. In WSGG model, the absorption coefficients and the weight factors of the gray gases are obtained by fitting the emissvity databases of a gas species obtained from other sources (usually line-by-line data). For the WSGG model used in FDS, a premixed H_2O-CO_2 LBL absorption coefficients was used to calculate the gray absorption coefficients and the weight factors. Total emissivity is calculated as,

$$\epsilon = \sum_{i=0}^{N_g} a_i(x)(1 - e^{-K_i P(Y_C + Y_H)L}) \tag{2}$$

where N_g, $a(x)$, K, P, Y_C, Y_H and L represent the number of gray gases, the weight factor, the absorption coefficient coefficients of the gray gases, total pressure of the mixture, molar fraction of CO_2, molar fraction of H_2O and pathlength, respectively. In this WSGG model, four gray gases plus one transparent gas representing the spectral windows are used. Based on the conservation of energy,

$$\sum_{i=0}^{N_g} a_i(x) = 1 \tag{3}$$

In the WSGG model used in this work (Bordbar *et al.* (2014)), the weight factors are considered as a polynomial function of temperature and the molar fraction ratio and absorption coefficients are polynomial of molar fraction ratio as,

$$a_i(x) = \sum_{j=0}^{4} b_{i,j} T_r^j \tag{4}$$

where T_r is defined as $T_r = T/T_{ref}$ ($T_{ref} = 1200$K). The $b_{i,j}$ in Eq.(4) is a polynomial function as,

$$b_{i,j} = \sum_{k=0}^{4} C_{i,j,k} M_r^k \tag{5}$$

and the absorption coefficient of gray gases in Eq.(2) is defined as,

$$K_i = \sum_{k=0}^{4} d_{i,k} M_r^k \tag{6}$$

The needed c and d coefficients were calculated and reported by Bordbar *et al.* (2014). With WSGG model in FDS, soot absorption coefficient in the form of effective absorption coefficient proposed by Sazhin and Sazhina (1996) is calculated as,

$$\kappa_s = b_1 c_m [1 + b_T (T - 2000)] \tag{7}$$

where $b_1 = 1232.4$, c_m is soot mass concentration and $b_T = 4.8 \times 10^{-4}$ K^{-1}. Then, the absorption coefficient of the mixture of H_2O, CO_2 and soot is obtained from the summation of the soot absorption coefficient, κ_s, and the absorption coefficient calculated by Eq. (6).

Because of using releatively coarse meshes in FDS simulations, the cells' temperature represent a bulk temperature by averaging over the cell volume. In the region where combustion occurs, the computed bulk temperature is usually lower than the true tempareature (McGrattan *et al.* (2012)). To prevent propogation of the error in the radiative source term, a correction factor, C, is employed with the emission term as,

$$I_{b,f}(x) = C\frac{\sigma T(x)^4}{\pi}, \; C = \min\left(C_{max}, \max\left[C_{min}, \frac{\sum_{\dot{q}'''_{ijk}>0}\left(\chi_r \dot{q}'''_{ijk} + \kappa_{ijk} U_{ijk}\right) dV}{\sum_{\dot{q}'''_{ijk}>0}\left(4\,\kappa_{ijk}\,\sigma\,T^4_{ijk}\right) dV}\right]\right) \tag{8}$$

The correction explained by Eq. (8) is applied to the cells in which $\chi_r q''' > 10$ kW/m^3, where χ_r is radiative fraction and q''' is total released energy. This criteria specifies the flaming region. The default values for C_{min} and C_{max} are set at 1 and 100, however, they can be changed to any arbitrary values. The radiative fraction, χ_r, is measured experimentally and for most of the fuels, it has been reported between 0.3 and 0.4. For Acetylene and Methane, the FDS default values used in this work are 0.49 and 0.2, respectively.

Here, the WSGG model in FDS is evaluated by comparing the numerical results with the experimental measurements of Hamins (2016). Hamins (2016) experimentally studied small and moderate-scale gaseous pool fires and measured time-averaged mass burning rate and radiative heat flux at different radial and vertical positions. In that study, the burners varying from 0.1m to 1.0m in diameter and total heat release rates from about 0.4 kW to 200 kW were studied. According to these conditions, the flames height was between 0.1 m to 2 m. Figure 1 shows a schematic diagram of the experimental setup and Figure 2 shows the geometry used in this work.

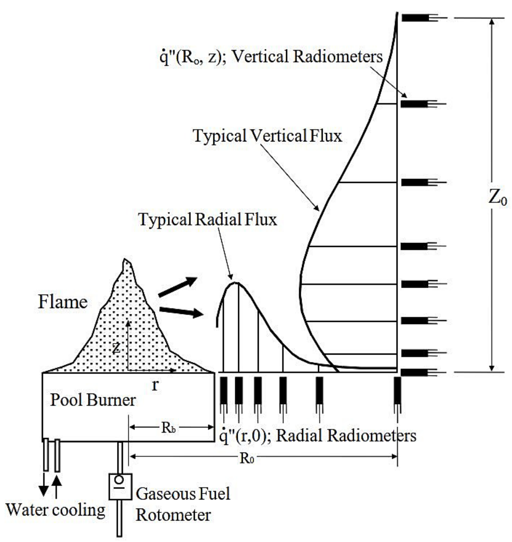

Figure 1. Experimental setup taken from Hamins (2016)

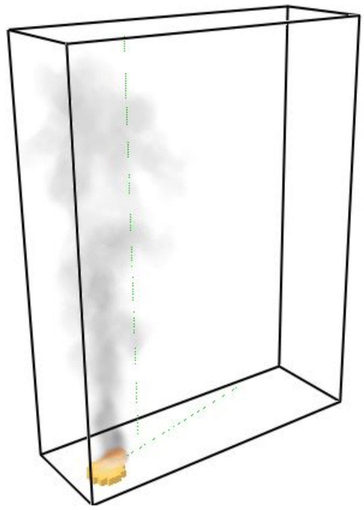

Figure 2. The FDS model built for Hamins gas burner experiments

3. RESULTS AND DISCUSSION

To validate the WSGG model in FDS, the predicted radiative heat flux were compared with the measurements of Hamins (2016) at different radial and vertical locations. The comparisons were done for Acetylene and Methane as heavily and lightly sooting fuels, respectively. In this work, three test cases for each fuel were selected to cover several burner's specifications such as diameter and heat release rates. Here, the test cases of 4, 8 and 12 for Acetylene and 3, 6 and 11 for Methane were chosen. Tables 1 and 2 present the details of the studied cases in which D is burner diameter, $\dot{m}$ is mass flux, R_0 is radial distance from the burner center to the vertical radiometer array, $\dot{Q}$ is heat release rate, $\dot{m}$ is mass loss rate, $\dot{Q}''$ is heat release rate per unit area, $\dot{Q}^*$ is dimentionless heat release rate, χ_{rad} is radiative fraction and D^* is dimensionless fire diameter and δx is mesh resolution. Figures 3 and 4 compare the measured and predicted radiative heat flux of Acetylene and Methane burners at different radial and vertical locations. As seen in Figure 3, the radiative heat flux predicted using WSGG model is overally in a good agreement with the measurements. For the test cases with lower burner diameter, the predicted heat fluxes are higher than the measured values and for the larger burner diameters, the predicted radiative heat flux is lower than the measurements, close to the burner. The reason is that when burner diameter incerases, the heat release rate increases and accordingly, the gas temperature within the flame increases. As explained previously, in FDS, the emission source term is calculated using the bulk temperature of the cell which is expected to be underestimated. This leads to predicting lower radiative heat fluxes compared to the experimental measurements in which the correction might not be effective. Additionally, the turbulence-radiation interaction has contribution to the radiative haet flux near the flame, but, this phenomena is not considered in FDS calculaitons. The higher errors are seen for both vertical and radial locations near the flame, but, they are more significant for the vertical measurements. Figure 5 indicates the uncertainity statistics of the measured and predicted heat flux of the studied cases, including relative standard deviations and the model bias factor.

Table 1. Specifications of the selected Acetylene test cases (Hamins (2016))

Test No.	D(m)	R_0(m)	$\dot{Q}$(kW)	$\dot{m}$(kg/s)	$\dot{Q}''$ (kW/m^2)	$\dot{Q}^*$	χ_{rad}	$D^*/\delta x$
4	0.1	0.13	1.29	0.027	164.2	0.37	0.27	6.7
8	0.35	0.51	20.4	0.424	212.0	0.26	0.22	8.1
12	0.35	0.69	62.4	1.29	648.6	0.78	0.42	12.7

Table 2. Specifications of the selected Methane test cases (Hamins (2016))

Test No.	D(m)	R_0(m)	$\dot{Q}$(kW)	$\dot{m}$(kg/s)	$\dot{Q}''$(kW/m^2)	$\dot{Q}^*$	χ_{rad}	$D^*/\delta x$
3	0.1	0.13	0.78	0.0155	99.3	0.22	0.13	11.0
6	0.35	0.4	11.2	0.226	115.9	0.14	0.08	6.4
11	0.35	0.63	27.0	0.546	280.3	0.34	0.15	9.1

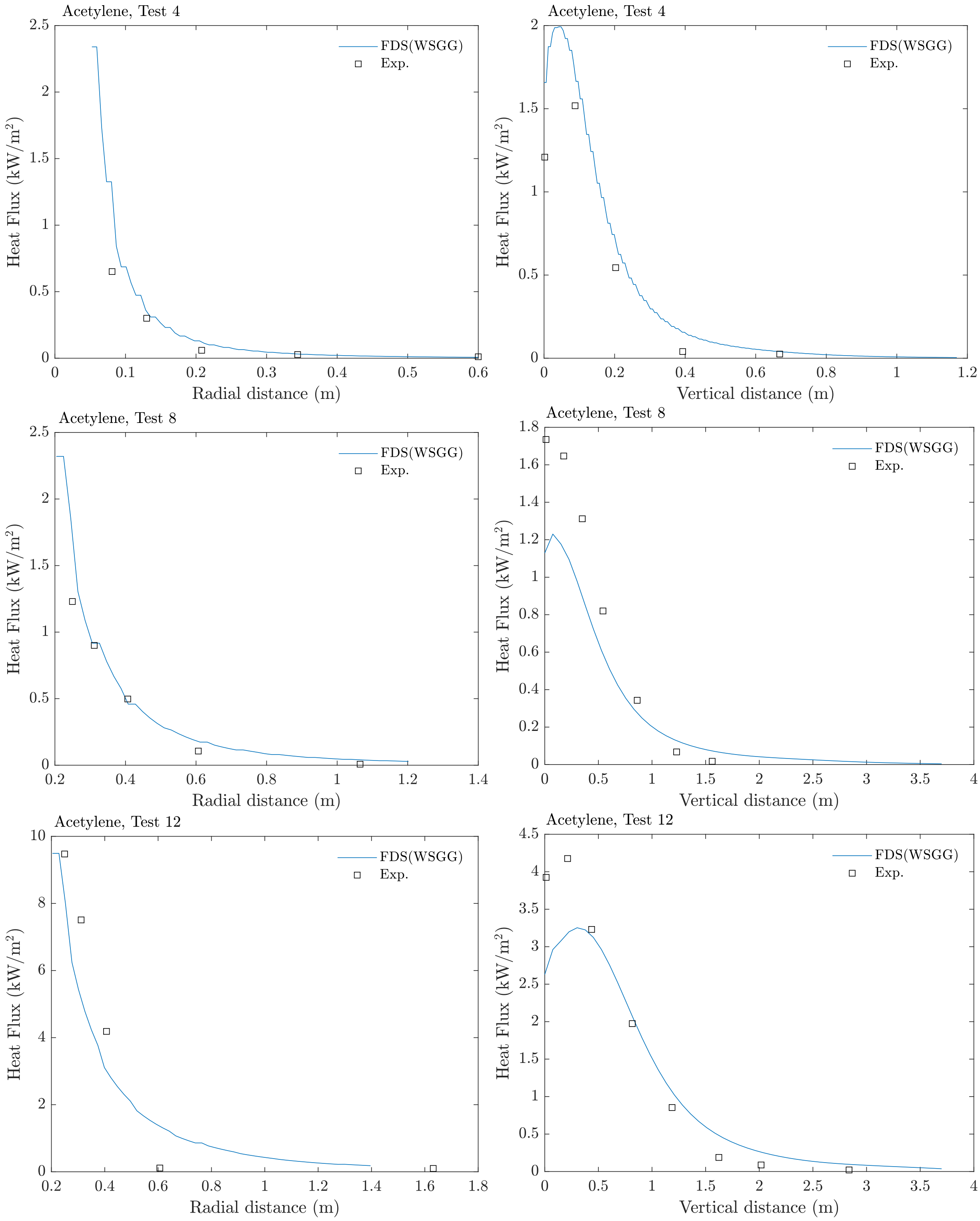

Figure 3. Comparison of predicted and measured heat fluxes for Hamins Acetylene test

4. CONCLUSION

To validate the WSGG model in FDS, Hamins Gas Burner was simulated and the predicted radiative heat flux along vertical and radial directions relative to the pool fire canterline were reported. Acetylene and Methane were chosen in this work due to their difference in soot production. Comparing the predicted radiative heat flux of Acetylene burner with the measurements, it can be concluded that the soot model used with WSGG model works well and the Methane cases as a lightly sooting fuel validates the WSGG model. The possible source of uncertainties are skipping Turbulence-Radiation interaction (TRI), setting parameters such as radiative fraction and heat release rate. Additionally, some numerical errors are added to the calculations from the LES turbulence model and the chemistry scheme which needs farther investigations. According to the comparisons presented in this work, it can be concluded that the WSGG model of FDS can be used for predicting the radiative heat flux.

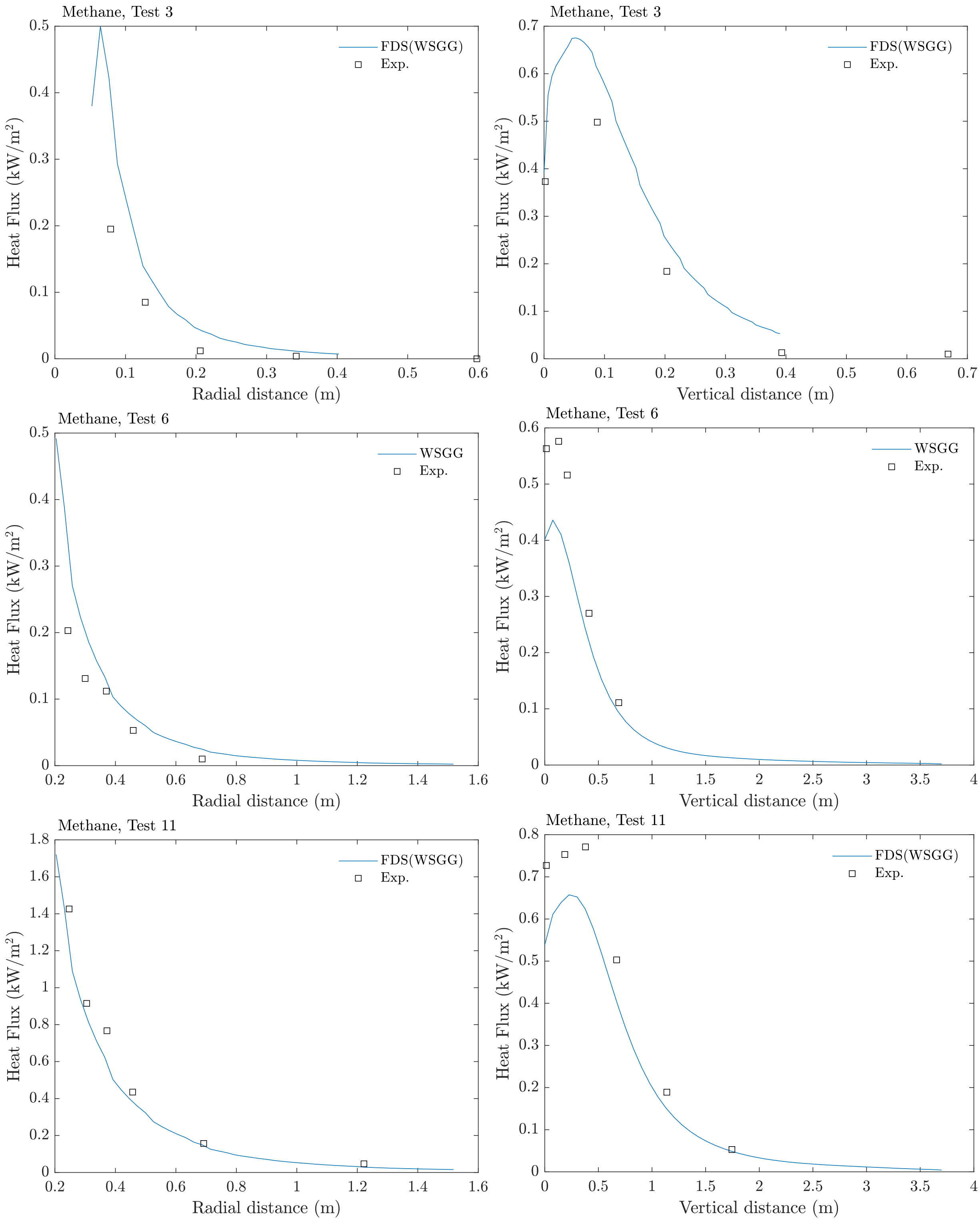

Figure 4. Comparison of predicted and measured heat fluxes for Hamins Methane test

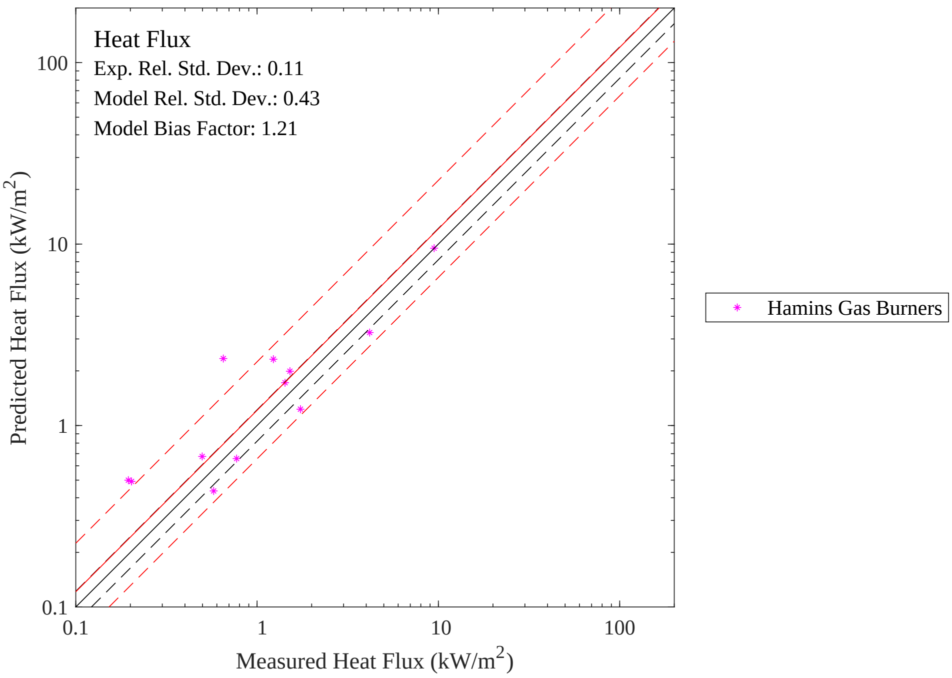

Figure 5. Uncertainity statistics

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