Response to reviewers' comments

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Title: CFD Simulation of a Natural Gas Combustion Burner

We thank the reviewer for the comments, which help to improve the clarity and quality of this manuscript. We considered all the comments carefully and made a necessary revision as suggested by the reviewer. We marked all the changes in the revised manuscript with yellow highlight.

Reviewer #1
It was unclear whether the studies for different k-ε are necessary as it was pointed out by the author that SKE has been proven to provide a reasonable prediction of temperature and chemical species concentration for natural gas combustion (page 2). A clarification is needed.

Response 1:
Three variant of k-ε turbulence model is evaluated in this work because they differ appreciably, and the newer k-ε variant such as RNG and RKE were specifically introduced to overcome the shortcoming of the standard k-ε. The standard k-ε (SKE) for instance can produce an unphysical –ve turbulence stresses and hence can produce unphysical result for strained turbulence flow. The newer variant, RKE still has a similar equation for turbulence viscosity (μ_t) as SKE, but the eddy viscosity (C_μ) is no longer a constant and instead is a function of velocity gradients to avoid a –ve normal turbulence stresses. Meanwhile, RNG uses an analytical equation for turbulent Prandtl number (Pr_t) to account for the interaction between turbulent dissipation and mean shear. Thus, RNG can provide a good prediction for rapidly strained flow, rotational and strong streamline curvature. In view with the shortcoming of SKE, we performed a comparison of turbulence models in this work. By looking at the results obtained, we agree with the reviewer that the difference on predictions of all three k-ε variant is not much owing to the simpler geometry of the combustion chamber used. However, the difference is clearly distinguishable from Figs. 6 and 7, and thus we are keeping the result as it is.

Action 1:
We added the following sentence in the introduction (page 2, line 27-30).

SKE is known to provide a reasonable prediction on the temperature and chemical species concentration for natural gas combustion, although it has a known issue to maintain a positive turbulence stresses besides giving a poor prediction of rotational and strained turbulence flow. The newer k-ε variant i.e., RKE and RNG are known to address the aforementioned issues.

We clearly mentioned the difference of the newer k-ε model in section 2.4 (page 9, line 1-21).

Reviewer #2
From Fig. 4C (location in between 0.05 to 0.15) the model prediction of P1 far overpredicts the Garreton and Simonin (1994) data by over 50 %. The difference must be commented.

Response 2:
We agree with the reviewer that the temperature prediction using P1 model at radial position X = 0.912 m is not great at location between 0.05 to 0.15, although temperature is correctly predicted at the position of the flame (Fig. 4A) and reasonably well predicted in other radial position. As we already introduce the P1 radiation model assume an isotropic spherical harmonic expansion of radiation intensity, which is not always accurate for many cases. In fact the most accurate model such as DO account for a discrete number of solid angle with respect to the hot surface, and hence supposedly more accurate than P1. We acknowledge that the difference between the two models is less pronounced in 2D model like the one in this work, but nevertheless the difference is observable (see Fig. 4). We believe the error is a follow through of poor gas fraction prediction at X = 0.912 m (see Fig. 5 at X ~ 0.9 m). The radiation through the gas inside the chamber is modelled using a weighted-sum-of-gray-gases model (WSGGM), thus error in gas composition prediction may follow through on the radiation heat transfer rate, since radiation account for about 90% of heat transfer in a combustion chamber. It is also known (ANSYS FLUENT, 2016) that P1 model tends to over-predict radiative fluxes from localized heat sources i.e. combustion flame.

Action 2:
We added the following sentence in section 3.2 (page 11, line 25 to page 12, line 3):

The large deviation of the predicted temperature at radial position of X = 0.912 m is a follow through of poor gas fraction prediction in the same region (see Fig. 5 at X ~ 0.9 m). The radiation through the gas inside the chamber is modelled using a weighted-sum-of-gray-gases model (WSGGM). The WSGGM uses a number of grey gases and weighting factor polynomials to model gas radiative properties, i.e. emissivity. Thus error in gas composition prediction may affect the radiation heat transfer rate, since radiation account for about 90% of heat transfer in a combustion chamber. In addition, P1 is known to over-predict the radiative fluxes from localized heat sources i.e. combustion flame at X ~ 0.9 m.

We had introduced explicitly the difference of DO and P1 in section 2.3.

Reviewer #3

How do the authors measure the time-varying temperature and mass fraction to obtain the data point in figure 6-7 and 10-11?

Response 3:
Data point for comparison was obtained from Garreton and Simonin (1994)'s work. The experimental data is measured at centreline of the combustion chamber, and the data presented is a time-averaged. Figs. 6, 7, 10 and 11 is not a time-varying; it is a position-varying time-averaged value. In ANSYS FLUENT, it is possible to record the data over finite time steps and to report them as statistical average. We mentioned the solution strategy explicitly in section 2.5 (page 10) as follows:

The simulation was firstly performed using first-order upwind scheme, steady-state SKE turbulence, DO radiation and FR/EDM. The unsteady-state solver and higher-order discretization scheme was then enabled after a converged solution was achieved. The thermophysical properties (i.e., specific heat, dynamic viscosity and thermal conductivity) of each chemical species at temperature range from 300 to 2500 K were introduced as a piecewise linear function. In partially premixed flame model, the GRI-MECH 3.0 associated with 325 mechanisms was used for more detail prediction. NASA polynomials (Thermochemical Data for Combustion Calculations) were used to model the gas properties as a function of temperature. The data were recorded for over 1000 time steps after a pseudo-steady solution was achieved and the value reported in this work is a statistical time-averaged.

Action 3:
We revised the following sentence in section 2.5 (page 10, line 16-17).

The data were recorded for over 1000 time steps after a pseudo-steady solution was achieved and the value reported in this work is a statistical time-averaged.

Reviewer #4
The authors need to comment on the significance of the model proposed against a more frequently used model (DTRM) for a more comprehensive discussion of the paper.

Response 4:
We are aware of DTRM radiation model. They are the simplest and cheapest to run, but can be CPU-intensive for a large number of rays. In term of hierarchical order DTRM is least complicated and the simplest compared to both P1 and DO. The DTRM has the following limitations, which both the DO and P1 does not have:

- The DTRM assumes that all surfaces are diffuse. This means that the reflection of incident radiation at the surface is isotropic with respect to solid angle.
- The effect of scattering is not included i.e. spectral emissivity is excluded.
- The implementation assumes either gray radiation or non-gray radiation, in the case of combustion both is needed.
- Solving a problem with a large number of rays is CPU-intensive.
- DTRM is not compatible with non-conformal interfaces or sliding meshes.
- DTRM is not compatible with parallel processing.

P1 model take into consideration the effect of radiation scattering and suitable for combustion where the optical thickness is large with little CPU demand. However, P1 is limited in term of solid angle, and since radiation in a complex geometry is affected by the solid angle, thus P1 do sometimes fails to give an accurate prediction for small optical thickness and complicated geometry. P-1 model tends to over-predict radiative fluxes from localized heat sources i.e. combustion flame.

The DO model is applicable to the entire range of optical thicknesses, making it possible to solve problems ranging from surface-to-surface radiation to participating radiation in combustion problems. It also allows the solution of radiation at semi-transparent walls. Computational cost is moderate for typical angular discretizations, and memory requirements are modest. DO model includes scattering, anisotropy, semi-transparent media, and particulate effects. Despite being the most comprehensive model, the CPU demand of DO model can be extensive.

Since both the DO and P1 is stated as most suitable for combustion and are much better option than that of DTRM, thus only DO and P1 was used in this work.

Action 4:
We added the following sentence in introduction (page 3, line 22-26).

It has to be noted that DTRM does not include the effect of radiation scattering and can only be accurate when a large number of rays is modelled (CPU-intensive). In addition the reflection of incident radiation at the surface is isotropic with respect to the solid angle, which is questionable, since the radiation should be a function of solid angle. All the aforementioned issues are addressed in the DO and P1 models.