# Mixing and entrainment of burned products in high Karlovitz number premixed jet flames

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## Abstract

Two large scale DNS of turbulent premixed combustion in jet flames are presented. The flames have the same jet Reynolds numbers of 5600 and Karlovitz number approximately equal to 40 and 400, respectively. These two high Karlovitz flames are analyzed to investigate the mixing and entrainment of fully burned products into the reaction and preheat zone of the flames. The simulations feature a 16 species, finite rate, chemical mechanism and up to 3 Billion grid points. In order to track the mixing of the coflow fluid into the flame, an equation for a tracer, i.e., a non-reactive, conserved, passive scalar with the same diffusivity of temperature, is solved in the DNS. In the higher Karlovitz number case, joint statistics of the local temperature and the tracer show that at locations where the temperature is close to that of the fresh mixture conditions, then deep in the preheat zone of the flame, up to 10% of the mixture is made of fluid coming from the coflow. This observation suggests that the flame is significantly diluted by burned products. The effects of this phenomenon on the local reactivity and dynamics of the flames are discussed. It is found that the local equivalence ratio is not affected significantly. The reaction rate of selected species is investigated. For methane, the reaction rate does not appear to be altered significantly. On the other hand, the oxidation rate of CO, which is supposed to consume almost completely the CO formed in the inner flame zone, is strongly affected by coflow mixing. Since the final CO emission is strongly sensitive to the balance between its production and oxidation, it is likely that the coflow mixing have a significant effect on the CO emission level at high Karlovitz.

## Introduction

In high Karlovitz number premixed combustion, the lenghtscales and timescales of the smallest turbulent structures are comparable or smaller than the corresponding characteristic scales of the flame. In this case, the inner zones of the flame structure, where the heating and the chemical reaction of the fresh mixture are concentrated, can be affected significantly since the smallest turbulent eddies can penetrate these layers, modifying the reactive-diffusive imbalance. The consequences for the flame dynamics are numerous. The local reaction rate can be altered with respect to the typical behavior of an unperturbed flame, inducing local quenching and a so-called broken-reaction regime. In addition, a remarkable widening of the thickness of the flame inner layers is often observed with strong consequences on the overall flame speed and global burning rate.

In addition to these phenomena, which have been studied extensively both by means of sophisticated experiments and direct numerical simulations (DNS), the intense turbulent transport that dominates high Karlovitz flames can induce mixing and entrainment of fully burned products into the low temperature regions of the premixed flame. This aspect can be very significant in jet and swirling flames, where the flames are stabilized with the heat and radical species provided by a stream of fully burned products, coming either from a pilot or from a recirculation region.

In the present work, two large scale DNS of methane-air flames at different Karlovitz numbers are analyzed to investigate the mixing and entrainment of fully burned products into the reaction and preheat zone of the flames.

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## DNS configuration, models, and methods

The flame configuration considered is a slot turbulent premixed jet flame surrounded by a coflow of burnt gases. The jet consists of a methane/air mixture with equivalence ratio $\Phi = 0.7$ and a temperature of 800 K and 500 K for the high Low and High Karlovitz cases, respectively. The background pressure is 4 atm. The temperature and equivalence ratio have been selected to be close to the typical conditions at the exit of the compressor in gas turbines. An elevated value of the pressure is chosen to optimize the numerical configuration as it allows high Reynolds and Karlovitz numbers avoiding excessive inlet velocities and slot widths. Based on one-dimensional simulations of freely propagating flames, the laminar flame speed are $S_L = 1$ m s$^{-1}$ and $0.25$ m s$^{-1}$, while the thermal thickness are $\delta_L = 110$ $\mu$m and 360 $\mu$m for the Low and High Karlovitz cases, respectively. The bulk velocities of the jets are $U$ = 100 m s$^{-1}$ and 90 m s$^{-1}$ while the coflows have velocity of 15 m s$^{-1}$ and 13.5 m s$^{-1}$.

For both cases, the Reynolds number $\mathrm{Re} = UH/\nu$ is 5600. The inlet velocities, jet widths, and laminar flame speeds yield a Karlovitz number $\mathrm{Ka} = \delta_L^2/\eta^2$ approximately equal to 40 and 400 for the two cases, with $u'/S_L$ around 10 and 35. The Kolmogorov scale is defined as $\eta = (\overline{\nu}^3/\tilde{\epsilon})^{1/4}$, where $\tilde{\epsilon}$ is the Favre averaged energy dissipation and $\overline{\nu} = \overline{\mu/\rho}$ is the averaged viscosity.

The domain is periodic in $z$, open boundary conditions are prescribed at the outlet in $x$ and no-slip conditions are imposed at the boundaries in $y$. The inlet conditions for the velocity field are obtained from an auxiliary simulation of fully developed turbulent channel flow.

The mesh is uniform in all three directions and the resolution is such that $\Delta/\eta < 2$ and $\delta_L/\Delta \sim 6$ for the Low $\mathrm{Ka}$ case. For the High $\mathrm{Ka}$ case, $\delta_L/\Delta \sim 20$. The Low $\mathrm{Ka}$ simulated with double the spatial resolution also without any significant change in the statistics. An analysis of the resolution requirements is available in Luca et al. [1]. The total number of grid points is about 350 Million and 3 Billion for the Low and High Karlovitz cases, respectively.

The reactive, unsteady Navier-Stokes equations are solved in the low Mach number limit [2] with an established finite-difference solver suitable for use on massively parallel high-performance computing platforms [3]. The mixture obeys the ideal gas equation of state and all transport properties are computed with a mixture-average approach [4]. The simulations feature finite rate chemistry, described by a skeletal methane mechanism with 16 species and 72 reactions [5], and customized source code for the evaluation of the analytical Jacobian of the reactive source terms [6]. In order to track the mixing of the coflow fluid into the flame, an equation for a tracer $ZMIX$, i.e., a non-reactive, conserved, passive scalar with the same diffusivity of temperature, is solved in the DNS. The boundary condition at the inlet for this scalar is equal to one in the central jet and zero in the coflow. All simulations were performed on the Cray XC40 supercomputer "Shaheen" at King Abdullah University of Science and Technology using up to 131,072 processors.

Figure 1 shows two-dimensional cuts of the vorticity and atomic oxygen mass fraction in the two cases. Due to the relatively lower flame speed in the High Karlovitz case, this flame is characterized by a significant larger length (measured in terms of the jet width $H$). For the same reason and due to the different tendency to entrain coflow fluid in the two cases, the High $\mathrm{Ka}$ flame is also characterized by a larger lateral spreading compared to the Low $\mathrm{Ka}$ case, as made evident by the visualization of the oxygen radical.

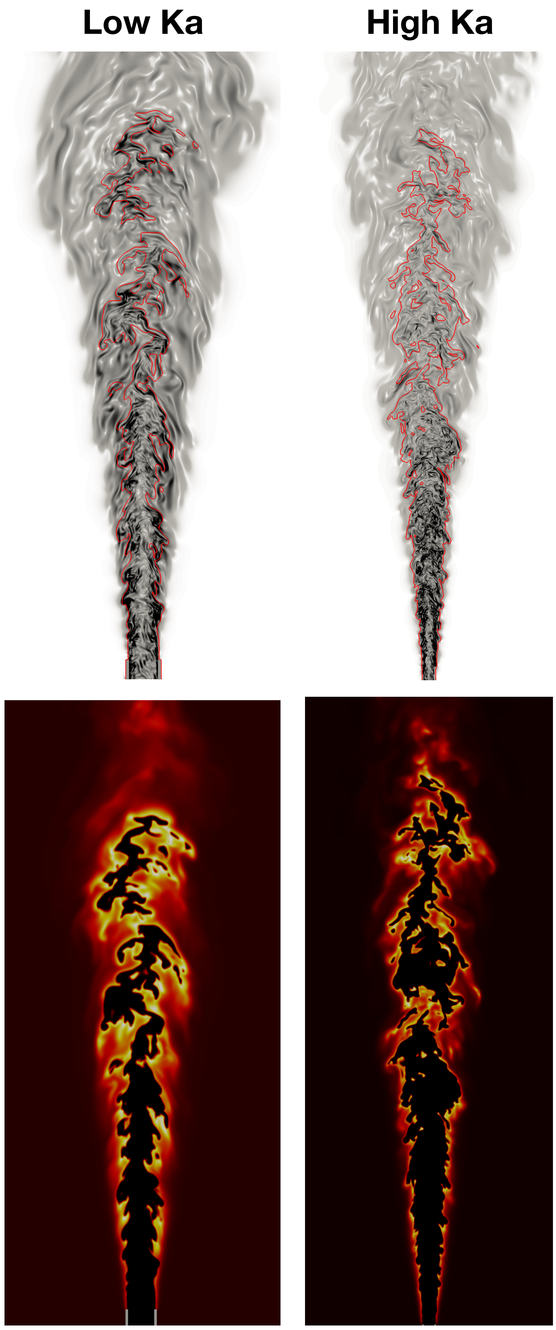


Figure 1: Two-dimensional cuts of the vorticity (top) and atomic oxygen mass fraction (bottom) for the two flame at different Karlovitz number. In the vorticity plots, the isoline of the temperature of maximum heat release rate in the unstreached laminar freely propagating flame is also shown.

**Entrainment and mixing of coflow**

In order to quantify the entrainment of coflow fluid into the burning flames, Fig. 2 shows scatter plots of temperature and mass fraction of the coflow fluid, identified by the passive scalar $ZMIX$. The results are shown for 4 different streamwise locations, corresponding to 10, 30, 70 and 100% of the flame length, which has been computed as the position on the centerline where the mean temperature is equal to the value at which the heat release rate peaks in the corresponding one-dimentional steady unstretched flame. In these plots, a value of $ZMIX$ equal to zero indicates that the local fluid is completely coming from the coflow stream injected at the domain inlet, while a value of one correspond to fluid originating from the central jet. While the value of $ZMIX$ is not directly influenced by combustion due to the lack of a source term in its equation, the temperature is subjected to both combustion and mixing. If combustion was absent, the plots would show a linear profile describing pure mixing between the hot coflow with $ZMIX = 0$ and the central jet characterized by the fresh mixture temperature, i.e., 800 and 500 K for the two cases respectively, and $ZMIX = 1$. The other limiting case would be observed if entrainment and mixing was negligible. In this case, the plot would shows a constant value of $ZMIX = 1$ at all temperature with a discontinuous drop of $ZMIX$ from one to zero at the maximum temperature.

From the analysis of the plot in Fig. 2, it can be observed that at the flame base, close to the nozzle exit, the mixing of coflow fluid into the flame is very strong. For both cases with different Ka, the scatter plot is not far from the pure mixing line. Moving downstream, combustion tends to overcome mixing and the profile become more and more horizontal, a behavior corresponding to pure premixed combustion. The horizontal profile extends over a rather large range of temperature, even if mixing is still dominant for very large temperature. However, even if in both cases the profile is approximately horizontal for $x > 0.5$L, the value of $ZMIX$ is not one. This means that combustion is actually happening in a premixed flame of methane and air diluted with the fluid coming from the coflow. Even very far from the inlet and close to the flame tip, in the high Ka the fresh mixture contains about 6% of coflow fluid. This behavior points out the fact that, for increasing Karlovitz, the flame should be not regarded as purely premixed.

**Effect on flame structure**

In a recent analysis of experimental data of an high Karlovitz flame, Wabel et al. [7] observed a similar behavior, pointing out that the local equivalence ratio in a high Ka flame might be influenced by mixing of the coflow or pilot fluid. In their experiment, Wabel et al. [7] used a coflow consisting of the burned product of a flame with a larger equivalence ratio compared to that of the main flame, therefore observed an actual stratification of the combustion.

In the present case, the fully burned product resulting from full combustion of the fresh mixture composition of the main jet have been used as coflow. Therefore, the mixing and entrainment has a relatively smaller effects on the local equivalence ratio observed in the flame, compared to the case investigated by Wabel et al. [7]. In particular, Fig. 3 shows scatter plots of temperature and equivalence ratio for different streamwise positions. In the present case, we followed Wabel et al. [7] using the definition suggested by Sweeney et al. [8] for the equivalence ratio:

$$phi = \frac{X_{CO_2} + 2X_{CH_4} + X_{CO} + 0.5(X_{H_2O}) + X_{H_2}}{X_{CO_2} + X_{O_2} + 0.5(X_{H_2O}) + X_{CO}} \qquad (1)$$

The local equivalence ratio is not constant across the turbulent flame; however, the fluctuations can be ascribed to the differential diffusion between different species. For very low temperature, i.e., in the unburned side of the flame, the local equivalence ratio is close to the nominal value of 0.7. In particular, it can be observed that, at the two downstream locations ($x = 0.7L$ and $x = L$) for the high Ka flame, where the scalar $ZMIX$ is around 0.93

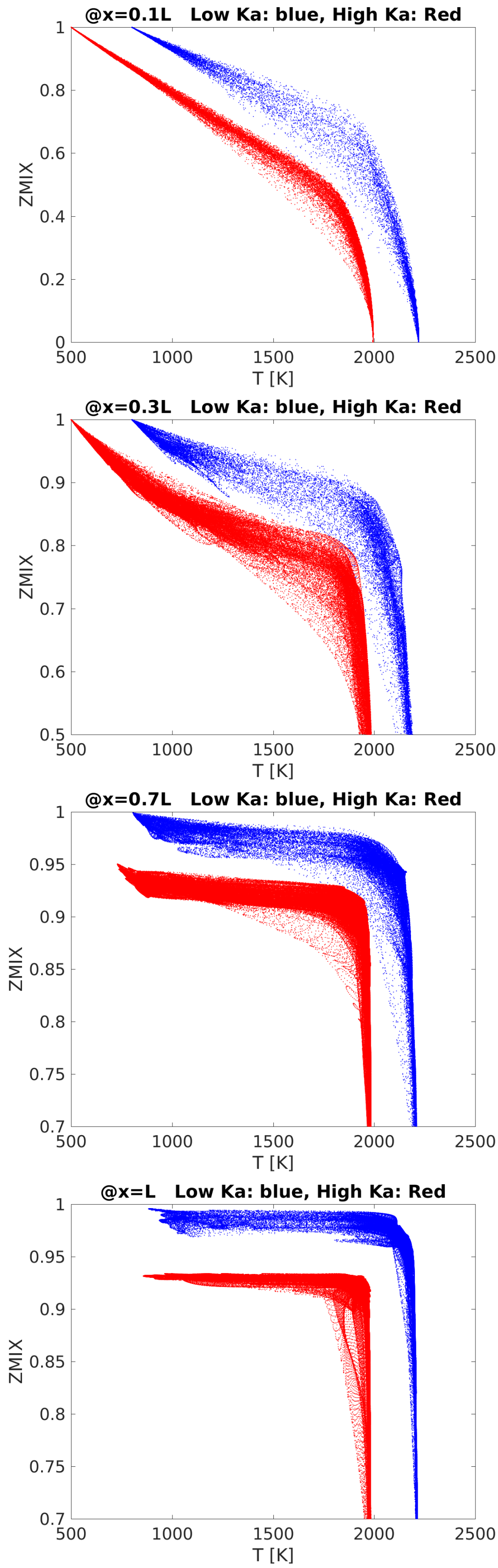


Figure 2: Scatter plots of temperature and mass fraction of the coflow fluid, identified by the passive scalar $ZMIX$. The results are shown for 4 different streamwise locations, corresponding to 10, 30, 70 and 100% of the flame length.

for a temperature of bout $1000K$, the equivalence ratio is not too far from $0.7$.

In addition, it is also interesting to assess the effect of the entrainment of coflow fluid on the local reaction rates. In Figs. 4 and 5, the reaction rates of the fuel (methane, $CH_4$) and CO are shown for two different streamwise locations and for the two cases. The corresponding profiles for one-dimensional unstreached laminar flames is also shown as reference. It can be observed that the effect of coflow mixing and entrainment is minor for the reaction rate of methane. In particular, the scatter plots in the two DNS cases do not differ significantly and both follow the one-dimensional profile.

Also for the CO reaction rate, the profiles do not appear very different. However, it should be noted that for large value of temperature, the CO reaction rate, which is supposed to be negative, shows important deviations from the one-dimensional profile, becoming much smaller in absolute value or even positive. Since the final emissions of CO in combustion systems strongly depend on the fine balance between the initial formation of CO in the colder side of the flame and the subsequent oxidation in the hotter part of the flame, the effect of coflow entrainment in the region of the flame where CO is supposed to be almost completely oxidized might have significant impact.


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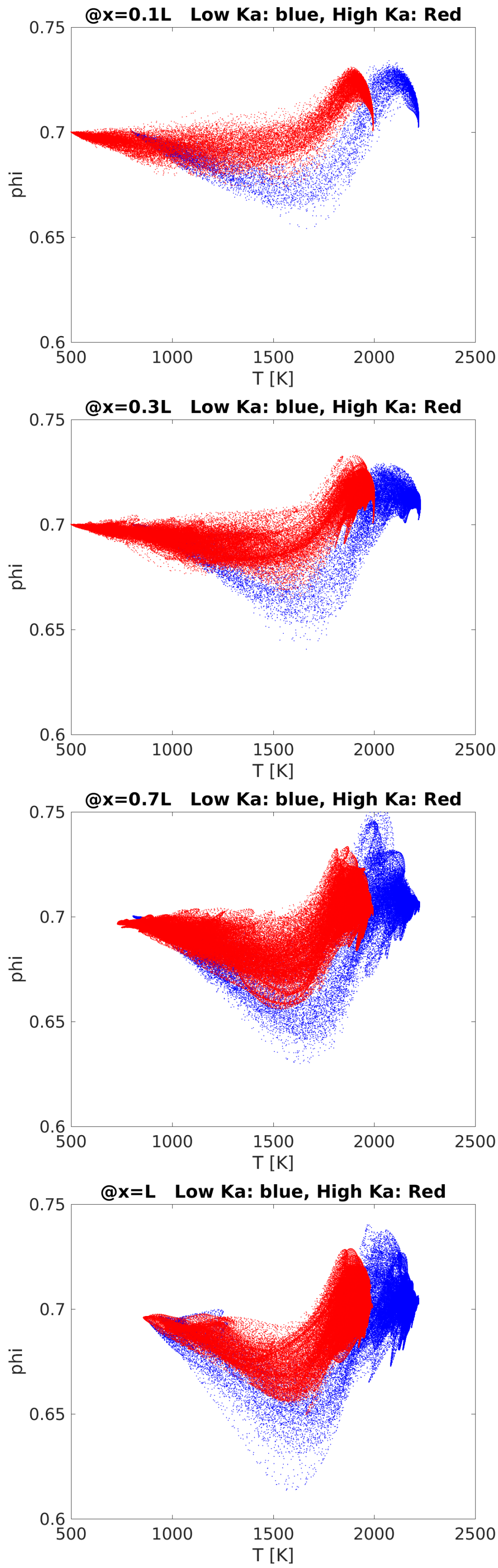


Figure 3: Scatter plots of temperature and local equivalence ratio, computed using eq. 1. The results are shown for 4 different streamwise locations, corresponding to 10, 30, 70 and 100% of the flame length.

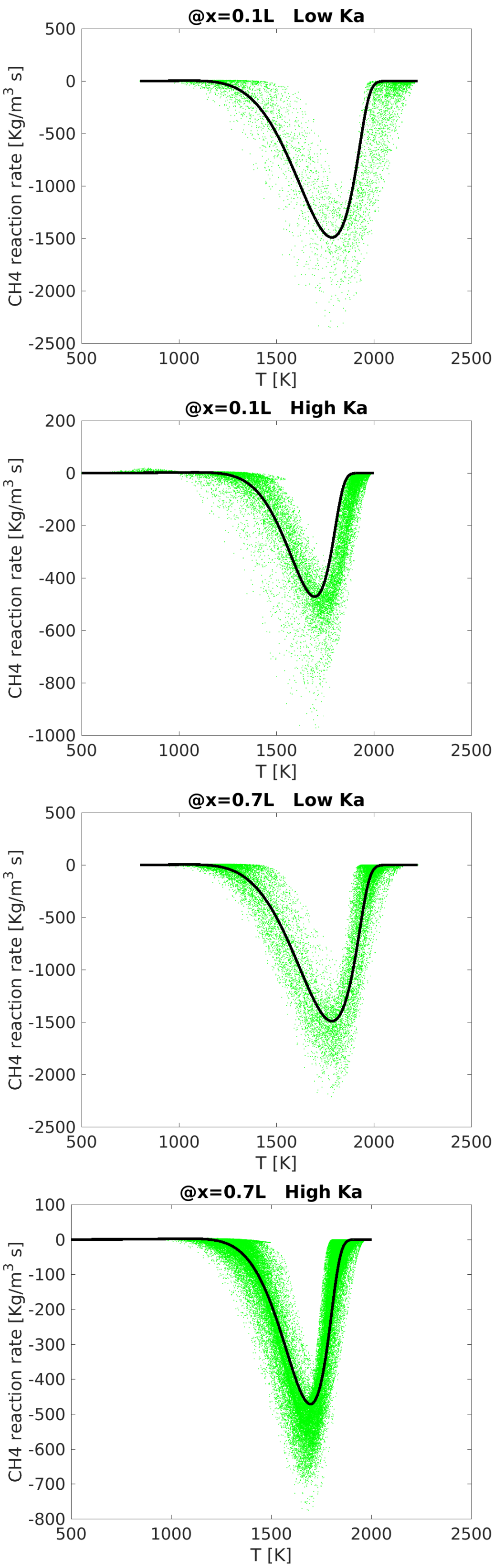


Figure 4: Scatter plot of temperature and methane ($CH_4$) reaction rate at two different streamwise positions for two DNS cases with different Karlovitz number.

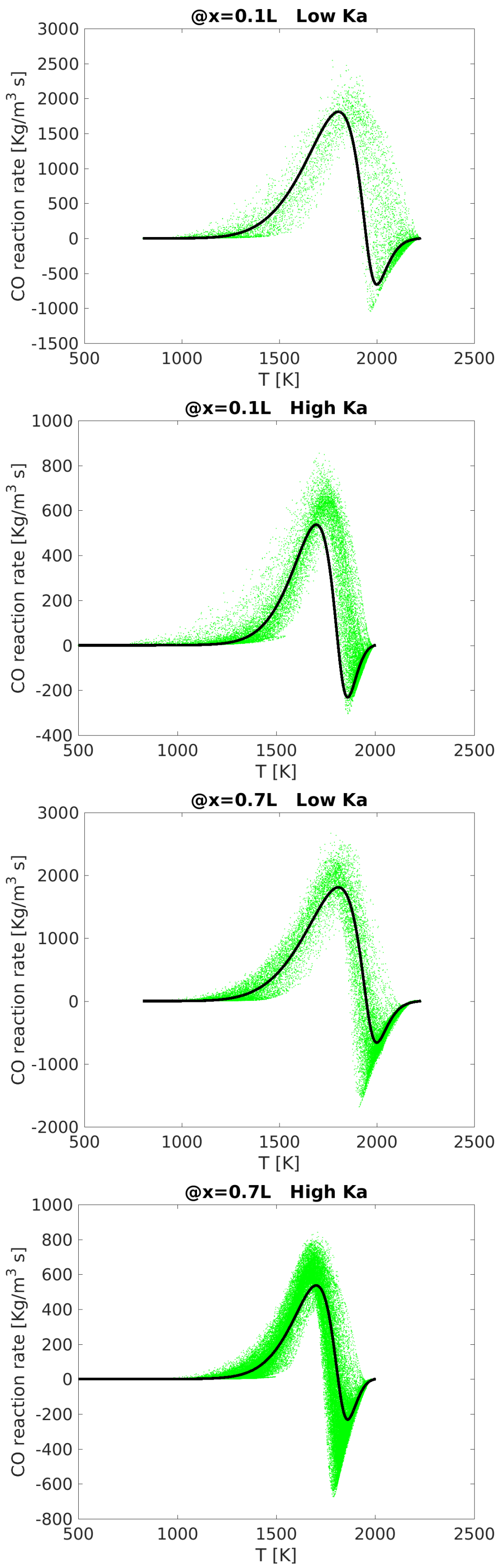


Figure 5: Scatter plot of temperature and CO reaction rate at two different streamwise positions for two DNS cases with different Karlovitz number.