Numerical Studies of Novel Inwardly Off-Center Shearing Jet-Stirred Reactor

Tianhan Zhang,* Hao Zhao,* and Yiguang Ju†
Princeton University, Princeton, New Jersey 08544

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A novel inwardly off-center shearing jet-stirred reactor is proposed and examined computationally. The inwardly off-center shearing jet-stirred reactor is compared with two traditional jet-stirred reactor designs, the outward cross-injector jet-stirred reactor and the concentric inward and outward jet-stirred reactor. The results show that the present inwardly off-center shearing jet-stirred reactor has significant improvement in terms of mixture uniformity and residence time distribution. Numerical results show the distributions of residence time in the two traditional jet-stirred reactors are wide and long tailed because of the formation of large and stable vortices, and the corresponding mean residence time of the two classical jet-stirred reactors deviates from the theoretical value by about 20%, while the new inwardly off-center shearing jet-stirred reactor has a much narrower residence time distribution and reduces the deviation to 8%, mainly attributed to the smaller vortices generated by an optimized jet arrangement. Moreover, the new inwardly off-center shearing jet-stirred reactor provides a fully optic-accessible platform for kinetic studies of alternative and real jet fuels.

I. Introduction

OVER the last few decades, there has been increasing interest in developing alternative fuels [1–3] and surrogate models for real fuels [4–8]. Among all kinds of experimental tools, jet-stirred reactors (JSRs) [9–14] are one of the most popular and important types of reactors for the development and validation of detailed chemical mechanisms. An ideal JSR creates a highly turbulent flow to accelerate rapid reactant and product mixing in the reactor. In the limit of rapid mixing, the temperature and concentration distributions inside JSR are uniform, and the distribution of flow residence time is extremely narrow. The utility of the information extracted from a JSR experiment hinges on the ability of a JSR geometry to satisfy the uniformity and residence time distribution requirements.

In terms of JSR geometry designing, several criteria of JSR design were proposed by David and Matras [15] to ensure fast turbulent mixing and avoid near-wall stagnation flow. First of all, jets need to be free flowing (i.e., not affected by the wall). In addition, another criterion requires the inlet jets to be highly turbulent, with a turbulence Reynolds number larger than 800. The third requirement is the sonic limit condition that sets the upper limit for the flow velocity at the injector nozzles to avoid choking. The last requirement is the recycling condition describing the restriction on the length-scale ratio between the injector tube and the reactor, which promises enough space for jets to mix up. Based on these criteria, several types of JSR geometries have been proposed. For example, a toroidal reactor was developed by Nenniger et al. [16] and Lignola et al. [10], in which multiple (32–48) jets are distributed on the outside wall of the JSR. The toroidal JSRs have been adopted for ethylene combustion [17], jet fuel [18], soot/nitrogen oxides (NOx) emissions [19], and so on. However, there exist large nonuniformities in terms of temperature, flow velocity, and residence time distributions inside the reactor; for example, the temperature nonuniformity could be as large as 100 K [16]. These nonuniformities were mainly caused by the unwanted internal circulations in the radial direction, thereby limiting the utility of the toroidal design. To solve the nonuniformities in toroidal JSRs, a cross-injector spherical JSR was proposed by Matras and Villermaux [20] and Dagaut et al. [21,22]. The typical outward cross-injector JSR is shown in Fig. 1. The uniformities of temperature and species were much improved by the cross-injector design; for example, the temperature variation was within 20 K [23], but the wide distributions of residence time remain an unresolved issue. The main issue for the cross-injector JSR is that the two pairs of jets create two vortices pointing in different directions, and the sum of two vortex vectors becomes a nonzero stable vortex together with a large recirculation zone.

As can been seen from the previous studies, even the JSR meets the requirements mentioned above, there are still other factors that can largely influence nonuniformities in JSRs, one of which is the arrangement of the jets and the corresponding vortex distribution. The jet arrangement, including jet locations and orientations, significantly affects the flowfield inside the reactor and correspondingly the temperature, concentrations, and residence time distributions. Quantitative understanding of the distributions of temperature, concentrations, and the residence time in a JSR is critical for kinetic model validation [24]. Although several concepts to improve the jet arrangement and turbulent flow distributions have been proposed [11,25], little attention has been paid on the distribution of the flow residence time [26,27] and uncertainty in the mean flow residence time. As a result, the uncertainty in the nonuniformities of species and residence time distributions inside the JSR are not known appropriately.

Motivated by the previously mentioned discussions, the goal of this study is to present and examine a new JSR design using inwardly off-center shearing (IOS) jets to improve fast and homogeneous turbulent mixing. Numerical simulations are carried out to simulate the distributions of species and residence time inside the IOS JSR. The temperature, fuel concentrations, and residence time distributions are used as a criterion to evaluate the performances of JSRs, and the results are compared with that of two other traditional JSRs. Moreover, the mean flow residence time is introduced to assess quantitatively the uncertainty of different JSR designs.

II. JSR Designs and Numerical Methods

Three different JSR designs are considered in this study. As shown in Figs. 1–3, the first design is the classical outward cross-injector (OCI) JSR designed by Dagaut et al. [21]. Four injectors are introduced from the center of the JSR and point in four different directions. The second JSR is the newly proposed concentric inward and outward (CIAO) JSR proposed by Davani and Ronney [12] with eight concentric inlets and four outlets. The last design is the present

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*Graduate Student, Department of Mechanical and Aerospace Engineering. Student Member AIAA.

†Robert Porter Patterson Professor, Department of Mechanical and Aerospace Engineering. Associate Fellow AIAA.

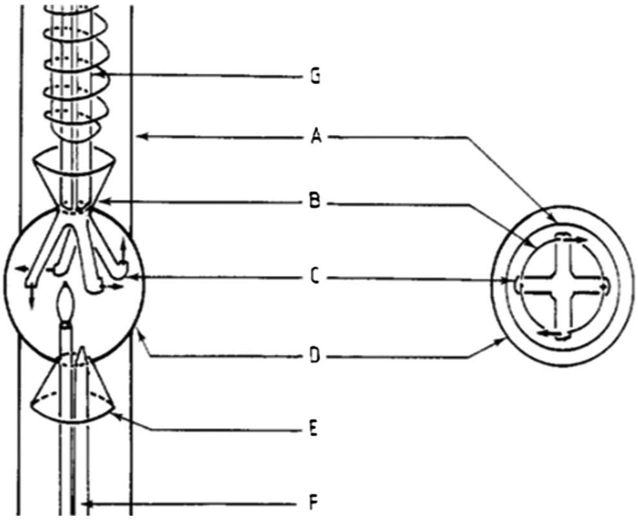

Fig. 1 OCI JSR [13].

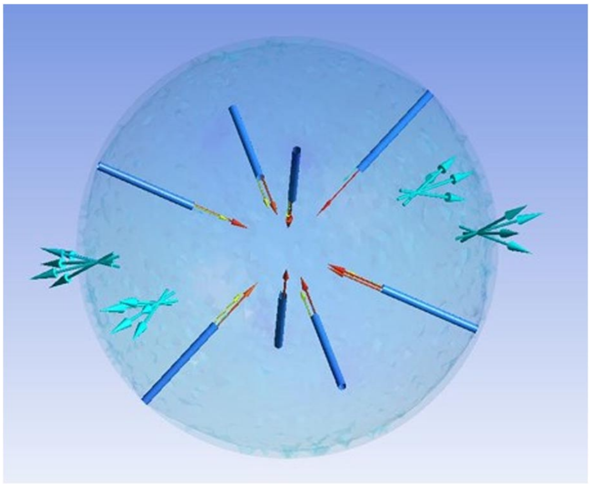
Fig. 2 CIAO JSR [19].

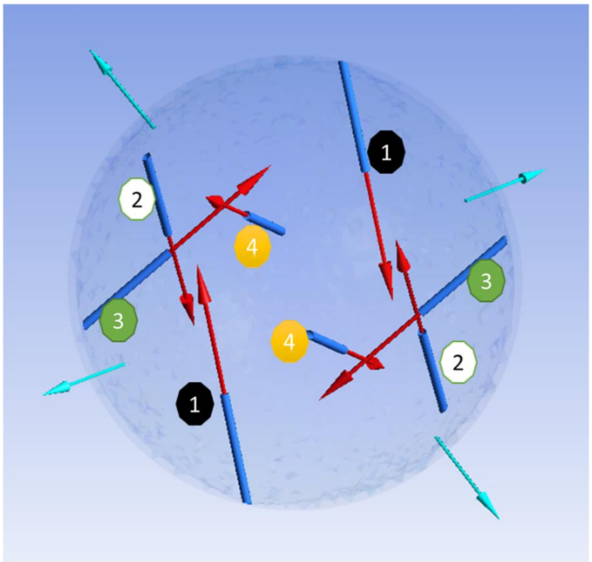

Fig. 3 IOS JSR.

IOS JSR, which has eightinjection nozzles and four exhaust gas exit holes on the wall. The basic idea is to generate four pairs of jets to induce four vortices with different directions. The vortices can promote the mixing inside the reactor, while at the same time, the magnitude of the net vortex is close to zero in order to avoid large recirculation loops in the reactor.

For better comparison in flow residence time, all three JSRs in the current work have the same size for the inlets, outlets, and reactors. The inner diameters of JSRs, inlet nozzles, and outlet nozzles are 50, 1, and 3 mm, respectively. The JSRs are initially filled with nitrogen. Starting from time $t = 0$, a methane/air mixture with a methane mole fraction of 0.5% is injected from the inlet nozzles to the JSR. The total pressure at the inlet exits is held at 104 kPa, and the environmental pressure at the outlets is 101.3 kPa.

Numerical simulations are conducted by using ANSYS 14.0-CFX. The mesh comprises tetrahedron cells, which are suitable for complicated geometry. The grid refinement is based on the curvature of the cell. The minimum cell dimension is 10 μm, with 10^6 as the number of cells. The maximum skewness, a commonly used parameter to evaluate mesh quality, is set below 0.80.

For the turbulence model, the $k - \varepsilon$ model is employed with 10–20% turbulence intensity at the inlet, which is defined as the ratio between the velocity fluctuation and mean inlet velocity. For the chemical source term, a methane/air 2-step global reaction mechanism is used for computational efficiency. The inlet and wall temperatures are fixed at 800 K.

An important parameter for JSR performances is the residence time distribution. Here, the particle tracking method is used to calculate the flow residence time. At the inlets, the particles are uniformly distributed once the flowfield computation is converged. By using a large enough number of particles (e.g., greater than 1000), a smooth distribution curve for the flow residence time can be achieved.

In addition to the particle tracking method, a transient simulation is also performed to calculate the mean residence time and to assess the uncertainty of JSRs. This method uses the steady-state flow solution as the initial condition and then changes the inlet gas composition from the methane/air mixture to pure air. As a result, the methane concentration decreases as a function of time as the air flows into the JSR. The temporal evolution of the average methane mass or mole fraction in the JSR represents the mean flow residence time. Physically, the relationship between methane mass fraction and the mean flow residence time can be derived as follows:

$$\rho V \frac{\mathrm{d}Y_{\mathrm{CH}_4}}{\mathrm{d}t} = -\dot{m} Y_{\mathrm{CH}_4} \tag{1}$$

$$Y_{\mathrm{CH}_4}(t) = Y_{\mathrm{CH}_4}(t_0) e^{-((t-t_0)/\tau)} \tag{2}$$

Here, ρ is the density, V is the reactor volume, $\dot{m}$ is the mass flow rate, Y_{CH_4} is the methane mass fraction, and

$$\tau \equiv \frac{\rho V}{\dot{m}} \tag{3}$$

is the mean flow residence time.

III. Results and Discussion

The comparison of the flow residence time distributions of three different JSRs is shown in Fig. 4. The abscissa is the residence time on a logarithmic scale, and the ordinate is the percentage of corresponding particles. The particles are injected from the inlets, and the initial positions are evenly distributed on the inlet surfaces. It is worth noting that the particle residence time distribution shown in Fig. 4 is a straightforward illustration but cannot be used to derive the mean residence time for the reactors. The reason is that the initial positions of the tracking particles are evenly distributed without considering the real (uneven) mass flow rate distribution on the inlet surface. However, particle tracking still provides important information for comparing the performance of different JSRs with the same inlet grid distribution. It can be seen from Fig. 4 that all of distribution functions in three JSRs have one main peak and a long tail toward the large residence time. Moreover, the position of the peak flow distribution time of each JSR is much smaller than its mean

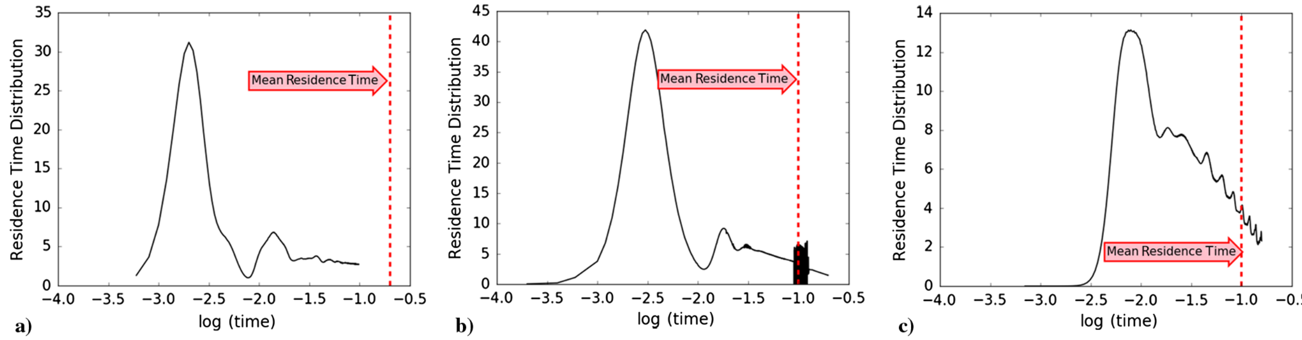

Fig. 4 Residence time distribution for a) the OCI JSR, b) the CIAO JSR, and c) the IOS JSR.

flow residence time calculated by the definition in Eq. (3). Note that for a perfect JSR the location of the peak flow residence time should be exactly at the mean flow residence time under the fast and perfectly mixed assumption. The main reason for this discrepancy is due to the finite mixing time and dynamics of the vortices inside the JSR. The theoretical result is calculated based on the assumption that all inlet flows will go through the whole volume with the same time histories. However, in a practical JSR, every flow particle will have different particle trajectories due to the effects of boundary layer and multiscale vortex motion. As such, some flow particles have shorter or faster pathways, and others have longer or shorter trajectories from inlets to outlets.

The flow pathways can be clearly seen from the streamlines and the velocity contours that are colored by local flow velocity shown in Figs. 5 and 6. Compared with other JSRs, the OCI JSR creates a large vortex as seen in Fig. 5a. An OCI JSR has two pairs of inlets, and each of them creates create a vortex that improves the mixing compared with previous toroidal JSRs. However, the jet distribution results in a net nonzero vorticity inside the reactor. As a result, a steady global vortex is formed, which can be clearly seen in Fig. 6a. The flow is almost stagnant near the center of the vortex, and this slow-motion zone is widely distributed along the global vortex tube in the reactor. For the particles entering this slow-motion zone, the residence time will be much larger than the theoretical value. On the other hand, for the particles away from the global vortex center, the residence time is significantly shortened due to the rapid flow motion. It can also be verified by Fig. 4a that the peak's position of the residence time distribution of the OCI JSR is about three orders of magnitude smaller than the mean flow residence time. This large difference implies that a great number of the inlet mixtures is recirculating in the center zone of the vortex in the JSR. As a conclusion, the global vortex greatly deteriorates the distribution of flow residence time. The CIAO JSR has a similar problem. All the inlet jets collide in the center of the reactor, creating a stagnation zone. After the collision, the inlet jets' velocities are heavily reduced such that a large percentage of the reactor volume can be hardly perturbed by the inlet jets, in which the particles have much longer residence time. Combining the advantages of vortex-assisted mixing in the OCI JSR and the simplified geometry in the CIAO JSR, the IOS JSR employs four pairs of inlet jets of which the velocity field is much more uniform. In addition, comparing the flow residence times of the three JSR designs, it can be seen that the present IOS JSR has the best performance in terms of the distribution of the flow residence time. It is seen that the difference between the residence time distribution peak and the mean value of the present IOS JSR is the smallest and the tail is the shortest among the three designs.

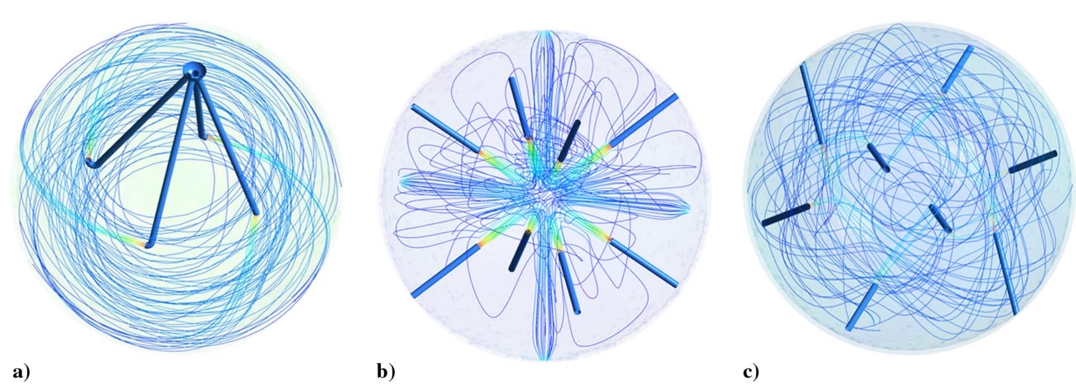

Fig. 5 Streamlines in a) the OCI JSR, b) the CIAO JSR, and c) the IOS JSR.

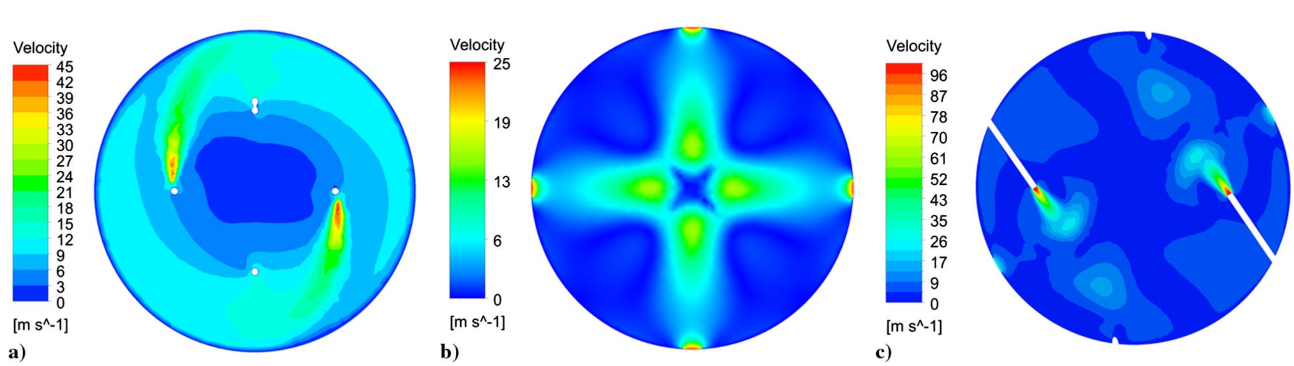

Fig. 6 Velocity contours in a) the OCI JSR, b) the CIAO JSR, and c) the IOS JSR.

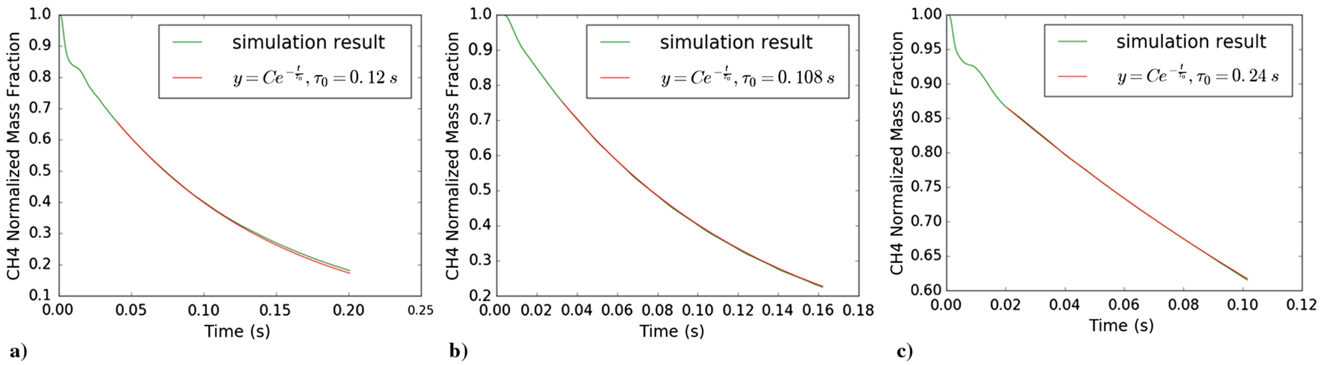

Fig. 7 Temporal evolution of methane mole fraction (green line) and the fitted curve (red line) in a) the OCI JSR, b) the CIAO JSR, and c) the IOS JSR.

To better evaluate performances of the three JSR designs, the transient simulation also is conducted. Figure 7 shows the comparisons between the transient simulation results (green lines) and the fitted curves (red lines). The green lines reflect the temporal evolution of the averaged methane mass fraction in the whole JSR volume, and the red lines are the theoretical time history of the methane mass fraction in Eq. (2). Here, the parameter τ is the actual mean residence time, which is calculated by fitting the exponential decay function of Eq. (2) with the simulation results. It is worth noting that, since the Reynolds numbers at the inlet are the same for all three JSRs, the total mass flow rate is proportional to the injector number. The OCI JSR has four injectors, and the other two have eight injectors; as a result, the OCI JSR's theoretical mean residence time is 0.2 s, while the CIAO JSR and the IOS JSR have the same theoretical mean residence time $\tau = 0.1$ s. However, Fig. 7 shows that the differences in the fitted mean residence time for the three JSR designs are very large. Specifically, the fitted mean residence times for OCI JSR, CIAO JSR, and IOS-JSR are 0.240, 0.120, and 0.108 s, respectively. The largest fitted mean residence time is that of OCI JSR and CIAO JSR, which is larger than the theoretical mean flow residence time by about 20%, while IOS JSR has the minimum difference from the theoretical value by only 8%. As has been pointed out earlier, in the jet-stirred reactor, there exist many different length and time scales of vortices, which create flow recirculation and broaden the distribution of flow residence time. As a result, the mixing process is much slower than the theoretical result, which assumes the methane fraction is uniform over the whole domain. This is the reason why the actual mean residence time is always larger than the theoretical value. Therefore, among three different JSR designs, IOS JSR still has the best mixing performance, which agrees with the results in steady-state simulation.

IV. Conclusions

A novel geometry of the inwardly off-center shearing jet-stirred reactor is proposed and examined numerically and compared with two traditional jet-stirred reactor (JSR) designs, the concentric inward and outward (CIAO) JSR and the outward cross-injector (OCI) JSR, in order to achieve improved turbulent mixing and a narrowly defined distribution of the flow residence time. The results show that there is significant nonuniformity in the distributions of the species and flow residence time in the two traditional JSR designs. Compared to the two traditional JSRs, the present inwardly off-center shearing (IOS) JSR has much improved performance in terms of mixture uniformity and narrower distribution of the flow residence time. There exist large recirculation zones in both CIAO JSR and OCI JSR, in which a large percentage of the reactants remains in the core of these large vortices much longer than the mean residence time, while the rest of the mixture exits the reactor directly through shortened streamlines from inlets to outlets. In contrast, the present IOS JSR design creates a fully mixed environment using inwardly shearing jets that cover the whole volume of the reactor and does not generate large vortices at the same time. Consequently, the IOS JSR has the smallest standard deviation of residence time distributions among all three JSR designs. As a result, the IOS JSR will provide merits to improve the flow residence time distribution and contribute to the development and validation of chemical kinetic models. In addition, its simplified geometry enables optical diagnostics with both in situ ultraviolet and infrared lasers, which can significantly extend the measure capability of the current JSRs for kinetic studies of jet fuels.

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P. Givi
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