Modeling of Cavity Residence Time via Modeled Lagrangian Particle Tracking

A. T. Norris, †
NASA Langley Research Center, Hampton, Virginia, 23681

ABSTRACT

One of the critical components in a scramjet is the cavity flame holder. In evaluating the sizing of this component, the residence time of the fuel in the cavity is a common parameter used. However, to obtain the residence time via CFD is an expensive undertaking. One method is to perform an LES simulation of the cavity and use Lagrangian particle tracking to obtain both the mean and probability density function of the time that the particles remain in the cavity. While this method affords a significant amount of information, it is very costly in CPU run time. A simpler method involves performing a time accurate RANS simulation of the cavity, and when converged, overlay a traceable scalar in the cavity region, and then record the decay of this scalar's flux at a downstream location. The time scale of the decay rate can then be estimated and a residence time inferred. This method is less computationally expensive than the LES approach, but still requires a time-accurate solution while only providing a mean cavity residence time evaluation.

In this paper a method of determining the mean cavity residence time as well as the Probability Density Function (PDF) of the residence time is proposed and demonstrated. This method is based on Lagrangian particle tracking modeled by the Generalized Langevin Equation and is implemented as a post-processing step for a steady RANS solution. Computational cost is on the order of minutes and the results are in agreement with values obtained by the LES and scalar decay methods.

INTRODUCTION

The cavity is a commonly used flame holding device in high-speed reacting flow paths and operates by providing a region where fuel and air can react to produce heat and chemical radicals to sustain combustion in the core flow. When analyzing the cavity operation, one of the important characteristics that needs to be determined is the fuel residence time. That is, the average amount of time a notional particle of fuel will spend in the cavity before being ejected into the core flow.[1] Too short a residence time, and the fuel will not have enough time to react and burn, and so the cavity will be extinguished. Too large a cavity and the increased size, weight and resulting heat load of this device will be detrimental to optimal performance of a high-speed engine.

However, despite the residence time being a very simple concept, the methods to obtain this quantity are not so straightforward. Experimental methods are not simple by the very fact that you have to build and then test a cavity in a supersonic wind tunnel, and even then, the methods of determining the residence time are not clear. From a numerical point of view, the situation is a little better with several established methods of calculating the residence time.

The most comprehensive method is to perform an LES simulation of the cavity flow and track notional fluid particles in the flow. By recording the amount of time particles spend in the cavity area before being ejected into the core flow, the statistics of the residence time can be obtained. A good description of this method can be found in the paper by Bonnani.[2] In principle, a similar result could be obtained from a Lagrangian Joint Velocity-Scalar PDF solver,[3] though no example has been found in the literature.

†Aerospace Engineer, Hypersonic Airbreathing Propulsion Branch, NASA Langley

Another method involves the "tagging" of a conserved species in a time-accurate RANS simulation and observing the decay of this species over time.[4] Specifically, the simulation is run to convergence and then a conserved scalar in the cavity is tagged by some method. The solution is then advanced and the flux of the tagged scalar flowing out of the cavity is recorded. The rate of decay of the flux measurement gives an estimate of the mean residence time.

One thing all these methods have in common is that they require a lot of computational effort. For an engine designer, where you are evaluating a range of conditions via RANS, the extra time involved in tagging a suitable scalar and then running the simulation as a time accurate case would be large. And in this case, you would only obtain a mean residence time, unlike the LES method where the PDF of the residence time can be obtained. However running all the cases as an LES simulation would be computationally expensive.

It should be noted that for one specific case there is an analytic solution. If fuel is only injected into the cavity, one can simply divide the mass of fuel atoms in the cavity by the fuel mass flow rate into the cavity, which yields a mean residence time. However this is not a common fueling situation in most practical applications.

In this paper a method of determining the mean cavity residence time, as well as the PDF of the residence time, from a steady RANS solution is proposed. The method is applied as a post-processing step to the RANS solution and only requires a few minutes of computational time to run.

LAGRANGIAN MODEL

Tracking Lagrangian particles to obtain the PDF of the cavity residence time is the approach used in the LES method. However, particle tracking in a steady RANS solution cannot provide any such information, as the particles will simply follow the mean streamlines. For the case of a cavity with no internal injection, this means the particle will either remain in the cavity or remain outside the cavity. There is a dividing streamline between the two zones that cannot be crossed in a deterministic model.

However, if the particle motion has a component that represents the turbulent diffusion process, it would be able to cross streamlines and, as a consequence, would represent the path of a particle in a turbulent flow. The particle path would then represent the Lagrangian motion of a particle in an unsteady turbulent flow whose Reynolds-averaged properties are given by the steady RANS solution.

From the Eulerian conservation equations, the fluid particle properties $X_i^+(t)$ and $U_i^+(t)$ evolve by

$$\frac{dX_i^+}{dt} = U_i^+ \tag{1}$$

$$\frac{dU_i^+}{dt} - \frac{1}{\rho}\frac{dP}{dx_i} = -\frac{1}{\rho}\frac{dp}{dx_i} + \nu\frac{d^2U_i^+}{dx_j dx_j} \tag{2}$$

where X_i^+ is the particle location, U_i^+ is the particle velocity, ρ is the density, P is the mean pressure, p is the fluctuating pressure and ν is the viscosity. The terms on the right hand side of Eq. 2 need to be modeled and, by using the Generalized Langevin Equations,[5 6] the modeled Lagrangian fluid particle equations can be written as

$$dX_i^+ = U_i^+(t)dt \tag{3}$$

$$dU_i^+ = -\frac{1}{\rho}\frac{dP}{dx_i}dt - C_T\omega(U_i^+ - \langle U_i\rangle)dt + (C_o\epsilon)^{1/2}dW_i \tag{4}$$

where $\langle U_i \rangle$ is the mean velocity, ω is the turbulent frequency and ϵ is the turbulent dissipation. There are two constants in the equations; C_o is a universal Kolmogorov constant and is assigned a value of 2.1 and C_T is a tuning constant and assigned an initial value of 1.0. The term dW_i represents independent Wiener processes which are independent Gaussian random variables with variance of the time step dt. That is:

$$dW_i dW_j = \delta_{ij} dt. \tag{5}$$

For the purposes of this study, $\langle U_i \rangle$, P, ρ, ω and ϵ are modeled by the values taken from the RANS solution at location X_i^+. The model can be expanded to include compressible effects,[8,9] which would involve additional terms, however the added complexity was not deemed necessary for this application as the flow in the cavity is always subsonic and thus the compressibility effects should be small.

Equation 3 gives the change in location of the particle due to the particle velocity while Eq. 4 gives the change in the particle velocity and has two main parts. The first two components on the right hand side represent a relaxation process, which causes the particle velocity to be influenced by the pressure gradient, mean flow velocity and turbulence time scale. The last component is the turbulence term, which provides the turbulent diffusion to the particle velocity, based on the turbulent dissipation.

Implementation is fairly straightforward, with the particle location and velocity updated via the Modified Euler Method (Explicit Midpoint Method)[10] and the mean flow field quantities interpolated from the RANS solution. The boundary conditions for walls are treated in a slightly different manner than those of RANS. The random component added to the particle motion makes it possible for a particle to cross a solid boundary. To prevent this nonphysical behavior, any particle that crosses the solid boundary is reflected back into the main flow. Periodic and exit conditions are treated as in a RANS solver, with the particles entering and exiting the solution domain as appropriate. Computational needs are small, with the whole process running on a single processor.

One item that needs some care is the selection of the time step used to advance the particle. Based on the recommendations of Pope,[6] the time step is required to be significantly less than the integral time scale of the mean flow field, T_L. That is:

$$dt \ll T_L = \frac{4}{3C_o\omega}. \tag{6}$$

For the cases described here, a value two orders of magnitude smaller than the integral time scale was selected.

RC19 GEOMETRY

The first test of the Langevin method is performed on the RC19 planar cavity experiment[11] shown in Fig. 1. The geometry of the experiment is that of a single planar cavity, 0.65 inches deep and 3.38 inches from the cavity lip to the end of the closeout. In this particular test, a nonreacting mixing case is simulated, with C2H4 injected into the cavity at the base of the rear closeout wall. As mentioned earlier, when the cavity is fueled directly, an analytic value for the mean residence time can be obtained, which will provide a useful benchmark against other methods and allow the tuning constant, C_T to be set.

A RANS simulation was performed for the conditions in Table 1. The computational domain (Fig. 2) consisted of a one inch thick slice of the full domain, with no end walls and two injectors. This was solved from upstream of the nozzle to just after the exit of the cavity closeout. Periodic boundary conditions were enforced for the sides of the slice. In addition, an LES simulation with particle tracking was performed in addition to an unsteady RANS case for the decay of a scalar. In all cases the cavity was defined as the volume under a straight line from the cavity lip corner to the cavity closeout corner. For the Langevin model, a series of particles were released at the exit of the cavity fuel injector and tracked. The amount of time each particle spent in the cavity was computed and the values averaged to obtain a mean cavity residence time.

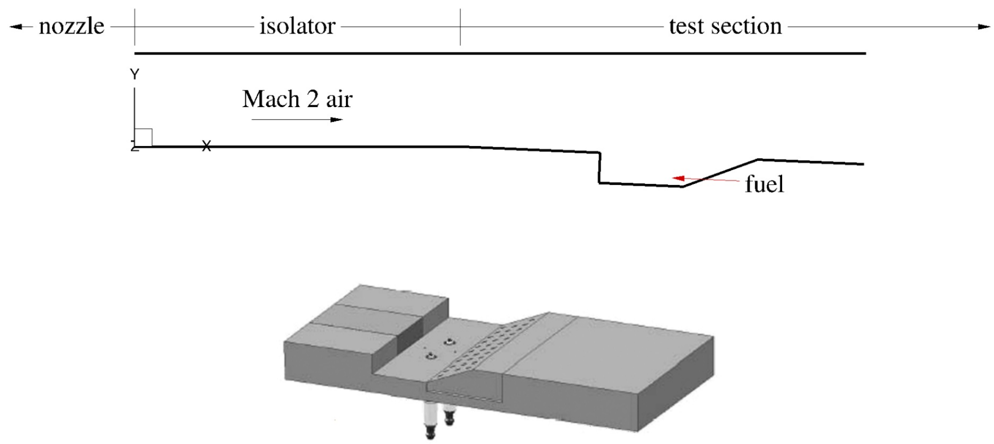

Figure 1. Sketch of the flowpath of the RC19 scramjet rig.[11] The upper diagram shows the side profile of the computational domain, while the bottom shows a perspective view of the cavity.

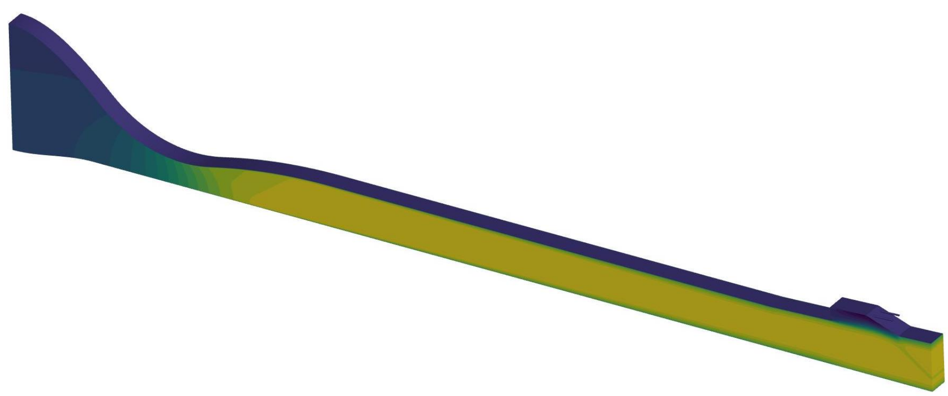

Figure 2. Illustration of the computational domain used for this study with flow from left to right.

The average residence times obtained by the different methods are given in Table 2. The Lagrangian model was run with 500 particles and a good agreement with the other mean residence times was obtained with a tuning constant of $C_T = 2.0$. Of particular note is that the computational time required to obtain the residence time is a matter of a few minutes, compared to the hours and/or days required by other numerical techniques. In all cases this estimate of computational time does not include the time required for the initial steady RANS solution to be performed. The path of the particles is illustrated in Fig. 7, where a small number of the particle paths are shown. The particle tracks illustrate what we would expect from tracking a particle, with the vast majority circling the cavity and exiting at the top.

Table 1. **Flow properties for RC19 cavity.**

Property	Value	Units
Grid Size	1,627,000	Cells
P_o	70	PSI
T_o	589	K
$\dot{m}_f$	56	SLPM
Mach	2.0	

Table 2. Mean residence time for RC19 cavity.

Method	Residence Time	Computional time
LES	1.73e-03 sec.	days
Decay	1.65e-03 sec.	hours
Analytic	1.75e-03 sec.	seconds
Langevin	1.71e-03 sec.	minutes

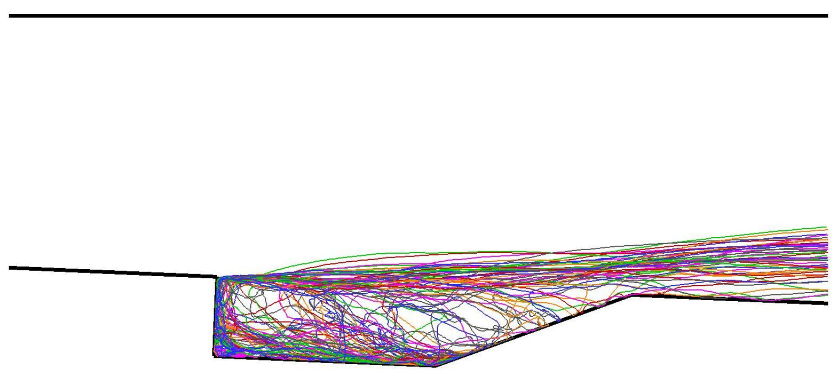

Figure 3. Paths of 50 notional fluid particles calculated by the Lagrangian model. Particle paths originate near the bottom right of the cavity and exit at the right.

In addition to the mean residence time, the PDF of the residence time can also be obtained from the Lagrangian model. In Fig. 4 the probability density function (PDF) of the residence time is shown for a sample of 500 particles compared to the PDF of residence time obtained from an LES simulation with over 500,000 particles tracked. Both distributions exhibit a similar shape, approximating a log-normal distribution, with fairly tight clustering of the residence times around the mean value.

LAZARUS RIG GEOMETRY

The other test of the Lagrangian model was conducted using the AFRL Lazarus rig,[12] shown in Fig. 5. This is an axisymmetric geometry with the fuel injected upstream of the cavity. The dimensions are similar to the previous example, with the cavity being 0.734 inches deep and 4.159 inches from cavity lip to end of cavity

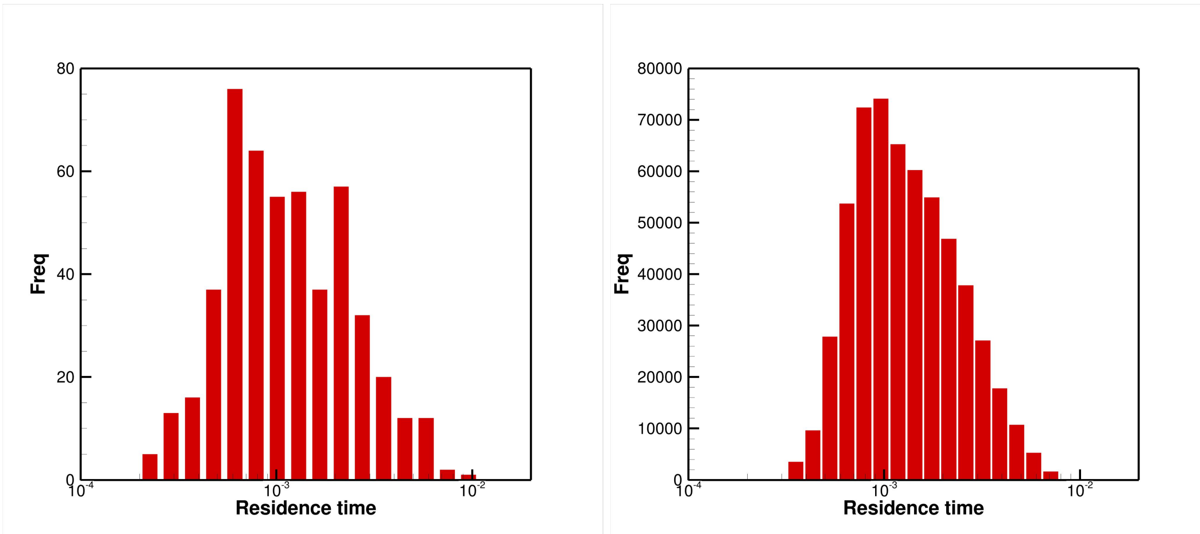

Figure 4. Histograms representing the probability density function of the cavity residence time distribution for the RC19 simulation. The left figure shows the results obtained from 500 particles using the Lagrangian model, while the right figure shows the results from over 500,000 tracked particles obtained from an LES study.

closeout. As in the previous example, the fuel is C2H4, and it is again a non-reacting case. However, in this experiment the fuel is not injected directly into the cavity but rather from an upstream location. Because of this, there is no analytic solution for the residence time as the mass flow of fuel into the cavity is an unknown. An asymptotic limit where all the fuel is assumed to be entrained in to the cavity can be evaluated however, which will give a lower bound to the residence time.

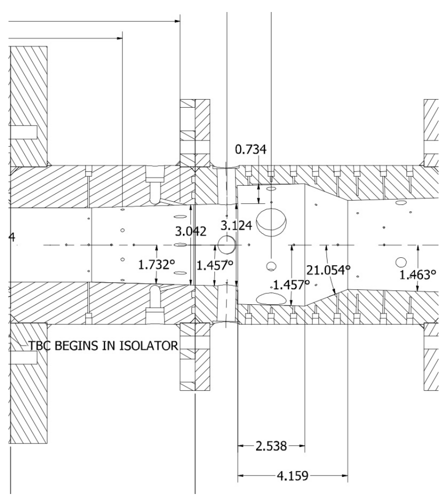

Figure 5. Sketch of the flowpath of the Laz scramjet rig[12].

The computational domain, shown in Fig. 6, consists of a 45 degree sector of the article flowpath, starting before the facility nozzle and ending just after the cavity closeout. One upstream injector is included and periodic boundary conditions are enforced on the sides of the sector. As with the RC19 cavity, the Lagrangian model was applied to the results of a steady RANS simulation, performed for the conditions shown in Table 3. The tuning constant from the previous test was left unchanged. In addition, a time-accurate RANS solution for the scalar decay method was also computed to obtain the mean residence time. The cavity was defined as the volume above a straight line connecting the cavity lip to the closeout corner and rotated around the axis. The notional fluid particles in this case were not released at the exit of the injector, but rather at a location just upstream of the cavity. This was to limit the number of particles that do not get entrained into the cavity and thus serve no part in evaluating the cavity residence time. Particles were not released directly in the cavity because it is not known where the fuel enters the cavity and so would skew the calculated residence time calculations.

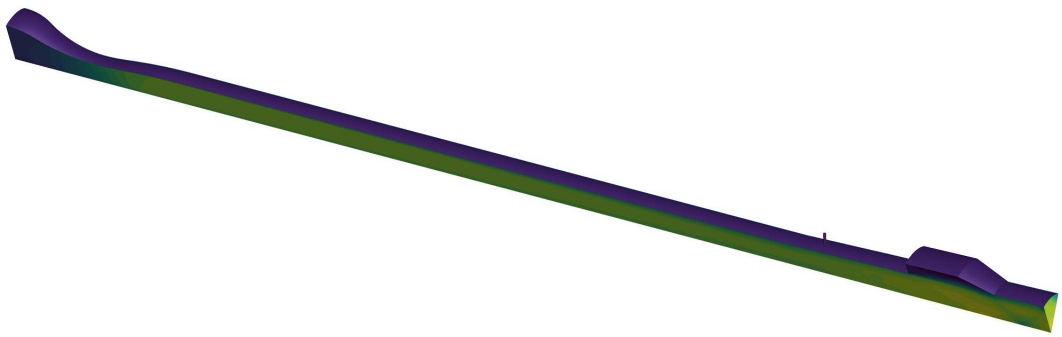

Figure 6. The computational domain used for the Lazarus Rig simulations. This is a 45 degree sector, with the flow starting in the plenum (left) and exiting just aft of the cavity (right). A normal injector is present upstream of the cavity.

Table 3. Flow properties for Lazarus simulation.

Property	Value	Units
Grid Size	1,289,000	Cells
P_o	50	PSI
T_o	397	F
$\dot{m}_f$	1076	SLPM
M	2.0	

The average residence time for the cavity is listed in Table 4 along with the value obtained by the scalar decay method and also the asymptotic limit for all the fuel being entrained into the cavity. As can be seen, there is a good agreement with the scalar decay value and Lagrangian model. The ratio between the asymptotic limit and the calculated residence time can be used to provide an estimate of the amount of fuel that does not get entrained into he cavity. In this case, the ratio suggests that only 8% of the injected fuel becomes entrained into the cavity.

Sample paths of the particles are shown in Fig 7, and again we see the trajectories that we would expect from a particle in a turbulent flow. Of note is that many particles just dip inside of the defined cavity volume and then escape downstream, rather than being entrained into the cavity recirculation. This is an artifact of the cavity definition and could be addressed with a more sophisticated definition of what defines the cavity volume. An option would be to define the cavity boundary as the dividing streamline between the core flow and the cavity flow. However, for simplicity, the simple linear definition of the cavity boundary was retained.

Table 4. **Mean residence time for Lazarus cavity.**

Method	Residence Time	Computional time
Limit	0.158e-03 sec.	seconds
Decay	1.89e-03 sec.	hours
Langevin	1.80e-03 sec.	minutes

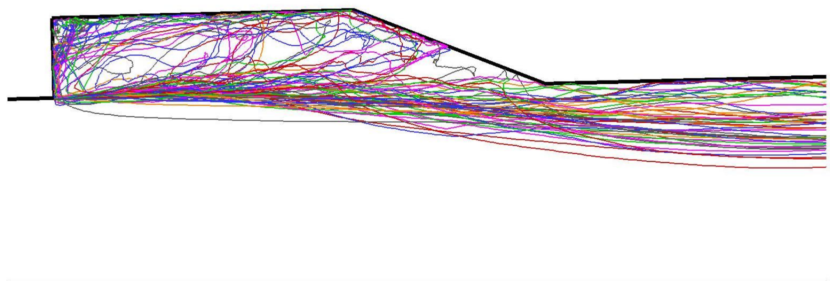

Figure 7. Particle paths of 50 notional fluid particles calculated by the Lagrangian model. The particles start just upstream of the cavity (to the left) and exit downstream to the right.

The probability density function of the residence time for a sample of 500 particles is shown in Fig. 8. At the current time no LES simulation of the results is available. This distribution shows a much increased range of residence times than the RC19 case. Part of this is the peak at about 1.0e-04 s, which represents the particles that just dip into the cavity and do not get caught up in the recirculation. The distribution of the residence times cannot be said to be log normal, but rather a bimodal combination of two approximately log normal distributions, one representing the fly-by particles and the other the particles entrained into the recirculating flow in the cavity.

CONCLUSIONS

A Lagrangian-particle-based model has been developed to obtain the residence time of a flame holding cavity. The method is based on the Generalized Langevin Equation working with the mean flow field obtained by a RANS simulation and operates as a post processing tool. The mean residence time obtained from the new model compares well to the results obtained from other methods. The shape of the probability density function of residence time compares well with that obtained from LES. The computational time required to obtain the results with the new model is several orders of magnitude quicker than the other methods. In the future, the model would benefit from further testing against LES results, as well as with reacting flows and more complex cavity shapes. However initial results presented here are promising.

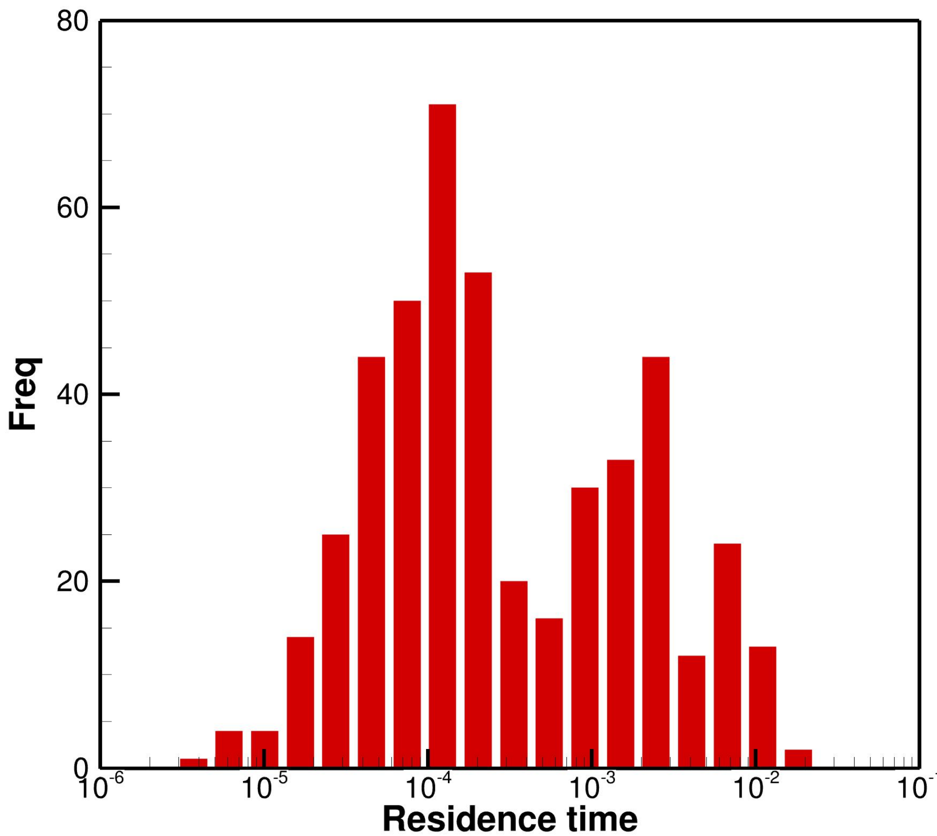

Figure 8. Histogram representing the probability density function of the cavity residence time distribution for the Lazarus Rig simulation. Results are from the Lagrangian model using 500 particles.

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