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VARIOUS APPROACHES TO COMPUTE FLUID RESIDENCE TIME IN MIXING SYSTEMS

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ABSTRACT

Residence time including mean residence time and residence time distribution (RTD) is a very important parameter to characterize a mixing system. In practice, tracer study has been widely used in experiments to obtain residence time distribution. There are several numerical approaches available to compute the average residence time and the residence time distribution of a system. This paper attempts to summarize those available approaches through an example.

NOMENCLATURE

$C(t)$	Species mass concentration function
C_l	Time constant
D	Diffusivity
$E(t)$	Residence time distribution function
$F(t)$	Cumulative residence time distribution function
I	Integration of mass concentration
Q	Volumetric flow rate
Sc_t	Turbulent Schmidt number
V	Vessel volume
Y_i	Mass fraction of species i
$\vec{X}_p$	Particle's location vector
$\vec{u}$	Velocity vector
f_i, g_i	RTD function
k	Turbulent kinetic energy
m	Mass of tracer species
r	Uniformly distributed random number
t	Time
ε	Turbulent kinetic energy dissipation rate
μ_t	Turbulent viscosity
ρ	Density
τ	Mean residence time
τ_e	Turbulent eddy lifetime
ζ	Normally distributed random number

INTRODUCTION

Mixing tanks have been widely used in various industries. Whether a tank is used as a reactor or a simple mixing device for two immiscible/miscible liquids, residence time is an important global parameter to characterize the system. For example, in a mixing tank reactor, if the reaction is isothermal and of first order, the conversion of the reactants in the reactor is purely determined by the residence time distribution. Even for a reaction system with high order reactions, residence time distribution gives us a knowledge of time window that reactions could occur. In an emulsion system, droplet size distribution is highly dependent on the shear history of droplet experimenting in the tank. In fact, the performance of any device in which a kinetic process occurs is highly dependent on the fluid residence time distribution.

Traditionally tracer study has been used successfully in experiments to obtain the residence time distribution. In such an experiment, inert chemicals, called tracer, is injected into the tank at time zero and then the tracer concentration at the outlet is monitored as a function of time. The concentration is usually measured by the conductivity of the fluid if the tracer is a solution or by spectrophotometry or colorimetry if a dye is used. The tracer can be introduced at inlet by either a step or pulse mode.

During the last few decades, computational fluid dynamics (CFD) has been increasingly used. At least three different approaches have been used to get the fluid residence time in a vessel. In the first approach, the tracer is treated as a species and the unsteady species transport equation is solved [1]. In the second approach, Lagrangian particles are released from the inlet and particles are tracked until they leave the domain [2]. The residence time can be obtained from the particle tracking. Another less well known method is to solve the average residence time equation directly [3–5]. Although it cannot get the time distribution, it provides the average residence time quickly at any point of the vessel.

The residence time distribution experimentally and numerically is usually obtained for a single device. A real industrial system usually consists of many devices which are interconnected together. The performance of such a system may depend on the total residence time of the fluid inside the system. Convolution integral can be used to combine the residence time distribution for individual device into the total fluid residence time distribution [6].

In this paper, we will review different numerical approaches in the calculation of the fluid residence time. We start with its definition, followed by different numerical choices to calculate it. The advantages and disadvantages of each method are discussed in the paper. We will also discuss the application of convolution integral in the calculation of RTD for complex systems. Finally, an example is shown to illustrate different methods. The paper focuses on the method which uses the transport equation to solve average residence time and on the application of convolution integral in combining individual RTD to a system's RTD.

RESIDENCE TIME AND RESIDENCE TIME DISTRIBUTION

The residence time theory has been generalized and popularized by the pioneering work by Danckwerts [7], Spalding [8] and Zwietering [9]. Since then, the theory has been refined and extended until it has become an important tool not only in chemical engineering, but also in environmental and pharmaceutical applications. Originally, residence time distribution was defined at the outlet of a vessel. If we release a lot of particles into a vessel, different particle takes different time to come out of the vessel. The time the particle spent in the system is called the residence time and the distribution of the various particles coming out the vessel with respect to time is called the residence time distribution (RTD). According to the definition, the residence time distribution can be written as

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} \tag{1}$$

where $C(t)$ is the measured tracer concentration at the outlet at time t. The average residence time of all particles can be calculated as

$$\tau = \frac{\int_0^\infty C(t)t dt}{\int_0^\infty C(t)dt} \tag{2}$$

In a pulse experiment, the tracer is only released at inlet during a short time period. The measured concentration as a function of time is referred to as the C curve in the RTD analysis. It can be seen that $E(t)$ is the normalized C curve. In a step experiment, a constant rate of tracer is added to the system from time zero continuously. The measured tracer concentration is monotonically increasing with time. The normalized measured concentration versus time profile is called F curve. The relation between $E(t)$ and $F(t)$ is

$$\frac{dF(t)}{dt} = E(t) \tag{3}$$

Here, $F(t)$ is the cumulative probability function of $E(t)$.

Although traditionally the residence time and its distribution function are defined only at the exit of a system, the concepts can be generalized and be applied to any spatial point in a system. As a result, residence time and its distribution are functions of space as well. In this paper, we will use residence time and its distribution in this general sense. Fluid residence time and its distribution will be calculated from a numerical pulse experiment. So $C(\vec{x},t)$, $E(\vec{x},t)$, and $\tau(\vec{x})$ will be our interested variables. From the tracer species transport equation, Danckwerts [7] and Spalding [8] were able to show the following two important results in a pulse experiment:

$$\begin{aligned} \int_0^\infty C(\vec{x},t)dt &= \text{constant everywhere in the domain} \\ &= m/Q \end{aligned} \tag{4}$$

$$\tau = \frac{V}{Q} \tag{5}$$

where m is the total tracer species quantity, Q is the volumetric flow rate and V is the vessel's volume.

The first result shows that if a steady stream (train of equal pulses) of tracer is injected at a vessel's inlet, the concentration of the tracer will be uniform throughout the vessel eventually.

As a result of this, the residence time distribution, $E(\vec{x},t)$, at different point in a vessel is directly related to the tracer species concentration, $C(\vec{x},t)$, at those points by a constant scaling factor through Eq. 1. The cumulative residence time distribution function, $F(\vec{x},t)$, is related to the following function by the same scaling factor:

$$I(\vec{x},t) = \int_0^t C(\vec{x},t)dt \tag{6}$$

Since I will approach to a constant value everywhere in the domain as time goes to infinity, it can be used to judge the convergence of the RTD in the unsteady tracer simulation. For a multiple inlet system, this still holds as long as the tracer mass injected from each inlet is proportional to its volumetric flow rate [10].

The second result shows that the mean flow residence time is always equal to the vessel volume divided by the volumetric flow rate. This holds irrespective of the flow pattern in the vessel. The flow pattern only affects the shape of the RTD. However, the first moment of the RTD, the mean residence time, is always constant. Theoretically, this result is valid only under the condition that the tracer is prevented from diffusing upstream out of the injection plane, which usually can be satisfied for convection dominated flows. This constraint can be used to check the accuracy of any numerical result regarding the RTD.

It should be noted that such a definition of the residence time leads to a quantity that is independent of time and is therefore applicable only to steady-state, incompressible flows. This limitation is essentially linked to the experimental procedure, which is based on recording a time-dependent tracer signal and assumes that the underlying transport field does not change in time. For a more general case of transient, compressible flows, residence time needs to be redefined and generalized. The interested reader can refer to [11–13]. In this paper, we will focus on the steady, incompressible flows and the traditional definition still holds.

NUMERICAL APPROACHES

Transport Equation of Tracer Species

The tracer pulse or step experiment can be simulated in terms of the traditional equations of transport. The tracer is treated as a separate species, but with the same properties as the original fluid. An unsteady species transport equation is solved to get the tracer's concentration along with the time, which is

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla\cdot(\rho\vec{u}Y_i) = \nabla\cdot\left[\left(\rho D + \frac{\mu_t}{Sc_t}\right)\nabla Y_i\right] \tag{7}$$

where Y_i is the mass fraction of the tracer species, $\vec{u}$ is the velocity field, ρ is the density of the fluid, D is the diffusivity of the tracer in the fluid, μ_t is the turbulent viscosity, and Sc_t is the turbulent Schmidt number.

In an experiment, tracer particles are only injected after the flow field is established. The same goes to the numerical simulation. Although the transport equation of the tracer species is transient in nature, usually the flow field is solved first with the steady state solver. Only after a converged solution is obtained, the flow field is frozen, species transport is set and the solver is switched into unsteady. As a result, only one equation is solved.

In an experiment a probe can, at least theoretically, be put into any position of the system, so the flow residence time at any point of the system can be measured. But installation issue of the probe may restrict the access of certain area and the extrusion of the probe may disturb the flow field. However, there is no such problems in a numerical experiment, and the concentration of the tracer species at any position of the system can be monitored along with the time. So this method gives a complete set of information in the residence time distribution of the system.

Note that, due to the transient nature of the equation, the equation has to be solved step by step in time. The time step used in the calculation is usually a fraction of the minimum cell residence time in the domain. The total time period usually needs to be at least several times of the mean residence time due to the usual long tail of a RTD curve. Therefore, the computational time could be large especially for a problem with large number of cells. That is the drawback of this method.

Lagrangian Particle Tracking Method

In most industrial applications, the complete information of the fluid RTD over the entire flow field may be not needed since the performance of a system can be estimated by the flow residence time distribution only at the exit point. For such cases, the Lagrangian particle method provides a much quicker solution. In this method, a lot of particles are released at inlet to mimic the tracer particles after the flow filed is established. Instead of solving an unsteady transport equation in the Eulerian reference frame, each particle's trajectory is traced in the Lagrangian reference frame. The particle's trajectory can be obtained by integrating the following equation:

$$\frac{d\vec{X}_p}{dt} = \vec{u}_p = \vec{u}(\bar{x}) + \vec{u}'(\bar{x}) \tag{8}$$

where the particle's velocity is always equal to the continuous phase local velocity, which includes the mean and the fluctuating part. The fluctuating part is used to consider the turbulent dispersion. In this paper, the random walk dispersion model implemented in ANSYS FLUENT [14] has been used, in which,

$$u_i' = \zeta\sqrt{2k/3} \tag{9}$$

where ζ is a normally distributed random number and k is turbulent kinetic energy. And it is assumed such a fluctuating velocity lasts during the lifetime of an eddy. The characteristic lifetime of the eddy is computed as

$$\tau_e = C_L k/\varepsilon \ln(r) \tag{10}$$

where C_L is a time constant, ε is the turbulent kinetic energy dissipation rate and r is a uniform random number between 0 and 1. When the time is reached, a new value of the instantaneous velocity is obtained by applying a new normal random number in Eq. 9.

The residence time distribution can be easily obtained by monitoring the particles coming out from the exit. To get meaningful statistics, in general a large number of particles usually are needed. In addition, special attention is needed if the inlet flow is not uniform. The number of particles at any point at inlet should be proportional to the local flow rate.

The advantage of this method is that it is very cpu effective. But the method only provides the residence time distribution where a large number of sampling particles can be collected so that the statistics is meaningful. That is why the method is usually used to get a RTD at a flow outlet. Another salient feature of this method is that the predicted RTD not only depends on the number of particles, but also on the turbulent dispersion model. As a result, the mean residence time at flow outlet computed from this approach does not necessarily satisfy the constraint Eq. 5.

Transport Equation for Average Residence Time

The transport equation for the average residence time has been derived initially by [3, 8] based on the definition of Eq. 1. Subsequently it has been studied by [5, 11]. For steady state, incompressible flow, the transport equation of the average residence time can be written:

$$\nabla \cdot (\rho \vec{u} \tau) = \nabla \cdot \left[\left(\rho D + \frac{\mu_t}{Sc_t} \right) \nabla \tau \right] + \rho \tag{11}$$

where τ is the mean fluid residence time, $D + \frac{\mu_t}{Sc_t}$ is an estimate of the local actual diffusivity, where D is the self-diffusivity of the fluid, which may be expressed by the ratio $\frac{\mu}{Sc}$ where Sc is the laminar Schmidt number.

If we ignore the diffusion (both molecular and turbulent diffusion) and add the unsteady term to Eq. 1, we obtain

$$\frac{D\tau}{Dt} = 1 \tag{12}$$

which is the expected result since the substantial derivative represents the variation of a variable following with an individual fluid particle, and the increase in residence time of an individual particle is, according to the definition of the τ, one unit residence time per unit elapsed time. This is also the basis of tracking the residence time using the particle tracking approach. Without diffusion, residence time will go to infinity at the wall and inside a recirculation zone. In reality, due to the molecular and turbulent diffusion it is always bounded.

At inflow boundaries where new fluid enters the computational domain, the mean residence time should be set to zero by definition. At walls, $d\tau/dn = 0$ is often used. The boundary condition on outflow boundaries depends on physical situation. A common assumption is the mass flux across an outflow boundary is dominated by convection. So the boundary value can be extrapolated from the inner points.

Equation 11 follows the standard form of the generic Eulerian convection-diffusion transport equation. And it can be very efficiently solved in a steady state solver. The transport equation provides the spatial distribution of the mean residence time over any point of the flow. It does not provide the distribution of the residence time though.

In practice, such mean residence time spatial distribution can be used to identify flow bypassing, channeling and dead zones in a flow field.

Convolution Integral

A real industrial system usually consists many devices, which are interconnected. The fluid coming out from an exit of one device will serve as input for the next as shown in Fig. 1. Sometimes the entire residence time distribution is desired to evaluate the system performance. The system may be too large to simulate in one model or, it may be preferred to simulate them individually since the focus of each device may be different (thus the physical models used may be different). As a result, we can build the model for each device. The residence time distribution can be obtained for each device from the simulation. Once the RTD of individual device is obtained, the RTD of the entire system can be computed by convolution integral. In general, a convolution integral is defined as a product of functions g_1 and g_2:

$$f(t) = g_1 \star g_2 = \int_0^t g_1(t-\tau) g_2(\tau) d\tau \tag{13}$$

where the symbol $g_1 \star g_2$ (occasionally also written as $g_1 \otimes g_2$) denotes convolution of g_1 and g_2.

In a general sense, convolution can be used to calculate the response of a system to arbitrary inputs by using the impulse response of a system. It has been used in many fields such as signal processing. In the context of residence time distribution, the g_2-function can be thought of as the system's response to an impulse signal, and g_1-function be the input signal to the system.

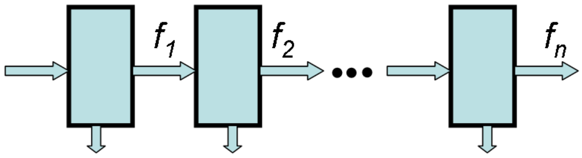

FIGURE 1. A system consisting of many devices

As a result, if the RTDs of each individual device in Fig. 1 are $g_1(t), g_2(t), \ldots, g_n(t)$, respectively, the total residence time distribution through the entire system will be

$$f_n(t) = g_1(t) \star g_2(t) \star \ldots \star g_n(t) \tag{14}$$

In practice, RTDs are usually represented by histograms. There is a simple but very effective way to compute convolution integral for functions in a histogram form. Let us start with a simple case where histograms of function g_1 and g_2 have the same bin size, i.e., the time interval for each bin is the same. Under such a special scenario, calculation of convolution integral can be easily done by the following procedure: given a bin in the g_1 function, its location and weight are known. The contribution of this bin to the integral can be visualized by first scaling the whole g_2 function by that weight factor and then shifting it according to the location of that bin. Conducting such operations for all the bins in the g_1 function, the convolution integral can be obtained by adding all those shifted functions together.

To illustrate the algorithm, let us assume that the g_1 and g_2 function have $n1$ and $n2$ bins, respectively. From the definition of residence time distribution, the f function will have $n1+n2$ bins at maximum. A segment of computer program in C to calculate convolution is shown here:

```
int n1, n2;
float g1[n1], g2[n2], f[n1+n2];

for(i=0; i<n1; ++i) {
for(j=0; j<n2; ++j) {
f[i+j] += g1[i]*g2[j]; }}
```

In practice, the bin size used even in a single function could be different. But, by reducing the bin size conceptually, any two histograms can be thought of having the same bin size eventually. Therefore, the above algorithm can be used for any functions.

TEST PROBLEM AND NUMERICAL RESULTS

Different information regarding residence time can be extracted from different approaches. To illustrate the differences, a 2D test problem is considered in this paper. The geometry of the test problem is shown in Fig. 2. It represents a typical flow problem which can be found in many mixing or heat exchanger applications , in which the flow is highly nonuniform with the presence of flow recirculation and short circuiting zones. The problem we considered here is symmetric and only half domain is needed in the CFD simulation. The fluid used is water with constant density of 1,000 kg/m^3 and the inlet average velocity is taken to be 1 m/s. The flow is fully turbulent. A commercial CFD software, ANSYS FLUENT [14], is used in the simulation. The Navier-Stokes (N-S) equations are discretized using the finite volume method and the realizable k-ε turbulence model is used. A pure quadrilateral mesh with a mesh size being 0.001 m is used to mesh the domain and the total mesh count is about 15,200.

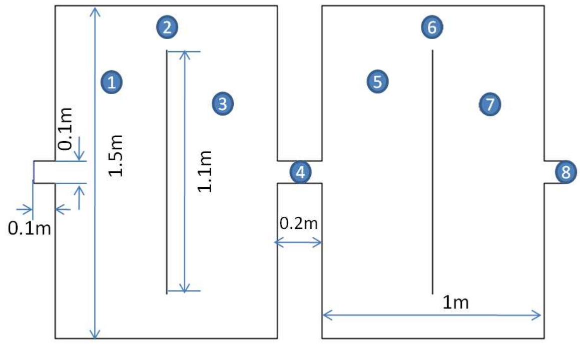

FIGURE 2. Geometry of the mixing device

The repetition of the geometry is specially designed here to illustrate the use of convolution integral in the residence time calculation later on. A periodic boundary condition is used for the inlet and outlet boundaries. The steady-state flow field can be easily obtained by using the segregated solver in FLUENT. The SIMPLE algorithm is used for the velocity-pressure coupling and the second order discretization scheme is used for all the solved variables. Figure 3 shows the contour plot of the velocity magnitude in the device. The red/yellow region in the pictures clearly shows a fast short circuiting passage and four blue regions represent four recirculation zones in the computational domain. Since the second stage of the mixing device is simply a repetition of the first stage, obviously the flow pattern just repeats itself as well.

Tracer Species Transport Approach

The tracer species approach is used first. In this method, the steady-state flow field is frozen. The solver is changed from the steady-state solver to the transient solver. Species transport equation of the tracer species is activated. The tracer species gets released from the inlet for a very short period of time to represent a pulse experiment. Then the solver keeps track of the propagation of the tracer species by solving Eq. 7 in time. The

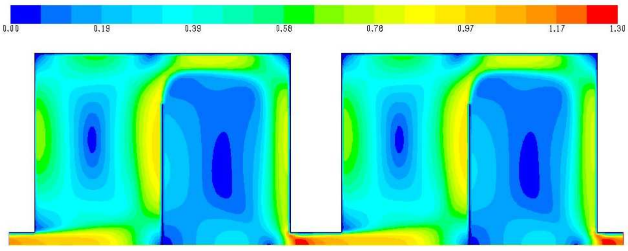

FIGURE 3. Contour plot of velocity magnitude within the device

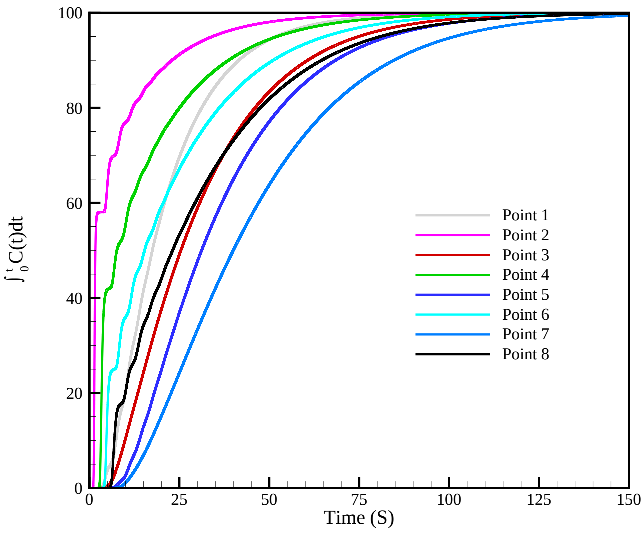

FIGURE 4. Time history of I at each monitored point

time step used in the simulation, 5×10^{-4} s, is small which only allows the species front, at maximum, to spread out less than one mesh size. This is used to guarantee the time accuracy of the simulation. In this study, tracer species is released only for the first 200 time steps, i.e., 0.1 s long in total. After that, tracer species is switched off. From the previous section, it is known that the residence time distribution at any point in the device is directly related to the species concentration through Eq. 1. For the demonstration purpose, eight points as shown in Fig. 2 are monitored. Point 1, 3, 5 and 7 are located in the center of the recirculation zones and Point 2, 4, 6 and 8 are located in the narrow flow passage zone. As the simulation goes on, the time history of species concentration at those points are monitored.

Equation 6 provides a natural condition to monitor the progress of mixing. At time infinity, the time integral of the tracer concentration converges to a single constant value, $I_\infty = \int_0^\infty Cdt = 100 kg/m^3 s$, at every point of the domain. The time history of the integral values at these points are drawn in Fig. 4. It is interesting to note that each curve represents the mixing rate of each corresponding point. In general, points in the circulation zones such as Point 1, 3, 5 and 7 have much slower mixing rate than Point 2, 4, 6 and 8. For example, to reach to 50% of I_∞, it takes about 21s, 26s, 31s and 40s for Point 1, 3, 5 and 7, respectively, which is much larger than 1s, 7s, 15s and 23s for Point 2, 4, 6 and 8, respectively, although the formers are at the upstream of the flow. The cumulative concentrations also increase fast initially and slow down at the later stage. This is due to the presence of a long tail in the species concentration history (which is directly related to the residence time distribution). This will be further discussed in the later section.

The transient simulation is run till the I-values for all the monitored points reach 99.9%I_∞, which translates to about 150 s in the total simulation time. The normalized species concentration which is also the residence time distribution has been plotted in Fig. 5 and 6. Figure 5 shows the residence time distribution curves for the points in the recirculation zone. For all the points, the RTD curve reaches to its peak quickly, then slowly decays to zero. Note that there is obvious oscillation for the curves, especially the one for the point in the first recirculation zone. In fact, the interval of the oscillation denotes the fluid turn-over time in the recirculation zone. As the fluid flows downstream, tracer species has been well mixed and curves become smoother. Similarly, the RTD curves for the points in the short circuiting regions are shown in Fig 6. The characteristics of the RTDs are quite different from the ones in the recirculation zones. In the recirculation zones, flow is diffusion dominated. The RTD curves are wide and their peak values are low. In the flow short circuiting zones, flow is convection dominated. Each RTD has multiple peaks. The time to reach the first peak is much shorter compared to the points in the recirculation zones. In addition, the curve decays much faster.

The mean resident time for each point is calculated out using Eq. 2 and the data are tabulated in Table 1. In the table, the time to reach 99.9%I_∞ is also shown. Another two columns of the data are the computed mean residence time by solving the mean residence time transport equation and by using the particle tracking method. They will be explained in a later section. It can be observed that, although the mean average residence time at exit of the device is about 30 s, to get this, actually we need to run the simulation for a much longer time period in the transient solver. In addition, for all the points the mean residence time is longer than the time where the peak of RTD occurs due to a long tail of the RTD curve. The mean residence time at exit can also be estimated by the ratio of the vessel's volume to volume flow rate. For this device, the volume is 1.52 m^3 and the flow rate is 0.05 m^3/s considering 1 m in the depth direction, so the mean average residence time is 30.4 s. Agreement of the simulation to this calculation provides another good check on the numerical accuracy.

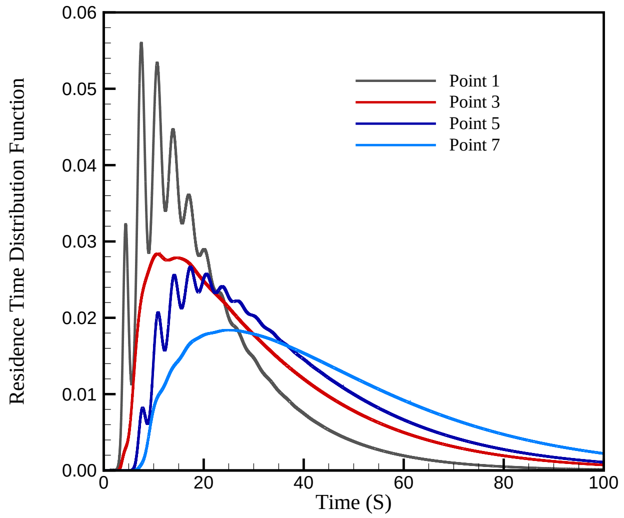

FIGURE 5. Residence time distribution at the monitoring points

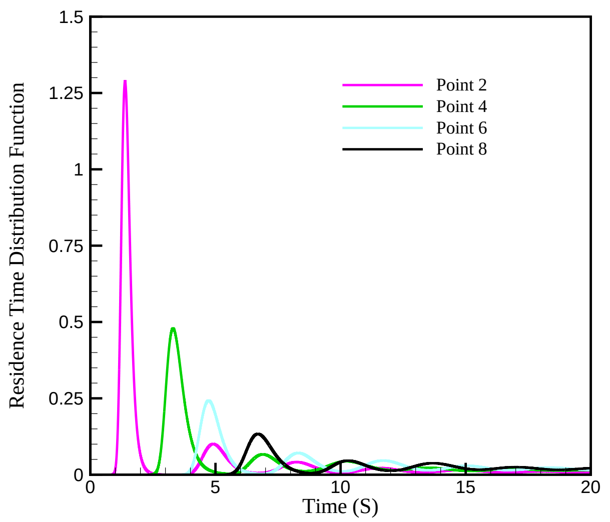

FIGURE 6. Residence time distribution at the monitoring points

To run the case to 150 s with a time step of 0.0005 s, it requires 3×10^5 time steps. On a single processor Linux machine, it takes about 10 hours to run it.

TABLE 1. Comparison of convergence and mean residence time at the monitored points

Point	99.9%I_∞ (s)	τ_{Tracer} (s)	τ_{MeanT} (s)	τ_{DPM} (s)
1	109.1	25.7	26.7	-
2	99.5	8.0	10.3	-
3	131.7	32.0	30.9	-
4	109.4	15.4	15.3	18.5
5	142.6	37.1	38.8	-
6	120.2	22.7	24.6	-
7	165.7	46.5	45.6	-
8	143.9	30.6	30.5	36.5

Convolution Integral

If we want to compute the RTD using the tracer species approach for the first stage of the device, we only need to run 109 s in the solver. But if two units are connected in serial, we will have to run 144 s to get the RTD to reach 99.9%I_∞. As more stages are connected to a system, a transient simulation will become very expensive. For such cases, the method using convolution integral will be very helpful. For example, we can construct the RTDs at Point 5, 6, 7 and 8 using the RTDs at Point 1, 2, 3 and 4. Using Eq. 14, we can obtain,

$$
\begin{aligned}
f_5(t) &= f_4 \star f_1 \\
f_6(t) &= f_4 \star f_2 \\
f_7(t) &= f_4 \star f_3 \\
f_8(t) &= f_4 \star f_4
\end{aligned}
$$

The constructed RTDs for the above four points are shown in Fig. 7 and 8 along with the RTDs obtained through the tracer approach. Figures clearly show the constructed RTDs agree very well with the ones directly obtained from the simulation. The biggest discrepancy occurs at the first curve for Point 5 although it is very small: the convolution computed RTD is sharper at peaks and valleys compared to the directly computed RTD. The reason is that the directly computed RTD is subject to numerical diffusion and discretization errors occurring in the second stage of the vessel while the convolution computed RTD is free of such errors.

This approach becomes very effective if more components are connected in a system in serial.

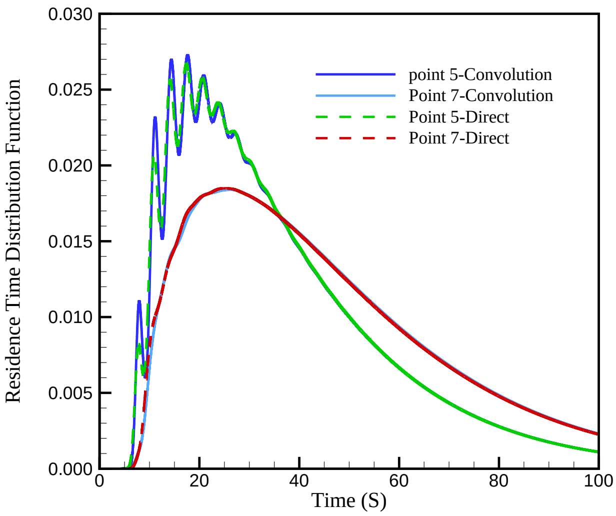

FIGURE 7. Comparison of RTD between computed from CFD and from convolution

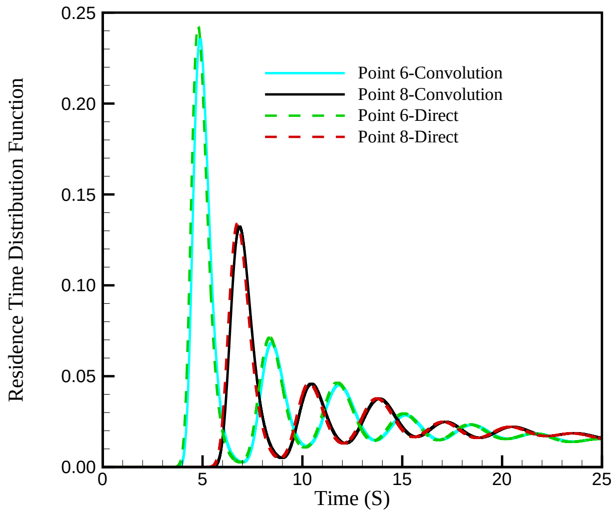

FIGURE 8. Comparison of RTD between computed from CFD and from convolution

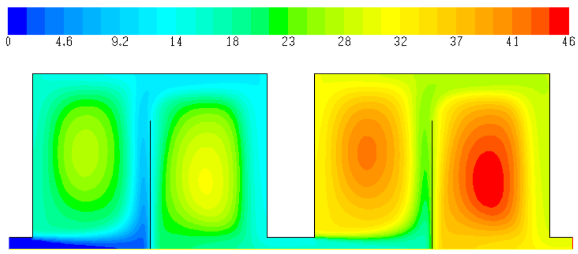

FIGURE 9. Spatial mean residence time distribution in the device

Mean Residence Time Equation Approach

Once a RTD curve is known, it has all the information of the residence time. Not only the mean residence time, its higher moments (e.g., its variance and skewness) can be computed out as well. If only the mean residence time is of the interest, solving the transport equation of the mean residence time is a much better solution. While it takes 10 hours to run the transient solver for 150 seconds in the first approach, it only takes several seconds to converge a steady state scalar equation! For this test problem, the transport equation of the mean residence time, Eq. 11, is solved in FLUENT as a user-defined scalar. The contour plot of the mean residence time is plotted in Fig. 9. It has clearly revealed four recirculation zones in the domain where large residence time is observed. The computed mean residence times at 8 monitored points are also compared to the values obtained from the earlier approach in Table 1. Generally the agreement is very good. The largest discrepancy occurs at Point 2. The tracer transport method is transient in nature, so the accuracy of results depends on solution parameters like time step size and total simulation time. The RTD curve at Point 2 has a very narrow peak around t=1.5 s. It may require a smaller time step to get a more accurate solution at that point. For the mean residence time equation method it is completely free of those transient related error sources.

Lagrangian Particle Tracking Approach

If the residence time distribution at the exit is needed, the particle tracking method can be used. In this study, ANSYS FLUENT's discrete particle method (DPM) is used to conduct the particle tracking. The resolution of the final RTD will highly depend on the number of particles released. To study its sensitivity, N=1,000, 10,000, and 100,000 are used in the simulation, respectively. Histograms of RTD at the outlet of the first section, i.e., location 4 in Fig. 2 are shown in Fig. 10 and 11 for the N=1,000 and N=100,000 case. To have a statistically meaningful curve, histogram with a bin size of 0.1s has been used in those figures. To evaluate the accuracy of those curves, the histogram of RTD with the same bin size from the tracer study is also shown in the figures. The histogram of the RTD is computed from the continuous RTD function (curve Point 4 in Fig. 6) by integration

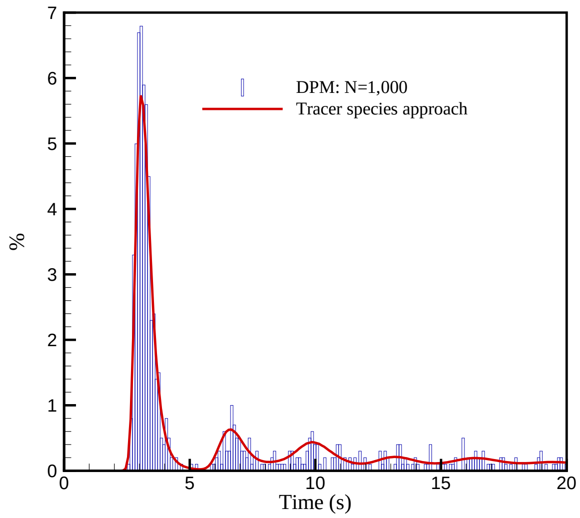

FIGURE 10. Histogram plot of residence time distribution from the DPM approach (N=1,000)

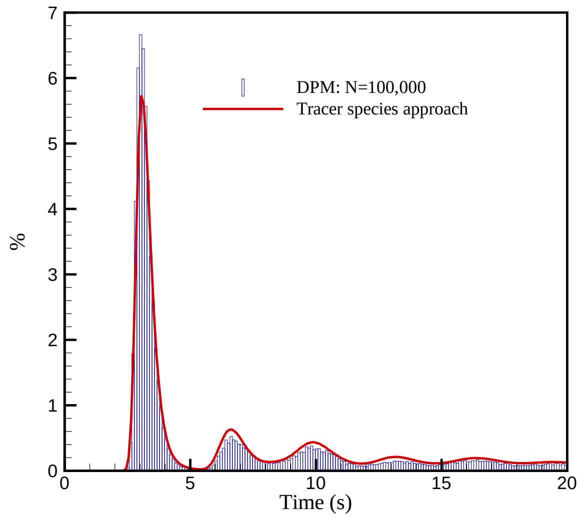

FIGURE 11. Histogram plot of residence time distribution from the DPM approach (N=100,000)

over each bin.

It can be seen that in general, the particle tracking approach can capture the trend very well. If a small number of particles are used, the stochastic error of the histogram will be large, especially in the long-time tail region. The histogram is not very smooth there. As the number of particles increases, the histogram becomes very smooth, closely following the RTD function we obtained from the tracer simulation. However, as the number increases, the computational cost increases as well. But this method is still less expensive compared to the tracer species approach. It takes several minutes to track 100,000 particles in the simulation.

The largest discrepancy in the figures is the peak values. The DPM approach overpredicts some peaks and underpredicts others in this case. It is mainly caused by the turbulent dispersion model which will be discussed in the next paragraph.

The mean residence time can be computed by averaging the residence time of each particle. The computed values are 17.9 s, 18.5 s and 18.7 s for N=1,000, 10,000, and 100,000, respectively. It seems that the mean residence time is not very sensitive to the number of particles. However, compared with the correct value, 15.2 s, and the values from other approaches, the DPM approach overpredicts the mean residence time by about 20% as shown in Table 1! This is mainly caused by inaccuracy of the turbulent dispersion model we used. In our simulation, a simple isotropic random walking model has been used. It seems that more advanced stochastic models are needed to capture the RTD correctly. The importance of turbulent dispersion can be illustrated by a simple exercise: switching off turbulent dispersion in the model, the computed mean residence time is only 3.13 s!

Besides the flexibility of changing particle numbers for different accuracy requirement, the particle tracking approach can be used to visualize the internal flow pattern as well. Figure 12 shows the trajectories of particles in the device. In this figure, 100 particles' trajectories are shown. And the trajectories are colored by the particle's residence time. It vividly reveals the recirculation zone and the nature of the flow being turbulent.

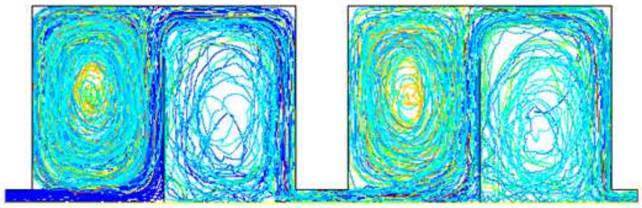

FIGURE 12. Particles' trajectories in the DPM calculation

CONCLUSIONS

Different numerical approaches to compute residence time information are summarized in the paper. An example is used to illustrate each method's advantages and disadvantages. Solving the unsteady transport equation of the tracer species is the most comprehensive approach, allowing user to get the detailed information. The computational cost is large due to the long tail of a RTD curve. The mean residence time can be conveniently obtained by solving a steady state transport equation. The computational cost is low and it can reveal spatial mean residence time distribution. The particle tracking approach is usually fast and can provide a quick and dirty solution for the RTD information at outlet. The method can capture the trend of RTD quite accurately. However, the mean residence time does not necessarily preserve the constraint of V/Q. It seems that more advanced turbulent dispersion models are needed to track the particles.

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