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DRAFT: RANS PREDICTIONS OF TURBULENT SCALAR TRANSPORT IN DEAD ZONES OF NATURAL STREAMS

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ABSTRACT

Natural stream systems contain a variety of flow geometries which contain flow separation, turbulent shear layers, and recirculation zones. This work focuses on stream dead zones. Characterized by slower flow and recirculation, dead zones are naturally occurring cutouts in stream banks. These dead zones play an important role in stream nutrient retention and solute transport studies. Previous experimental work has focused on idealized dead zone geometries studied in laboratory flumes. This work studies the capabilities of computational fluid dynamics (CFD) to investigate the scaling relationships between flow parameters of an idealized geometry and the passive scalar exchange rate. The stream geometry can be split into two main regions, the main stream flow and the dead zone. For the base case simulation, the depth-based Reynolds number is 16,000 and the dead zone is 0.5 depths in the flow direction and 7.5 depths in the transverse direction. Dead zone lengths and the main stream velocity were varied. These flow geometries are simulated using RANS turbulence model and the standard $k-\omega$ closure. Scalar transport in dead zones is typically modeled as a continuously stirred tank with an exchange coefficient for the interface across the shear layer. This first order model produces an exponential decay of scalar in the dead zone. A two region model is also developed and applied to the RANS results. Various time scales are found to characterize the exchange process. The volumetric time scale varies linearly with the aspect ratio. The simulations showed significant spatial variation in concentration leading to many different time scales. An optimized two region model was found to model these different time scales extremely well.

NOMENCLATURE

A_{cp} Area of exchange between core and perimeter, $[m^2]$
C Average concentration in the dead zone, $[kg/m^3]$
C_0 Initial concentration in the dead zone, $[kg/m^3]$
C_c Concentration of the core region, $[kg/m^3]$
C_{mc} Concentration of the main channel, $[kg/m^3]$
C_p Concentration of the perimeter region, $[kg/m^3]$
D Main channel depth, $[m]$
E Exchange velocity, $[m/s]$

E_{cp} Exchange velocity between core and perimeter, $[m/s]$
h_D Average dead zone depth, $[m]$
h_E Depth of dead zone/main channel interface, $[m]$
k Nondimensional exchange coefficient, $[1]$
L Dead zone length, $[m]$
T_0 Time scale at late time, $[s]$
T_{avg} Average residence time of the dead zone, $[s]$
T_{conv} Convective time scale of main channel, $[s]$
T_{vol} Volumetric time scale of exchange, $[s]$
U Average main channel velocity, $[m/s]$
V_c Volume of the core region, $[m^3]$
V_p Volume of the perimeter region, $[m^3]$
W Dead zone width, $[m]$
W_p Width of the perimeter region, $[m]$

FIGURE 1: A natural dead zone caused by an obstruction in a stream.

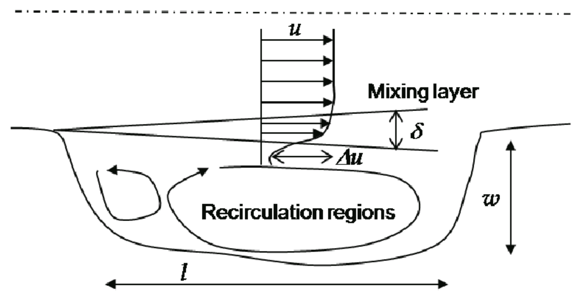

FIGURE 2: Schematic of a typical dead zone showing the mixing layer and streamwise velocity profile.

INTRODUCTION

In studying the mixing properties of turbulent flows, residence times can be important descriptors of the system. Within a system, there can exist dead zones, regions of slower fluid flow and longer residence times. These dead zones can significantly affect the overall behavior of the system. Chemical engineers have extensively studied residence times as they apply to reactor design [1, 2]. This work investigates the mixing and residence times as they apply to natural streams. As complex ecological and fluid systems, streams may contain dead zones. These dead zones can be formed by natural erosion and deposition process as well as by structures introduced by humans. Regardless of origin, dead zones, through turbulent mixing processes, are regions of increased retention for dissolved substances such as nutrients for aquatic life or pollutants introduced by humans.

While dead zones can generally be identified by visual inspection, dead zones contain a set of consistent characteristics. Figure 1 shows a typical dead zone in a small stream caused by a root protruding into the channel. Physically a dead zone is formed as a cutout into the bank. Separating the dead zone from the main channel flow is a mixing layer where mass and momentum are exchanged, Figure 2. A mixing layer forms due to the difference in velocity magnitude between the fast moving flow of the main channel and the slower moving dead zone. The slower fluid in the dead zone is cause by the flow separating at the upstream corner of the dead zone. The separation causes recirculation inside the dead zone. The recirculation generally takes the form of one large eddy, but additionally eddies can be present depending on the dead zone geometry.

This work focuses on dead zones with an idealized rectangular geometry. This geometry is directly applicable to some erosion control structures built into streams. Naturally formed dead zones are generally more rounded and irregular. This work seeks to come up with results for the idealized geometry that can then be used with modification for more complex geometries.

Early work on quantifying the transport properties of dead zones focused on developing a simplified model for the interaction between the dead zone and the main channel. Valentine and Wood [3] conducted laboratory experiments on simplified dead zones. These experiments found that the exchange process can be modeled as a first order system by assuming the dead zone to be perfectly mixed (see theory section for more details). Valentine and Wood [4] found that the exchange coefficient was approximately constant for a variety of dead zone geometries. This first order dead zone model was then combined with the axial dispersion model used by Levenspiel [2] to model the response of the combination of steam and dead zone.

Engelhardt et al. [5] later conducted large scale experiments on irregularly shaped dead zones in the River Elbe. These experiments showed that the exchange process relies on coherent eddies shed from the upstream corner of the dead zone. As these eddies travel downstream through the mixing layer, their influence penetrates into the dead zone. These structures are quasi-two dimensional. Hinterberger [6] compared depth-averaged LES simulations with full 3D LES and found that the depth averaged simulations predicted significantly higher exchange rates than either

3D LES or experiment. Kimura and Hosada [7] compared laboratory experiments to numerical results using the depth-averaged equations. The depth averaged equations captured the same average velocity trends as the experiments. The largest differences were in the mixing layer. Engelhardt [5] also found that the exchange process for the irregular dead zones had many time scales and thus could not be represented as a first order system. Additional experiments on the River Elbe by Kozerski et al. [8] showed that the exchange process is complicated by a dead zone having regions of distinctly different flow characteristics. In this cases, the dead zone can be modeled as a combination these subregions. Each subregion is modeled as a first order system.

Recently Uijttewaal et al. [9] conducted laboratory flume studies on series of dead zones. A series of dead zones is less likely to appear naturally in streams, but can be found where human made structures have been introduced to control erosion or help habitat restoration. These experiments varied geometric and flow parameters. The exchange coefficient was generally insensitive to changes in geometry and the flow. The dye concentration studies show that the system can be approximated as a first order system. However, the system is more complicated as the exchange coefficient changes over time. The particle tracking results show a primary eddy located near the center of the dead zone with a secondary eddy in the upstream corner of the dead zone. The existence of the secondary eddy is hypothesized to contribute an additional time scale to the exchange process.

Weitbrecht [10] also conducted experiments on a series of dead zones in a laboratory flume. These experiments focused on parametric studies for many different geometric features. Weitbrecht found that the aspect ratio of the dead zone determines how many eddies will be present. For aspect ratios around unity, only one eddy is present. As the aspect ratio is increased or decreased, secondary eddies are formed. Using a combination of dye concentration and particle tracking studies, Weitbrecht found that the exchange coefficients generally matched the results of Valentine and Wood, and Uijttewaal [4, 9]. However, the coefficient varied slightly based on the geometry of the dead zone. Weitbrecht proposed using a modified hydraulic diameter to combine geometry terms.

McCoy et al. [11] further looked at series of dead zones using LES and RANS studies for the same geometry as Uijttewaal. McCoy's results show a strong dependence of the entrainment velocity on depth. Fluid from the main stream tends to be entrained near the bottom surface of the dead zone and at the upstream side. This result suggests depth averaging does not appropriately capture the details of the entrainment velocities.

Bellucci et al. [12] conducted an analytical investigation of the advection-diffusion equation for semi-enclosed basins assuming a constant eddy diffusivity. The residence times of these basins could be characterized by multiple time scales. Using an eigenvalue analysis Bellucci et al. showed that the average concentration of a passive scalar will always become exponential at late time. These results are applicable to flows with recirculation like dead zones.

The objective of this work is to determine the scales that are important to the residence time of regular shaped dead zones. Currently, field researchers need to conduct lengthy studies to determine the residence times of dead zones in streams. A better understanding of the important scales could lead to predicted residence times based of easily measured geometric or flow parameters. This paper first introduces two dead zone models. Results are presented for several numerical studies along with the analysis on the performance of the dead zone models.

THEORY

There are two broad types of dead zones series that have been studied, those formed by obstructions protruding into the main flow and those formed by cutouts into the bank, Figure 3. The obstruction type causes the flow to accelerate around the obstruction as the stream width is decreased. The acceleration and subsequent separation leads to major variation between the first dead zone in the series and the last. This type is more similar to erosion control structures placed in rivers. For the cutout type, the only differences between the first and last dead zone in a series are due to the developing mixing layer. This type is more representative of naturally formed dead zones in streams.

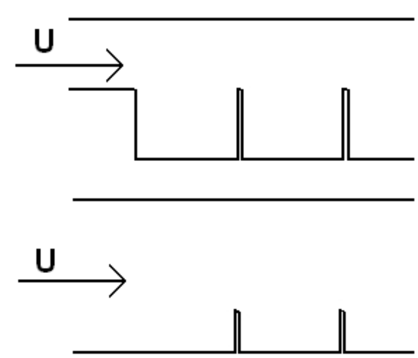

FIGURE 3: A comparison of the two ways dead zones are formed viewed from the top. Top: Dead zone is formed by a cutout into the bank, Bottom: Dead zone is formed by obstructions in the main channel.

With both dead zone types, there are common geometry parameters. Figure 4 shows the standard definition for dead zone geometry. The dead zone length, L, is defined in the streamwise direction. The width, W, is defined in the transverse direction. There are three different depths, the main channel depth, D, the depth at the interface between the dead zone and the main channel, h_E, and the average depth of the dead zone, h_D. U is the

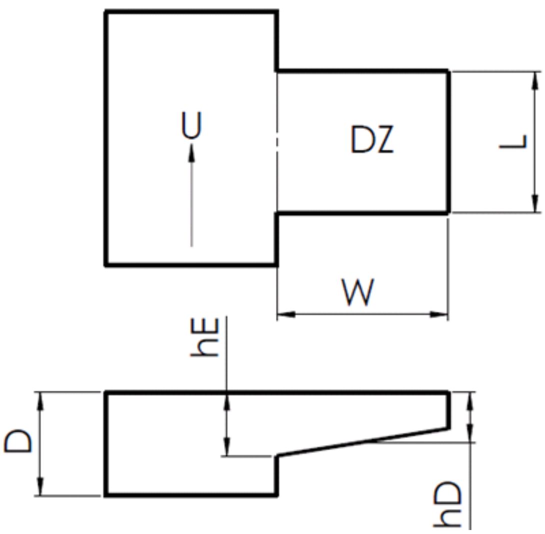

FIGURE 4: Definitions of typical dead zone parameters.

average velocity in the main channel.

First Order Model

The most commonly used model for residence time in a dead zone is the first order model. This model assumes that the dead zone contains a passive scalar at a uniform concentration and that the main channel has a different uniform concentration. Exchange between the main channel and dead zone is only specified by the entrainment velocity, E. The uniform concentration in the dead zone is equivalent to a perfectly mixed region, also called a continuously stirred tank reactor (CSTR). Using the entrainment velocity, a non-dimensional exchange coefficient, k, can be formed as a ratio of velocities, Equation 1.

$$k = \frac{E}{U} \tag{1}$$

Using the definition of k, a mass balance can be written for the mass of the passive scalar in the dead zone, Equation 2, where M is the mass of scalar in the dead zone, C is the concentration of scalar in the dead zone, and C_{mc} is the constant scalar concentration of the main channel. Using the definition of k, the definition of concentration as mass per volume, and assuming the concentration of the main channel is zero, the mass balance turns into a first order differential equation, Equation 3. Using the initial concentration C_0, the differential equation can be solved for the concentration as a function of time, Equation 4.

$$\frac{\mathrm{d}M}{\mathrm{d}t} = -Eh_E L(C - C_{mc}) \tag{2}$$

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -\frac{kUh_E}{Wh_D}C \tag{3}$$

$$\frac{C}{C_0} = \exp\left(-\frac{t}{T}\right) \text{ where } T = \frac{Wh_D}{kUh_E} \tag{4}$$

The first order model is completely defined by the time scale T. An exponential curve can be fit to an experimental normalized concentration curve to determine the model time scale. Generally, the exponential fit is done for the entire concentration time series. This method gives a single time scale that is a best fit for all the data. Alternatively, the exponential fit can be done at each data point. This method gives the time scale at each data point. The series of time scales can be used to assess how well the first order model represents the experimental data. If the time scale changes significantly over time, a more complicated model is needed to capture the dead zone system.

Two Region Model

The experimental results of Weitbrecht et al. [10] show that dead zones have a large primary eddy approximately located at the center of the dead zone. The primary eddy separates the dead zone into two regions. There is the core region of the primary eddy where the average velocity is small and the higher momentum perimeter region. As an extension of the first order model and following the method used by Kozerski et al. [8], the dead zone can be divided into two perfectly mixed CSTRs. The core region, C_c, exchanges scalar with the perimeter region based on an exchange velocity E_{cp}. The perimeter region, C_p, exchanges scalar with both the main channel and the core region. The surface area of exchange between the core and perimeter regions is A_{cp}.

For simplicity, the perimeter region is defined as a uniform width, W_p, rectangular band that runs around boarder of the dead zone. The core region is the remaining volume at the center of the dead zone, Figure 5. Using the conservation of mass for a passive scalar, Equations 5 and 6, two coupled differential equations, can be derived to model the two regions. These equations can be efficiently solved numerically. The average concentration of the dead zone is the volume weighted average of the two regions as shown in Equation 7.

$$\frac{\mathrm{d}C_p}{\mathrm{d}t} = -\frac{Eh_E L C_p + E_{cp} A_{cp} (C_p - C_c)}{V_p} \tag{5}$$

$$\frac{\mathrm{d}C_c}{\mathrm{d}t} = -\frac{E_{cp} A_{cp} (C_c - C_p)}{V_c} \tag{6}$$

$$C = \frac{C_c V_c + C_p V_p}{W L h_D} \tag{7}$$

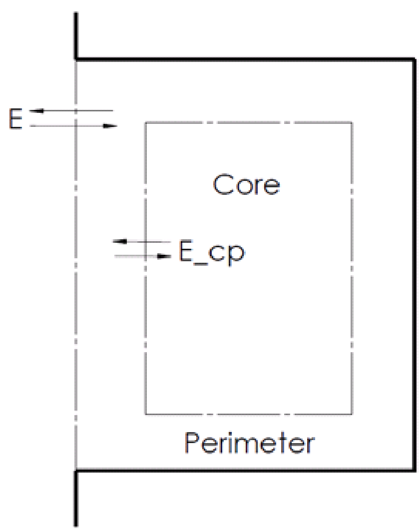

FIGURE 5: Definition of two region geometry. The perimeter region has a uniform width and surrounds the core region.

Time Scales

There are many different time scales that are important to transport within a dead zone. The convective time scale, T_{conv} in Equation 8, is the time it takes fluid in the main stream to travel the length of the dead zone. This time scale dictates how long an eddy in the mixing layer will affect the dead zone. The average residence time, T_{avg} in Equation 9, can be found by integrating the normalized concentration curve.

A volumetric or turnover time scale, T_{vol} in Equation 10, is defined as the ratio of the dead zone volume to the volumetric flow rate into the dead zone. This time scale is equal to the time scale of the first order model. T_0 is the exponential time scale of the system at late time that is predicted by the analysis of Bellucci [12]. For a perfectly mixed dead zone $T_0 = T_{vol} = T_{avg}$.

$$T_{conv} = \frac{L}{U} \tag{8}$$

$$T_{avg} = \int_0^\infty \frac{C}{C_0} \mathrm{d}t \tag{9}$$

$$T_{vol} = \frac{W h_D}{E h_E} \tag{10}$$

METHODS

This work looks to study the time scales that are important to the passive scalar transport within a dead zone. Parametric studies are run for both bulk velocity, U, and dead zone length, L. The RANS equation is simulated for each geometry using the commercial finite volume solver Star-ccm+. The turbulence is modeled using the standard $k-\omega$ closure with wall functions. The free surface is modeled as a rigid slip boundary. This approximation is reasonable as the Froude number is below 0.3, meaning free surface effects are small. The smallest Reynolds number based on the main channel depth is 8000 ensuring that the flow is turbulent.

Table 1 shows the parameters used for all of the simulations. The base case and cases 7, 8, and 9 replicate the experimental conditions used by Weitbrecht et al. [10]. Figure 6 shows the geometry used. As these dead zones are formed by obstructions into the flow, data was collected in dead zones #8 to avoid the irregular flow around the first obstruction. Due to the short length of the dead zones in cases 7 and 8, 15 dead zones were used and data was collected in dead zone #14. The depth of the dead zone is uniform and the same as the main channel for all cases, $h_E = h_D = D$.

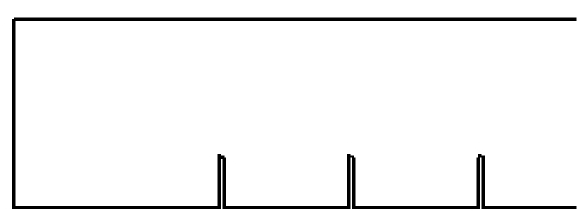

FIGURE 6: Plan view of the geometry used. Dead zones #1 and #2 are shown. Geometry contains ten dead zones in total.

Numerical Method

Using the defined geometry, structured hexahedral grids were created. Each grid is refined near the walls and in the

TABLE 1: Summary of Parameters for Each Case

Case #	L (m)	W (m)	D (m)	U (m/s)	W/L
Base	1.25	0.5	0.046	0.16	0.4
2	1.25	0.5	0.046	0.08	0.4
3	1.25	0.5	0.046	0.12	0.4
4	1.25	0.5	0.046	0.14	0.4
5	1.25	0.5	0.046	0.18	0.4
6	1.25	0.5	0.046	0.20	0.4
7	0.25	0.5	0.046	0.16	2.0
8	0.45	0.5	0.046	0.16	1.1
9	0.65	0.5	0.046	0.16	0.77
10	0.94	0.5	0.046	0.16	0.53

mixing layer. The appropriate grid resolution was determined through a grid convergence study. The inlet section has a prescribed fully developed turbulent profile. This profile was generated from a separate simulation on a periodic channel with the same cross-section. The free surface is approximated as a slip wall. The bank opposite the dead zones is modeled as a slip wall and the rest of the walls have the no-slip condition.

To verify that the RANS model was implemented correctly, a case was run identical to McCoy's simulations [11]. These simulations use the same geometry as Uijttewaal's [9] experiments. Results using this implementation match McCoy's RANS results for transverse velocity and turbulent kinetic energy profiles.

The first step in the solution procedure is to solve for the time averaged flow field. This is a steady solution of the RANS equation. In order to run passive scalar study, the simulation must be transient. To do this, the time averaged flow field is mapped to the transient simulation and frozen in time. This method allows the passive scalar to be advected and diffused using the time averaged velocities and eddy diffusivities. The turbulent Schmidt number is set equal to one. The passive scalar is initialized with a concentration of one inside the dead zone and zero in the main channel. The average concentration inside the dead zone is calculated as a volume average of the concentration inside each cell. The initial condition automatically normalizes the concentration to be at one at time zero. The transient simulation is allowed to run until the dead zone concentration is small which, which was found to be 2000 s.

Two Region Optimization

The two region model can be applied to these simulations. However, there are three unknown parameters, the exchange velocity, E, the core-perimeter exchange velocity, E_{cp}, and the width of the perimeter region W_p. The applicability of the two zone model can be evaluated by comparing the model results to the RANS simulation results. Using the optimization code SNOPT [13], E, E_{cp}, and W_p are varied to minimize the square of the difference between the concentration curves of a RANS simulation and the model. SNOPT is a robust implementation of a sequential quadratic programming algorithm used to iteratively optimize nonlinear problems. For the two zone model to match, the optimized model should also have a physically realistic value of W_p.

RESULTS

Results from the ten simulations summarized in 1 are presented here. First the exchange velocity, E, is calculated as the area average velocity into the dead zone. The exchange coefficient is calculated by dividing E by U. This gives exchange coefficients of approximately 0.02 which is in the range of past experiments [4, 9, 10]. The exchange velocity can also be used to calculate the volumetric time scale, T_{vol}. By dividing T_{vol} by the convective time scale, T_{conv}, a ratio is formed that compares the transport in the dead zone to the transport in the main channel. Figure 7 is a plot of the this ratio of time scales to the W/L ratio. Also plotted are the experimental results of Weitbrecht and Uijttewaal [9, 10]. Weitbrecht used two different experimental methods. The PIV data was collected by tracking particles on the free surface. Dye injection and concentration studies were used to get the PCA data. Uijttewaal's experiments use a different geometry where h_E and h_D are less than D. Overall, the trend is increasing with W/L ratio and appears linear. The largest W/L ratio case was omitted from the linear fit. Such slender dead zones begin to exhibit different behavior where there are multiple eddies stacked along the dead zone width. The RANS results match the experimental trend and have similar numerical values. The T_{vol}/T_{conv} ratio should approach zero as the W/L ratio approaches zero as this limiting case would be simple channel flow.

Figure 8 shows the normalized concentration plot for the base case. At first glance, this plot looks somewhat exponential and approaches zero at late time as expected. Figure 9 fits the first order model to the concentration curve at each point in time. From this plot, it is clear that the dead zone does not have a single time scale. The time scale is initially equal to T_{vol} as the dead zone starts out perfectly mixed. As time progresses, the scalar is quickly advected out of the dead zone by the fast moving fluid in the perimeter region. The scalar remains at higher concentration in the slow moving core region. This uneven distribution causes the time scale to increase over time. Also, shown in Figure 9 is the late time scale T_0 predicted by Bellucci's [12] analysis. The average time scale is shown for reference and is always bounded by T_{vol} and T_0.

Due to the uneven distribution of scalar in the dead zone, the two region model is a good candidate to describe the dead zone. Optimizing the two region model parameters to match the concentration plot of the base case gives Figure 10. The concentration plots match so closely that the lines are overlaid on top of each other. The RMS difference is 0.17%. Such a close match suggests that the two region model describes the transport process in the RANS simulations.

The optimization found the best match when the perimeter region is 0.14 m wide. Figure 11 shows an overlay of the optimized core region size on a contour plot of the concentration from the RANS simulation. The optimized core region somewhat matches the size of the region of higher concentration at the center of the dead zone. This correlation suggests that the model does match the behavior of the RANS simulations.

Figure 12 shows the concentrations for the two regions. These model results show that the concentration of the perimeter region quickly drops while the concentration remain high in the core region. This behavior was also observed in the RANS simulations. Table 2 shows the model parameters E, E_{cp}, and W_p

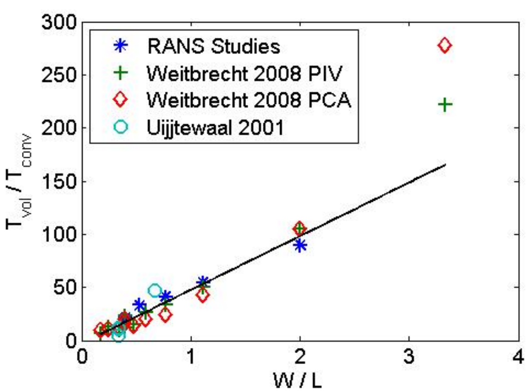

FIGURE 7: Plot of the ratio of the volumetric time scale to the convective time scale vs. the width to length ratio.

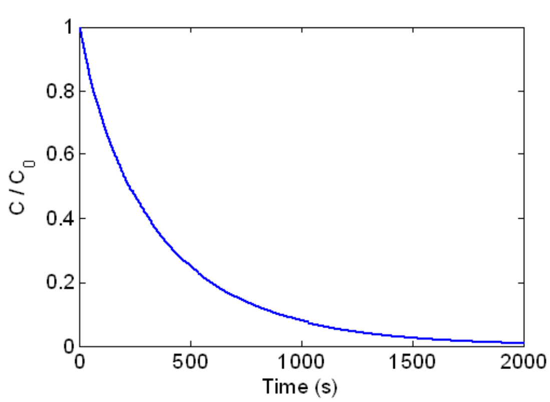

FIGURE 8: Plot of normalized concentration vs. time for the base case.

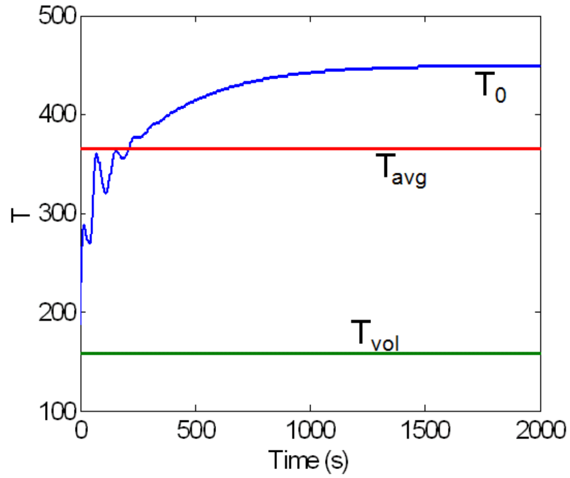

FIGURE 9: Plot of the dead zone time scale vs. time. Plotted for reference are the volumetric, average, and late time scales.

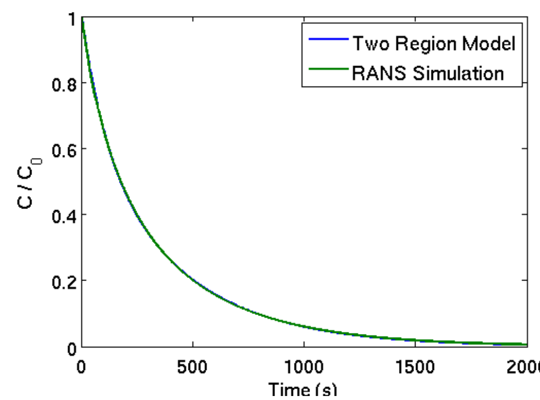

FIGURE 10: Comparison of the concentration plot for the base case and the optimized two region model.

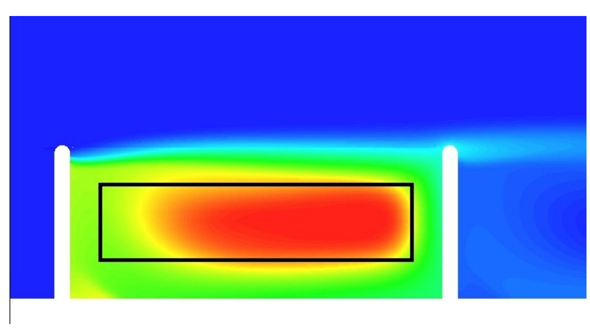

FIGURE 11: Plot showing the size of the core region based on the optimized two region model.

for the the ten cases. E_{cp} is generally an order of magnitude less than E which causes the core region to retain scalar longer. In the two region model, E sets T_{vol}, E_{cp} sets T_0, and W_p sets T_{avg}.

TABLE 2: Summary of Two Region Model Results

Case #	E (m/s)	E_{cp} (m/s)	W_p (m)	% Error
Base	0.0018	0.00032	0.14	0.16
2	0.0009	0.00033	0.10	0.17
3	0.0015	0.00039	0.12	0.15
4	0.0017	0.00045	0.12	0.12
5	0.0021	0.00043	0.13	0.14
6	0.0023	0.00046	0.13	0.14
7	0.0031	0.00007	0.080	0.11
8	0.0027	0.00044	0.094	0.090
9	0.0024	0.00025	0.12	0.17
10	0.0020	0.00031	0.11	0.15

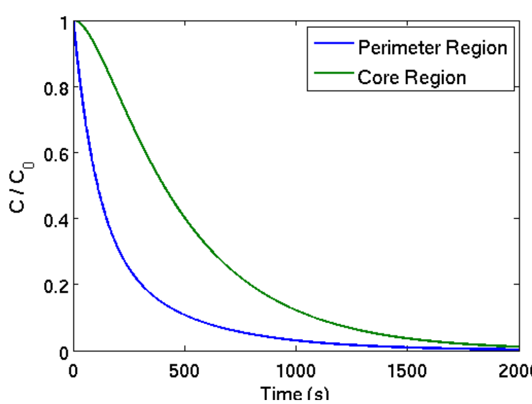

FIGURE 12: Plot of the normalized concentration for the perimeter and core regions.

The uneven distribution of the scalar in the RANS studies calls into question the perfectly mixed assumption used in the first order model. To be perfectly mixed, the dominant mode of transport would need to be turbulent diffusion. This idea can be tested by initially placing scalar only in the core region and then using a averaging technique. The concentration in the dead zone is averaged in both the vertical and streamwise directions.

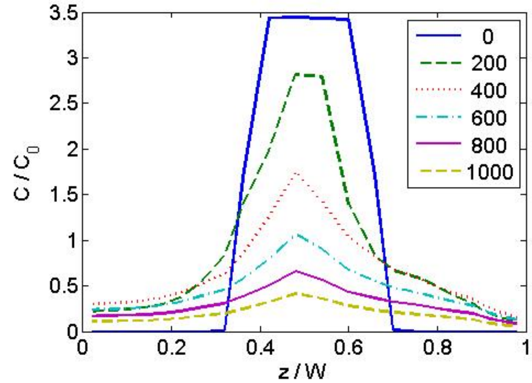

FIGURE 13: Plot of the concentration averaged in the vertical and streamwise directions. Concentration is initially added to the core region only.

Figure 13 shows the resulting line plots for the averaged concentration versus the transverse location for several different times. Bellucci [12] used this technique to determine if the transport is advective or diffusive in nature. If the dead zone were dominated by turbulent diffusion the line plots would quickly flatten to a uniform distribution. The fact that there remains a peak concentration suggests that advection is the main cause of scalar transport in the RANS simulations.

CONCLUSIONS

RANS simulations of series of dead zones were carried out for a range of lengths and average velocities on similar geometry to past experiments. The time averaged velocity field generally matches the experiment with a large eddy at the center of the dead zone with additional eddies depending on the W/L ratio. The exchange velocities, E, for the simulations matches the range of values found by experiment.

With the calculated exchange velocities, the volumetric time scales were calculated. When T_{vol}/T_{conv} is plotted vs the W/L ratio, the simulations match the increasing trend of the experimental results. This plot could be useful for estimating the T_{vol} of an actual dead zone from just a width, length, and average velocity measurement. For a perfectly mixed dead zone, T_{vol} would completely describe the residence time of the dead zone.

The passive scalar simulations showed that the dead zone is not perfectly mixed. The core of the primary eddy retain scalar longer than the perimeter region. This lead to multiple time scales being present in the dead zone. The dead zone time scale begins equal to T_{vol} and increases with time. At late times, the time scale becomes constant and is defined as T_0. The average residence time is bounded by T_{vol} and T_0. An averaging technique showed that the dead zone is not well mixed and that the exchange process is advection dominated.

The nonuniform concentration distribution in the dead zone lends the RANS results to be approximated using a two region CSTR model. This model uses a core region and a perimeter region. The exchange properties and the size of these dead zones is optimized to match the concentration plots from the RANS simulations. The two zone model matches the RANS results extremely well in both the physical size of the core region and the concentration of the dead zone. While this model yields insight into the mechanism for transport within a dead zone, it does not have predictive capability.

Additional work is needed to verify the results of the RANS passive scalar studies. Due to the unsteady behavior of the dead zone, it is possible the RANS equation is not capturing part of the transport process. Large eddy simulation could be used to investigate this limitation. This work focuses on rectangular shaped dead zones. Detailed field work is needed to determine if these trends hold for more complicated natural dead zones.

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