PARAMETERIZATION OF MEAN RESIDENCE TIMES IN IDEALIZED RECTANGULAR DEAD ZONES REPRESENTATIVE OF NATURAL STREAMS

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5 ABSTRACT

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Three-dimensional Reynolds averaged Navier-Stokes modeling, validated against experi-6 mental data, is used to parameterize the flow features and time scales in idealized rectangular 7 cavities for a wide range of width-to-length ratios, $0.4 \leq W/L \leq 1.1$, and Reynolds number 8 based on the depth, $5000 \le Re_D \le 20300$, representative of isolated dead zones in small nat-9 ural streams. The flow features for this parameter range are similar to open cavity flows and 10 consist of a mixing layer spanning the entire length of the dead zone together with a single 11 main recirculation region. The Langmuir time scale (ratio of dead zone volume to discharge) 12 based on the assumption of a well-mixed dead zone is found to be a function of the mean 13 rotation time scale (inverse of average rotation rate) within the dead zone, the momentum 14 thickness of the upstream boundary layer, and the dead zone width. The entrainment coeffi-15 cient, used to relate the exchange velocity to the average free- stream velocity, is shown to be 16 directly related to the upstream boundary layer momentum thickness non-dimensionalized 17 by the width of the dead zone. Using passive tracer to quantify the mean residence time 18 showed that the dead zone can be characterized by two perfectly mixed regions including a 19 core or secondary region around the center of the eddy and a surrounding primary region 20 that interacts directly with the free-stream through the mixing layer. A two-region model is 21

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developed to obtain time scales associated with the primary and secondary regions within the dead zone using an optimization procedure based on the computational data. The time scale associated with the primary region is representative of the Langmuir time scale and is found to be a strong function of the aspect ratio W/L and the Reynolds number. The secondary region time scale represents the long-time asymptotic behavior of the tracer concentration and is found to be a strong function of the dead zone geometric parameters only.

²⁸ Keywords: Dead Zones/Cavities, Mean Residence Time, Surface Transient Storage, RANS

29 INTRODUCTION

As complex ecological and fluid systems, streams may contain dead zones which are 30 parts of the surface channel that have zero mean downstream flow and that exchange water 31 with the main channel. These dead zones can be formed by natural erosion and deposition 32 processes as well as anthropogenic structures. Regardless of origin, dead zones, through 33 turbulent mixing processes, provide refugia for aquatic life and provide transient storage for 34 dissolved substances such as nutrients or pollutants introduced by humans. In the case of 35 both nutrients or pollutants, knowledge of dead zone residence time is critical for under-36 standing reactions and how long the solutes stay in the system. 37

While irregular dead zones found in natural streams can generally be identified by visual 38 inspection, they contain a consistent set of flow and geometric characteristics as shown in 39 Figure 1(a). Figure 1(b) shows a typical dead zone in a small stream caused by a root 40 protruding into the channel. Physically, a dead zone is formed as a cutout into the bank. 41 Separating the dead zone from the main channel flow is a mixing layer where mass and 42 momentum are exchanged, as shown in figure 1(a). The slower moving fluid in the dead zone 43 is caused by the flow separating at the upstream corner of the dead zone. The separation 44 causes recirculation inside the dead zone. Figure 1(c) shows a schematic of the idealized 45 dead zone geometry with streamwise length, L, and transverse width, W. The depth, D, 46 into the paper is assumed uniform for channel and the dead zone; however, in natural dead 47 zones some variations in depths may occur. The recirculation generally takes the form of one 48

⁴⁹ large eddy for typical dead zones in streams, but additional eddies can be present depending ⁵⁰ on the dead zone geometry, width-to-length ratio (W/L), and stream flow rate or Reynolds ⁵¹ number $(Re_D = UD/\nu)$, where U is the average free-stream velocity and ν is the kinematic ⁵² viscosity.

There are two broad types of dead zones that have been studied, those formed by ob-53 structions protruding into the main flow and those formed by cutouts into the bank. The 54 cutout type involves a cavity in the bank of the stream. The flow separates at the beginning 55 of the cavity and recirculates within the dead zone. The obstruction type is formed by a 56 protrusion into the main channel that causes the flow to accelerate. This acceleration leads 57 to larger flow separation and higher velocity gradients near the upstream corner of the dead 58 zone. Obstruction type dead zones are characteristic of erosion control structures or a down 59 tree extending into the channel. Cavity type dead zones are common in natural streams and 60 field work has found that they generally have aspect ratios (W/L) less than one (Jackson 61 et al. 2012). 62

The transport phenomena involved in dead zones (Valentine and Wood 1979; Gualtieri et al. 2010) are similar to flow features observed in cavity flows relevant to many engineering applications. Of importance are contaminant mass exchange processes in river embayments and main channels (Chang et al. 2006; Engelhardt et al. 2004), shear layer instabilities and relevant heat and momentum transfer processes over aircraft wings (Lin and Rockwell 2001; Lawson and Barakos 2011), and cavitation due to impingement of the shear layer on downstream end of the cavity in naval applications (Liu and Katz 2008).

In studying the mixing properties of turbulent flows, residence times can be important descriptors of the system (Nauman 2008; Levenspiel 1967). The flow characteristics of the mixing layer, the recirculation within the dead zone and the geometry of the dead zone can significantly affect the overall behavior of the system and mean residence times. Currently, researchers use labor-intensive tracer tests to determine the residence time of dead zones experimentally (Gooseff et al. 2005). The response of an entire stream system to a release of a dissolved substance would require the analysis of many individual dead zones. Therefore, it
is important to develop simplified yet accurate models of the transport processes that occur
within a dead zone. The goal of these simplified models would be to facilitate quick and
accurate estimation of the appropriate residence times associated with a given dead zone.

The objective of this work is to characterize the time scales present in an idealized dead 80 zone. In general, each time scale is a function of the relevant nondimensional groups, Re_D , 81 W/L, W/D, and Fr. This work explores the nondimensional relationship using parametric 82 numerical studies. Many experiments (Valentine and Wood 1979; Uijttewaal et al. 2001; 83 Weitbrecht et al. 2008) have found that dead zone time scales are approximately two orders 84 of magnitude larger than the time scale of the main stream. A physical explanation for this 85 difference in scales is proposed using simple scaling arguments combined with the parametric 86 results. Such a large parametric study requires the use of an efficient numerical method, 87 Reynolds Averaged Navier Stokes (RANS), as opposed to detailed Large Eddy Simulations 88 (LES). A simplified model is also introduced as an extension of the Continuously Stirred Tank 89 Reactor (CSTR) model. The model parameters lend insight into the transport phenomenon 90 and can be correlated to the important nondimensional groups. Developing this model could 91 help predict dead zone time scales without time consuming field measurements. 92

This work focuses on dead zones with an idealized rectangular geometry (Figure 1(c)). 93 Range of parameter variation investigated in this work corresponds to the dead zones occur-94 ring in natural streams: length ($0.45 \le L \le 1.25 \ [m]$), width ($0.5 \le W \le 1.25 \ [m]$), depth 95 $(0.023 \le D \le 0.092 \ [m])$, and stream mean velocity $(0.11 \le U \le 0.248 \ [m/s])$. This varies 96 the Reynolds number based on the depth, $Re_D = DU/\nu$, over the range 5000-20300 and 97 aspect ratio W/L over the range 0.4-1.1 typically observed in natural streams. The depths 98 used correspond to shallow stream levels. For these parameter ranges, the flow features ob-99 served consist of a large primary recirculation zone within the cavity. In addition, the mixing 100 layer spans the entire length of the cavity. The developed models are thus only applicable 101 to dead zones with such flow characteristics. 102

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Review of Relevant Studies

As shown in figure 1(a), the flow structure in a dead zone typically involves a mixing 104 layer at one end and a recirculating region within the cavity bounded by walls on three sides 105 and can depend on the flow Reynolds number, the cavity shape, and the aspect ratio (W/L). 106 Lawson and Barakos (2011) found that for low speeds and small aspect ratios (large L), a 107 distinct recirculation region is not observed. The mixing layer does not extend all the way 108 to the downstream corner of the cavity and the flowfield is classified as closed cavity flow. 109 As Re_D is increased and/or W/L is increased, an open cavity flow is obtained. The present 110 work focuses on such open cavity flows. 111

Weitbrecht et al. (2008) studied the flow patterns inside groyne fields by varying $0.35 \leq$ 112 $W/L \leq 3.4$ for Reynolds number (Re_D) on the order of 7500. They showed that for W/L < 1.5113 0.7, there exist two gyres side-by-side within a cavity: a main primary gyre that is driven 114 by momentum exchange with the main stream and interacts with the mixing layer, and a 115 secondary gyre rotating in the opposite direction and driven by momentum exchange with 116 the primary gyre. The secondary gyre is in contact with the upstream edge of the cavity and 117 has no momentum exchange with the free-stream. For $0.7 \le W/L \le 1.5$, the flow structure is 118 replaced by a large single gyre exchanging momentum with the free-stream. For W/L > 1.5, 119 the single gyre system becomes unstable, and is replaced by multiple gyres on top of one 120 another. Given these flow regimes, the momentum exchange between the free-stream and 121 the cavity will depend on the aspect ratio. 122

Open cavity flow structures of dead zones can also be represented by lid-driven cavity flows which have been studied extensively (Koseff and Street 1984; Shankar and Deshpande 2000). Although these types of flows exhibit similar circulation patterns within the cavity, they lack momentum transport across the top boundary as is present in lateral dead zones in streams. The interactions between the mixing layer, the recirculation regions within the cavity, and the free-stream are critical in understanding mass and momentum transfer mechanisms in dead zones.

Several studies have been carried out in quantifying the mass transport in dead zones. 130 Residence times (Nauman 2008; Levenspiel 1967) have been used as important descriptors 131 in quantifying the mixing and transport properties of these turbulent flows. A number of 132 definitions have been used to characterize the mean residence times in dead zones. The 133 hydraulic residence time or Langmuir time scale (τ_L) , also called the flushing time or the 134 volumetric time scale, is obtained from the ratio of the volume of the dead zone to the vol-135 umetric discharge out of the dead zone (Langmuir 1908; Kozerski et al. 2006; Weitbrecht 136 et al. 2008). The Langmuir time scale, like other dead zone time scales, is inversly propor-137 tional to the exchange rate; a small time scale indicates rapid exchange (rapidly decreasing 138 concentration) and vice versa. For a rectangular dead zone with uniform depth equal to the 139 main channel depth, D, the Langmuir time scale is given by 140

$$\tau_L = \frac{V}{Q} = \frac{WLD}{LDE} = \frac{W}{E},\tag{1}$$

where V is the volume of the dead zone, Q is the volumetric flow exchanged between the 142 dead zone and the main stream, and E is the average exchange velocity. However, exchange 143 velocity is not known a priori. In order to estimate the exchange velocity, Valentine and Wood 144 (1977) suggest that the entrainment velocity is some fraction of the average main stream 145 velocity, that is $E = k_e U$, where the factor k_e is termed as the entrainment coefficient. This 146 assumption is based on the intermittency of turbulent mixing layer that can be related to 147 the free-stream velocity through some factor. A majority of the research in this field has 148 concentrated on accurately measuring and quantifying the exchange coefficient (Valentine 149 and Wood 1977; Uijttewaal et al. 2001; Kurzke et al. 2002; Kozerski et al. 2006; Chang et al. 150 2006; Hinterberger et al. 2007; Weitbrecht et al. 2008; McCoy et al. 2008; Constantinescu 151 et al. 2009). However, measurement of exchange velocity and the entrainment coefficient in 152 natural streams is not straightforward. 153

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The entrainment coefficient and the mean residence times can be obtained by use of a

conservative tracer experiments that fills the entire dead zone (Gooseff et al. 2005; Briggs 155 et al. 2009). Valentine and Wood (1979) conducted laboratory experiments on simplified 156 dead zones and found that the exchange process can be modeled as a first order system by 157 assuming the dead zone to be perfectly mixed region or CSTR. With the perfectly mixed 158 dead zone assumption, a mass balance can be written for the mass of the passive scalar in 159 the dead zone, as shown in equation 2, where M is the mass of scalar in the dead zone, C160 is the scalar concentration in the dead zone, and C_{mc} is the constant scalar concentration 161 in the main channel. Using the definition of concentration as mass per unit volume, and 162 assuming the concentration in the main channel is zero, the mass balance turns into a first 163 order differential equation (equation 3). Using the initial concentration difference between 164 the dead zone and the main stream, $(C - C_{mc})_0 = (\Delta C)_0 = C_0$, the differential equation can 165 be solved for the concentration as a function of time (equation 4). 166

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 $\frac{dM}{dt} = -Q\left(C - C_{mc}\right) = -Q\Delta C \tag{2}$

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- 170 171

 $\frac{dC}{dt} = -\frac{Q}{V}\Delta C = -\frac{E}{W}\Delta C \tag{3}$

$$\frac{C}{C_0} = \exp\left(-\frac{t}{\tau_L}\right) \text{ where } \tau_L = \frac{W}{E}, \text{ and } E = k_e U \tag{4}$$

The first order model is completely defined by the Langmuir time scale, τ_L . Knowing the 172 time series of concentration, an exponential fit can be applied to a normalized concentration 173 curve to determine the Langmuir time scale. This method gives a single, unique time scale 174 that is a best fit for the entire time series. Valentine & Wood (Valentine and Wood 1977) 175 found that the exchange coefficient was approximately constant for a variety of dead zone 176 geometries. This first order dead zone model was then combined with the axial dispersion 177 model used by Thackston and Schnelle (1970) to model the response of the combination of 178 stream and dead zone. 179

Recently, Uijttewaal et al. (2001) conducted laboratory flume studies on series of dead
 zones or groyne fields. The exchange coefficient was generally insensitive to changes in geom-

etry and the flow. Dye concentration studies showed that the system can be approximated as a first order system for early time. At late times, some geometries exhibited a second-order time scale. 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 et al. (2008) also conducted experiments on a series of dead zones in a labo-188 ratory flume. These experiments focused on parametric studies for many different geometric 189 features. Weitbrecht et al. (2008) confirmed that the aspect ratio of the dead zone de-190 termines how many eddies will be present. A modified hydraulic diameter, WL/(W+L), 191 was proposed as the effective length scale to combine the geometric terms, and showed that 192 the entrainment coefficient increases with an increasing Reynolds number based on the hy-193 draulic diameter. Their study did not consider the effect of the depth on the entrainment 194 coefficients. 195

McCoy et al. (2008) further looked at series of dead zones using LES and RANS studies for the same geometry as Uijttewaal et al. (2001). McCoy's results show a clear 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. Their work suggests that depth averaging does not appropriately capture the details of the entrainment velocities.

Based on above studies, for flow past rectangular cavities the entrainment coefficient 201 varies over a wide range 0.01 - 0.04, and considerable uncertainty has been observed in 202 these measurements. These results also indicate that the exchange velocity is two orders 203 of magnitude smaller than the average free-stream velocity. This suggests that different 204 scaling, other than the standard approach of $E = k_e U$, should be possible and needed to 205 relate the exchange velocity to other physical parameters present in the problem. Therefore, 206 a systematic parametric study varying the length, depth, width, and bulk velocity for simple 207 rectangular dead zones can be performed to better quantify their effect on the residence time 208

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and is the focus of the present work.

Owing to the complexity of the flow field and mixing process within the dead zone, the 210 simplified first order model has its limitations, as the concentration within the dead zone 211 is not uniform. Engelhardt et al. (2004) conducted large scale experiments on irregularly 212 shaped dead zones in the River Elbe. These experiments showed that the exchange process 213 relies on coherent eddies shed from the upstream corner of the dead zone. Hinterberger et al. 214 (2007) compared depth-averaged LES with full 3D LES and found that the depth averaged 215 simulations predicted significantly higher exchange rates than either 3D LES or experiment. 216 The errors introduced by depth averaging requires that numerical simulations must be three 217 dimensional to accurately predict exchange rates and thus time scales. Kimura and Hosoda 218 (1997a) compared laboratory experiments to numerical results using the depth-averaged 219 equations. The depth averaged equations captured the same average velocity trends as the 220 experiments. 221

Engelhardt et al. (2004) 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. (2006) showed that the exchange process is complicated by a dead zone having regions of distinctly different flow characteristics. Under such circumstances, Kozerski et al. (2006) showed that the dead zone can be modeled as a combination of these sub regions. Each sub region is modeled as a first order system.

Bellucci et al. (2001) conducted an analytical investigation of the advection-diffusion 228 equation for semi-enclosed basins assuming a constant eddy diffusivity. The residence times 229 of these basins could be characterized by multiple time scales. Results of the eigenvalue anal-230 vsis showed that the volume averaged concentration of a passive scalar will always become 231 exponential at late times. Bellucci et al. (2001) showed that the eigenvalue analysis results 232 are applicable to flows with recirculation like dead zones. The characteristic time (T_0) asso-233 ciated with asymptotic exponential decay of the concentration curve has also been used to 234 characterize the residence time (Nauman 2008; Bellucci et al. 2001). A mean residence time 235

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 (T_{avg}) can be obtained by the first moment or area under the concentration plot normalized by the initial concentration and is given as, $T_{avg} = \int_0^\infty \frac{C(t)}{C_0} dt$.

The time scales mentioned above $(\tau_L, T_{avg} \text{ and } T_0)$ are generally different for dead zones in natural streams. Recently, Jackson et al. (2012) conducted field experiments on dead zones in natural streams to find considerable variability in obtaining these time scales. This work showed that the dead zone is not perfectly mixed, but has regions marked by primary, secondary, and tertiary eddies, that tend to retain different concentrations of the passive tracer. For a perfectly mixed dead zone $\tau_L = T_{avg} = T_0$. For realistic dead zones, τ_L is the minimum time scale and T_0 is the maximum.

The paper is arranged as follows. The computational approach and its validation with 245 available experimental data on multiple grownes is briefly discussed below. The validated 246 approach is then applied to perform parametric studies on a single dead zone by varying 247 the flow velocity, dead zone width, length, and depth. The main goals of these parameteric 248 studies are (i) to quantify the Languir time scale and the entrainment coefficient by relating 249 them to simple geometric and flow parameters, and (ii) to develop a simple model that can 250 be used to predict the residence time within the dead zone. A two-region model is developed 251 that extends the applicability of standard the first-order model. The parameters for the 252 model are also related to the geometric parameters and flow Reynolds number. 253

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MATHEMATICAL FORMULATION AND COMPUTATIONAL APPROACH

The mathematical formulation is based on Reynolds Averaged Navier Stokes Equations with the standard k- ω model in three dimensions. The k- ω and k- ϵ two equation models are widely used and have been tuned and validated for many different applications including separated flows similar to a dead zone. The k- ω model was selected for its computational efficiency, validation history, and similarity to past work (McCoy et al. 2008). This model introduces two additional transport equations shown in equations 7 and 8, which add com²⁶¹ putational expense. The time-averaged equations for an incompressible flow are,

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \tag{5}$$

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$$\frac{\partial \bar{u}_j \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + (\nu + \nu_T) \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j},\tag{6}$$

where ν_T is the eddy viscosity, ν is the kinematic viscosity, P is pressure, and ρ is density. The overbar represents time-averaged quantity. In addition, the turbulence closure for eddy viscosity ($\nu_T = k/\omega$) is obtained by solving the k- ω equations,

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$$\overline{u}_{j}\frac{\partial k}{\partial x_{j}} = \tau_{ij}\frac{\partial \overline{u}_{i}}{\partial x_{j}} - \beta^{*}k\omega + \frac{\partial}{\partial x_{j}}\left[\left(\nu + \sigma^{*}\nu_{T}\right)\frac{\partial k}{\partial x_{j}}\right]$$
(7)

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$$\overline{u}_{j}\frac{\partial\omega}{\partial x_{j}} = \alpha \frac{\omega}{k}\tau_{ij}\frac{\partial\overline{u}_{i}}{\partial x_{j}} - \beta\omega^{2} + \frac{\partial}{\partial x_{j}}\left[\left(\nu + \sigma^{*}\nu_{T}\right)\frac{\partial\omega}{\partial x_{j}}\right],\tag{8}$$

where standard model constants are used: $\alpha = 13/25$, $\beta = 9/125$, $\beta^* = 0.09$, $\sigma^* = 0.5$. Once the mean velocity profile is obtained, a transient scalar (\bar{C}) advection-diffusion problem is solved by first initializing the dead zone with $\bar{C} = 1$,

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$$\frac{\partial \overline{C}}{\partial t} + \overline{u}_j \frac{\partial \overline{C}}{\partial x_j} = \left(\frac{1}{Sc}\nu + \frac{1}{Sc_T}\nu_T\right) \frac{\partial^2 \overline{C}}{\partial x_j \partial x_j}; \quad Sc_T = \frac{\nu_T}{D_T}$$
(9)

where Sc_T is the turbulent Schmidt number (on the order of unity).

The RANS equations are solved for each geometry using the commercial finite volume solver Star-ccm+ (User Guide 2009). The turbulence is modeled using the standard k- ω closure with wall functions. The free surface is modeled as a rigid slip boundary. This approximation is reasonable when the Froude number is small (Fr << 1) meaning free surface effects are small (Nakayama and Yokojima 2003). The Froude number in the present work ranges between 0.16 < Fr < 0.32 and is listed in Table 1. Recent work by (Kimura and Hosoda 1997b) at $Re_D \sim 4500$ and over a range of Froude numbers, showed that the unsteady flow oscillations can become important in mass exchange for Fr >> 0.33. However, since the present work deals with higher Reynolds numbers and lower range of Froude numbers, free surface effects are not significant. Similar treatment of the free surface has been used by Hinterberger et al. (2007) and McCoy et al. (2008). All no-slip walls are assumed to be smooth. The bank opposite the dead zone is modeled as a slip wall as its effect is not relevant to this work.

The first step in the solution procedure is to solve for the time averaged steady flow 290 field. Here we use steady RANS approach to obtain the flowfield. In order to confirm that 291 the steady RANS approach predicts the same results, as URANS, a full three-dimensional 292 unsteady RANS study for the baseline case in Table 1 was also conducted. The differences 293 between the steady and unsteady RANS were less than 0.22%. Thus, steady RANS calcu-294 lations were employed to first obtain the flowfields as it is computationally less intensive. 295 In order to run the passive scalar study, however, a transient simulation is performed by 296 advecting the scalar with the mean steady velocity field and eddy diffusivities. To do this, 297 the time averaged flow field is mapped to the transient simulation and frozen in time. The 298 turbulent Schmidt number is set equal to a value of 0.9 which is the same as Baik et al. 299 (2003), Santiago et al. (2007), and Gualtieri et al. (2010). The passive scalar is initialized 300 with a concentration of one inside the dead zone, up to a line joining the upstream and 301 downstream corners of the dead zone, and zero in the main channel. The average dead zone 302 concentration is calculated as the volume average of all the cells within the dead zone. The 303 initial condition automatically normalizes the concentration to be at one at time zero. The 304 transient simulation is allowed to run until the dead zone concentration is small (~ 0.005), 305 which was found to be on the order of 4000 seconds. 306

307 Validation Study

Before using the above approach to perform parametric studies on a single dead zone, detailed validation of the mean flow quantities together with grid refinement study is performed for a series of dead zones for which experimental data are available. Flow in series

of dead zones have been studied extensively, both experimentally by Weitbrecht and Jirka 311 (2001), Weitbrecht et al. (2008), and Uijttewaal et al. (2001) and numerically by McCoy 312 et al. (2008), Constantinescu et al. (2009), and Hinterberger et al. (2007). These studies 313 involved series of groups formed by obstructions protruding into the main flow as well as 314 those formed by cutouts into the bank. The flow separates at the beginning of the cavity and 315 recirculates within the dead zone. The obstruction type is formed by a protrusion into the 316 main channel that causes the flow to accelerate. This acceleration leads to larger flow separa-317 tion and higher velocity gradients near the upstream corner of the dead zone. Computations 318 involved varying the groyne length to change the aspect ratio, $0.2 \leq W/L \leq 3.4$, as well as 319 varying the freestream velocity to change the Reynolds number ($8000 < Re_D < 39000$). Ui-320 ittewaal et al. (2001) conducted experiments on cavity-type dead zones in series which 321 involved different depths in the main stream compared with the dead zone. On the other 322 hand, majority of the data by Weitbrecht et al. (2008) is on protruding-type dead zones 323 with uniform depths in the main stream and the dead zone. 324

For these cases, systematic grid refinement study was conducted by generating structured 325 grids. Each grid is the most refined in the shear layer between the dead zones and the main 326 channel. The grid coarsens in the spanwise direction away from the dead zone. Near the 327 walls of the dead zone as well as near the stream bed, the grid is refined to obtain a well 328 resolved wall layer. For all cases, the minimum and maximum grid resolution along the 329 depth of the channel is 10 and 78 in wall units. Similar resolutions are within the dead zone 330 as well as inside the mixing layer. First, a periodic, turbulent channel flow is simulated and 331 the mean velocity profile is used as an inlet condition to obtain a fully developed turbulent 332 flow. A no-slip condition is used at the walls and a convective outflow boundary condition 333 is used at the outlet. A slip condition is used at the centerline of the stream. 334

For all cases, the mean flow, mixing layer characteristics and the dead zone recirculation was compared with the experimental data as well as RANS results by Constantinescu and co-workers (McCoy et al. 2008; Constantinescu et al. 2009) to obtain reasonable agree-

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ment (Drost 2012). The mean flow, mixing layer characteristics, and dead zone recirculation 338 compared well with published RANS results. Figure 2 shows the mean streamline pat-339 terns predicted for three-different W/L ratios, namely 0.4, 0.77 and 2. For large lengths 340 (W/L = 0.4, say), the dead zone has one main eddy that is centered slightly downstream of 341 the dead zone center. There is a secondary eddy in the upstream corner of the dead zone. 342 The secondary eddy has significantly less momentum than the primary eddy. As the dead 343 zone length is decreased, the secondary eddy gets smaller and eventually vanishes around 344 W/L = 0.77. As the length is decreased further, the main eddy separates into two eddies 345 stacked in the spanwise direction. Such a flow pattern has been reported experimentally 346 by Weitbrecht et al. (2008) and provides an important qualitative validation of the present 347 predictions. Specifically, predicting the mean flow patterns accurately is critical as that can 348 alter the residence times and scalar dispersion time scales significantly. As will be shown 349 later, majority of the dead zones that occur naturally in the stream fall in the range of W/L350 that provides a single primary recirculation gyre (similar to the W/L = 0.4 case). However, 351 being able to predict the different flow patterns validates the RANS model. 352

For more quantitative validation, we compare variations of mean velocity and turbulent 353 kinetic energy in the main stream and the dead zone with available experimental data. 354 Figure 3a shows a velocity profile plot in the spanwise direction. This particular case was 355 chosen mainly because it was also studied numerically by McCoy et al. (2008) and thus it 356 allows direct comparison of the present predictions to theirs. In general, the RANS results 357 from the present work matches well to the RANS simulations by McCoy et al. (2008). With 358 refined grids used in the present work, the mean velocity is closer to the experimental data in 359 the main channel. Both RANS profiles differ slightly from the experimental results inside the 360 dead zone. Figure 3b shows a turbulent kinetic energy profile in the spanwise direction. The 361 turbulent kinetic energy (TKE) also shows the same behavior as the experiments, however, 362 the distribution is slightly narrower and the peak in the mixing layer slightly larger in 363 the present predictions compared to the experimental data. The TKE peak is lower and 364

closer to the experimental data in the present simulations compared to that of McCoy et al. 365 (2008). The TKE is a difficult quantity for a RANS model to capture perfectly compared to 366 the experimental data, however, its overall prediction is fairly consistent with experimental 367 measurements. This numerical error is a limitation of the $k-\omega$ turbulence model, wherein, 368 all turbulence scales are modeled based on two transport equations. Large eddy simulations 369 (LES) (Constantinescu et al. 2009) are capable of predicting the flowfields much more 370 accurately, however, are computationally intensive. Given a large number of parametric 371 variations conducted in the present work, use of a LES approach is difficult and RANS 372 presents an acceptable tradeoff for the computational efficiency needed. 373

Finally, to thoroughly validate all aspects of the flow and scalar dispersion, the Langmuir 374 time scale was computed by tracking dispersion of a passive scalar initially uniformly placed 375 within the dead zone. For accurate prediction of the Langmuir time scale, it is critical that 376 the mean flowfield, the turbulent kinetic energy, the exchange mechanisms between the dead 377 zone and the free stream, and the scalar transport are captured correctly. Thus, this quantity 378 helps validate all processes improtant for further analysis to be used in the present work. As 379 W/L is varied over a wide range, the recirculation flow patterns within the dead zone changes 380 significantly and thus can alter the Langmuir time scale. As shown in figure 4, the Langmuir 381 time scales are very well predicted by the RANS results compared to the experimental 382 data (Weitbrecht et al. 2008; Uijttewaal et al. 2001). Here the convective time scale, 383 $T_{conv} = L/U$. Weitbrecht et al. (2008) conducted both particle tracking velocimetry, PTV, 384 and dye concentration, PCA, studies. This validation study establishes sufficient confidence 385 on the predictive capability of the RANS approach for the residence time computations 386 conducted on single dead zones in this study. 387

388 PARAMETRIC STUDY RESULTS

This work investigates the time scales that are important to the passive scalar transport within a dead zone. Parametric studies are run by varying the bulk velocity, U and dead zone length, L, width, W, and depth, D. Table 1 shows the parameters used for all of the

simulations. The base case is listed first and all additional cases modify a single parameter 392 from the base case. Cases 2-7 vary the length (labeled as L cases), 8-11 vary the velocity (the 393 U cases), 12-14 vary the width (the W cases), and finally 15-17 vary the depth (the D cases). 394 Figure 1(c) shows a planview of the geometries used. The depth is constant throughout the 395 main channel and dead zone. The grid resolution used for these cases was selected to be 396 finer than the validation cases. The minimum grid resolutions in wall units were 1.06 in all 397 directions, whereas the maximum resolution was $\Delta Y_{\text{max}}^+ = 59.6$ in the vertical direction and 398 $\Delta X_{\text{max}}^+ = \Delta Z_{\text{max}}^+ = 119.2$, along the streamwise and spanwise directions, respectively. 399

Before running simulations with dead zone geometries, a fully developed turbulent inlet 400 condition was generated. Lien et al. (2004) conducted experiments in turbulent channels 401 that could be used to estimate the entrance length. However, adding such a long region to 402 each simulation would greatly increase the computational cost of each simulation. For this 403 work, the inlet condition is generated by simulating a simple periodic channel with the same 404 cross section as the eventual inlet surface. The periodic channel is allowed to evolve until 405 it reaches a stationary state. The inlet condition involving the velocity field and k and ω 406 values are taken from an arbitrary cross section of the periodic channel. 407

The results from the 17 studies shown in table 1 are used to obtain trends for changes in dead zone geometry and flow conditions. In order to analyze and interpret the results for the various mean residence times, the following time scales are used. The convective time scale, T_{conv} in equation 10, is the time it takes fluid in the main stream to travel the length of the dead zone.

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$$T_{conv} = \frac{L}{U}.$$
(10)

⁴¹⁴ Typically, the characteristic velocity associated with the mixing layer $(U_m = 0.5U)$ is used ⁴¹⁵ to define the convective time scale; however, the average free-stream velocity is used here ⁴¹⁶ for simplicity. A time scale based on the average rotation rate (Ω) within the dead zone can ⁴¹⁷ also be defined,

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$$T_{rot} = \frac{1}{\Omega} = \frac{2}{\overline{\omega}_v}.$$
(11)

Note that the average rotation rate within the dead zone can be easily obtained from the average vorticity ($\overline{\omega}_v$) which can be obtained by computing the circulation (Γ) within the dead zone.

$$\Gamma = \int \mathbf{u} \cdot \mathbf{d}l = \int_{A} \omega_{v} dA = A\overline{\omega}_{v}, \qquad (12)$$

where A is the area of the dead zone, $\overline{\omega_v}$ is the average vorticity within the dead zone, and the mean circulation is computed along a closed path (**d***l*) encompassing the dead zone at the free surface. It is possible to consider an average of circulation evaluated at all planes in the plan view. However, it was done at the free surface mainly because majority of the data collected in field measurements is only at the free surface. In order to verify that the trends are unaltered, we have also estimated Γ based on average of circulation over all planes, and the general trends presented in the paper are not affected significantly.

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Entrainment Coefficient Scaling

One of the main goals of parametric studies is to obtain detailed data on the Langmuir 431 time scale, τ_L , and develop a simple relationship for the entrainment coefficient, k_e . As 432 mentioned earlier, the Langmuir time scale depends on the exchange velocity between the 433 main stream and the dead zone and is difficult to measure in the field. Instead, Valentine 434 and Wood (1977) suggest that the entrainment velocity is some fraction of the average main 435 stream velocity, and given by the entrainment coefficient. For a majority of streams and river 436 dead zones, the observed entrainment coefficients are within the range of 0.01 - 0.04 (Jackson 437 et al. 2012; Jackson et al. 2013). However, a definitive relation between k_e and some 438 measurable geometric and flow parameters of the dead zone is needed. 439

First, the Langmuir time scale in the first order continuous stirred reactor (CSTR) model, is obtained by using the dead zone geometry and the mean exchange velocity E obtained directly from the steady flowfield predicted by the RANS results, $\tau_L = W/E$. Since the exchange velocity is typically defined through the exchange coefficient and the mean freestream velocity, $E = k_e U$, the Langmuir time scale versus W/U is first plotted to obtain nearly a linear relationship as shown in figure 5, the inverse slope of which gives the entrainment coefficient, $k_e \sim 0.01$. This is within the experimental range observed (0.01-0.03) for data on real dead zones in natural streams (Jackson et al. 2012).

The relationship between the Langmuir time scale, the mean free-stream velocity, and 448 the width of the dead zone can also be interpreted using some measure of net circulation 449 within the dead zone. The circulation within the dead zone (equation 12) can be estimated 450 by integrating the velocity along a closed loop encompassing the edges of the dead zone at 451 the free surface and the center of the mixing layer (line joining the upstream and downsteam) 452 corners of the dead zone). Using the characteristic mixing layer velocity $(U_m = 0.5U)$ as an 453 approximate model to the actual mean streamwise velocity at the center of the mixing layer, 454 the net circulation is simply obtained as, 455

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$$\Gamma \sim U_m L = 0.5 U L. \tag{13}$$

Using equation 12, the average vorticity in the dead zone is given as,

$$\overline{\omega}_v = \frac{\Gamma}{A} \sim \frac{0.5UL}{WL} = 0.5 \frac{U}{W}.$$
(14)

Thus, $W/U \sim 1/(2\overline{\omega}_v)$. This was confirmed by actually computing the average vorticity 459 within the dead zone based on the mean flow field at the free surface. It was found that 460 W/U correlated linearly with $1/\overline{\omega}_v$ for most cases, except for some cases where the length 461 or depth were varied. That is attributed to the fact that, the characteristic mixing layer 462 velocity (U_m) is just an approximate model and may not be the exact velocity along the 463 line joining the upstream and downstream ends of the dead zone. This result suggests that 464 the Langmuir time scale must be related to the rotation time scale, $T_{rot} = 2/\overline{\omega}_v$, and is 465 confirmed as shown in figure 6(a). This figure shows that the Langmuir time scale varies 466

linearly with the rotation time scale and that the fit for all cases is much better than that 467 against W/U shown in figure 5. This physically means that the Langmuir time scale is 468 governed mostly by the average recirculation in the dead zone. Faster circulating fluid will 469 reduce the residence time. The average rotation rate is dependent on the free-stream velocity 470 as well as the geometry of the dead zone, implicitly including all main parameters associated 471 with the problem, namely the geometric features L, W, and D, and the average free-stream 472 velocity, U. It should be noted that the inverse slope of the plot of τ_L versus $1/\overline{\omega}_v$ is also 473 related to the entrainment coefficient and shows a value on the order of 0.015. 474

This relation incorporates the dead zone flow characteristics through the average rotation 475 rate; however, it does not explicitly include the mixing layer parameters. The driving force 476 for the rotation inside the dead zone is the turbulent boundary layer upstream of the dead 477 zone or the bed shear stress. The boundary layer is well characterized by the momentum 478 thickness (θ) as defined in equation 15 where u is the average streamwise velocity as a function 479 of the distance away from the wall and u_0 is the average streamwise velocity far from the 480 wall. Physically, the momentum thickness is the width of flow at u_0 that would be needed 481 to replace the momentum lost due to the boundary layer. In this work, the momentum 482 thickness is calculated at the free surface in the spanwise direction, mainly to be as away 483 from the influence of the boundary layer that forms near the stream bed. Depth-averaging of 484 the parameter is possible, however, since primary interest is in the momentum thickness in 485 the lateral direction, that the stream bottom may bias the distribution considering that the 486 streams are shallow. The rotation time, T_{rot} , scaled by the ratio of the dead zone width, W, 487 and the boundary layer momentum thickness, θ , is approximately linearly correlated with 488 the Langmuir time scale as shown in figure 6(b) and below, 489

$$\theta = \int_0^\infty \frac{u}{u_0} \left(1 - \frac{u}{u_0} \right) dy \tag{15}$$

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$$\frac{W}{k_e U} = \tau_L \sim 0.5 \frac{W}{\theta} \frac{1}{\overline{\omega}_v} \sim 0.5 \frac{W}{\theta} \frac{2W}{U} \implies k_e \sim \frac{\theta}{W}$$
(16)

While the trend of figure 6(b) is clearly linear for the W cases, the other data points 493 have a significant standard deviation from the linear fit. The important output of this 494 figure is that the slope is approximately 0.5. Using equation 16, this slope implies that the 495 entrainment coefficient, k_e , is related to the ratio of the momentum thickness (θ) to the 496 dead zone width (W). This provides a scaling argument for why experiments (Valentine 497 and Wood 1979; Uijttewaal et al. 2001; Weitbrecht et al. 2008) have consistently found 498 k_e to be in the range 0.01 – 0.03. Obtaining an approximate Langmuir time scale using 499 equation 16 is straightforward without requiring tracer tests. Only measurements of the 500 upstream momentum thickness (θ) and the average rotation rate (or average vorticity, $\overline{\omega}_n$) 501 are required. The momentum thickness of the upstream boundary layer can be obtained 502 by measuring the mean velocity profile normal to the stream or can be estimated using 503 correlations for boundary layer development based on the flow Reynolds numbers. The 504 rotation time scale can also be obtained by measuring the velocity profile along the center 505 of the mixing layer (U_m) and using equation 13 to obtain the mean circulation and average 506 vorticity within the dead zone. Alternatively, an estimate for average vorticity within the 507 dead zone can be obtained by using equation 14. 508

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TWO REGION MODEL RESULTS

When using the first order model, the Langmuir time scale fully defines the normalized 510 concentration plot and thus could be used to predict the response of a dead zone to changes 511 in the main channel concentration. Figure 7 shows the mean streamlines within the dead 512 zone and an instantaneous passive scalar contour plot at a simulation time of 5000s. It is 513 observed that a single recirculation is present within the dead zone, which has been observed 514 for majority of the test cases studied here. The scalar contour plot, figure 7(b), also shows 515 non-uniformity within the dead zone. The main recirculation eddy separates the dead zone 516 into two regions, the core region of the main eddy where the average velocity is small and the 517 perimeter region where the velocity and mixing are larger. Figure 8 shows the time history 518 of the average scalar concentration for the base case. The temporal evolution of scalar 519

concentration in a perfectly mixed dead zone is exponential as shown in equation 4. On 520 a semi-log plot, an exponential would make a linear trend. Figure 8 shows the temporal 521 evolution of the scalar concentration normalized by the initial concentration within the 522 dead zone. The time is also normalized by the primary zone time scale as shown for three 523 different cases W/L = 0.345, 0.4, 1.11. In addition, for the baseline case of W/L = 0.4, a 524 linear curve corresponding to the primary zone (which is also close to the Langmuir) time 525 scale is plotted. It is clear from this figure that up to one non-dimensional time unit, the 526 concentration evolution nearly follows the linear evolution, which suggests that the initial 527 scalar evolution is mainly governed by direct exchange between the primary zone and the 528 main stream through the mixing layer. A similar plot was also produced by Weitbrecht 529 et al. (2008) from their experiments. However, figure 8 does show some positive curvature 530 confirming that more than one time scale exists and that the dead zone is not perfectly 531 mixed. It is also important to note that nearly 75-80% of the scalar mass has escaped within 532 the first non-dimensional time unit, similar to the observations by Weitbrecht et al. (2008). 533 The remaining tracer mass exits slowly and involves time scale of a secondary zone thus 534 indicating the need for at least a two-zone model. The predicted results are consistent with 535 recent field measurements conducted by Jackson et al. (2012). 536

Without a well-mixed dead zone, the first order model is not accurate to completely 537 describe the long-time evolution of the tracer field. As an extension of the first order model 538 and following the method used by Kozerski et al. (2006), the dead zone can be divided into 539 two perfectly mixed CSTRs, one in the perimeter of the main eddy (primary region) and one 540 in the core of the main recirculation (secondary region), see figure 7(b). The primary region, 541 with volume V_p and concentration C_p , exchanges scalar with the main channel based on the 542 exchange volume flow rate, Q_{pm} . In this region, the flow velocity and turbulent diffusivity are 543 large which facilitate rapid mixing. The secondary region, with volume V_s and concentration 544 C_s , exchanges scalar with just the primary region based on the exchange volume flow rate, 545 Q_{ps} . This model does not specify the exact shape of the secondary region, only the volume 546

and the exchange volume flow rates. Using the conservation of mass for a passive scalar, two
coupled differential equations (17 and 18), can be derived to model the two regions.

$$\frac{dC_p}{dt} = -\frac{Q_{pm}}{V_p}C_p - \frac{Q_{ps}}{V_p}\left(C_p - C_s\right) \tag{17}$$

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$$\frac{dC_s}{dt} = -\frac{Q_{ps}}{V_s} \left(C_s - C_p\right) \tag{18}$$

⁵⁵² The governing equations can be solved analytically to obtain,

$$\begin{bmatrix} C_s \\ C_p \end{bmatrix} = k_s \begin{bmatrix} 1 \\ 1 - \frac{\tau_{sp}}{\tau_s} \end{bmatrix} e^{-\frac{t}{\tau_s}} + k_p \begin{bmatrix} 1 \\ 1 - \frac{\tau_{sp}}{\tau_p} \end{bmatrix} e^{-\frac{t}{\tau_p}},$$
(19)

where τ_s and τ_p are the negative reciprocals of the eigenvalues of the system, the vectors on the right hand side are the eigenvectors, and $k_s = \frac{\frac{1}{\tau_p}}{\frac{1}{\tau_p} - \frac{1}{\tau_s}}$, $k_p = \frac{\frac{1}{\tau_s}}{\frac{1}{\tau_s} - \frac{1}{\tau_p}}$ are constants determined by the initial conditions of 1 for both regions. The time scales for scalar exchange between different regions are given as $\tau_{sp} = \frac{V_s}{Q_{ps}}$, $\tau_{pm} = \frac{V_p}{Q_{pm}}$, and $\tau_{ps} = \frac{V_p}{Q_{ps}}$. Then, the time scales for the primary (τ_p) and secondary regions (τ_s) are given by,

$$\tau_p, \ \tau_s = 2 \left[\frac{Q_{pm}}{V_p} + \frac{Q_{ps}}{V_p} + \frac{Q_{ps}}{V_s} \pm \sqrt{\left(\frac{Q_{pm}}{V_p} + \frac{Q_{ps}}{V_p} + \frac{Q_{ps}}{V_s}\right)^2 - \frac{4Q_{pm}Q_{ps}}{V_pV_s}} \right]^{-1}$$
(20)

The mean dead zone concentration is volume weighted summation of the mean concentrations in the primary and secondary regions, $C_{DZ} = \frac{C_s V_s + C_p V_p}{V_p + V_s} = \frac{C_s \tau_{sp} + C_p \tau_{ps}}{\tau_{sp} + \tau_{ps}}$. The mean dead zone concentration can be expressed as,

$$C_{DZ} = (1 - k_W) e^{-\frac{t}{\tau_s}} + k_W e^{-\frac{t}{\tau_p}}, \quad k_W = \frac{\tau_{sp} \frac{\frac{1}{\tau_s}}{\frac{1}{\tau_s} - \frac{1}{\tau_p}} + \tau_{ps} \frac{\frac{1}{\tau_s}}{\frac{1}{\tau_s} - \frac{1}{\tau_p}} \left(1 - \frac{\tau_{sp}}{\tau_p}\right)}{\tau_{sp} + \tau_{ps}}, \quad (21)$$

where k_W represents a single weighting factor. If it is assumed that $\tau_p \ll \tau_s$ and $\tau_{sp} \sim \tau_s$,

then weighting factor simplifies to,

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$$k_W \sim \frac{\tau_{ps}}{\tau_{sp} + \tau_{ps}} = \frac{V_p}{V_p + V_s},\tag{22}$$

and can be thought of as the ratio of the primary region volume to the entire dead zonevolume.

569 Two Region Model Fitting

Given the three model parameters, τ_p , τ_s , and k_W , the average concentration is known 570 at all times using equation 21. Without a method for determining the model parameters, 571 this model is only a mathematical exercise. Tuning the model is accomplished by fitting the 572 model to the concentration results from the parametric RANS studies using an optimiza-573 tion procedure. The difference between concentration plots from the model and a RANS 574 simulation is minimized. A MATLAB-based optimization code, SNOPT (Gill et al. 1994), 575 does the minimization using a robust implementation of a sequential quadratic programming 576 algorithm for nonlinear problems. 577

Using SNOPT (Gill et al. 1994), τ_p , τ_s , and k_W are varied to minimize the square of the 578 difference between the temporal evolution of mean concentration curves in the dead zone 579 obtained from the RANS simulation and the two region model. The weighting factor is 580 constrained to be between 0.25 and 0.75 to ensure that both optimized time scales have a 581 significant influence on the concentration plot. A maximum error of 2.05% was obtained 582 between the mean dead zone concentration from the model and the RANS study (see Drost 583 (2012) for details on the optimization procedure). These results show that this model can 584 accurately fit the RANS results a posteriori. 585

The average k_W value was found to be 0.55 with a standard deviation of 0.17, indicating that the dead zone volume is almost equally split between the primary and secondary regions. The primary time scale, τ_p , obtained from the two-region model was compared with the Langmuir time scale as shown in figure 9(a). It is observed that τ_L and τ_p are roughly on the same order and show direct linear correlation between them. The primary region time scale compared with the rotational time- scale in the dead zone, T_{rot} , also shows a linear fit (figure 9(b)) indicating that as the rate of rotation within the dead zone is increased, the primary region residence time decreases. This suggests that the primary region time scale, τ_p , provides a good estimate of the Langmuir time scale. Both time scales are correlated to rotation of the dead zone. This matches the reasoning for creating the two region model, that primary region seemed to contain the majority of the recirculating fluid.

The secondary region time scale, τ_s , was found to be generally two to four times larger than the primary region time scale for all cases verifying the presence of at least two distinct time scales within the dead zone. The larger time scale, τ_s governs the asymptotic behavior of the concentration plot in time. The separation of time scales causes τ_p dominating the exchange with the main stream at early times when the dead zone is approximately perfectly mixed. At late times, τ_s limits the exchange rate. This is similar to the multiple time scales observed by Uijttewaal et al. (2001).

The two region model has been shown to be able to fit RANS results with small error. However, to make the model predictive, the model parameters need to be estimated based on dead zone geometry and flow conditions. Accordingly, the primary and secondary region time scales can be related to the geometric paramters, L, W, D, and free-stream average velocity, U, by forming non-dimensional groups and assuming a power law relationship. The convective time scale T_{conv} is used for non-dimensionalization as it is the smallest possible time scale in the system.

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$$\frac{\tau_p(\text{or }\tau_s)}{T_{conv}} = a \left(\frac{W}{L}\right)^b \left(\frac{W}{D}\right)^c \left(\frac{WU}{\nu}\right)^d$$
(23)

The specific non-dimensionalization groups are not unique, but any other combination will lead to equivalent results. Using four independent simulations and this power law, four equations define the constants a, b, c, and d. Averaging the results from all the independent groups of four from the 17 simulations, gives the relationships,

$$\frac{\tau_p}{T_{conv}} \sim 15 \left(\frac{W^3 D}{L^3} \frac{U}{\nu}\right)^{\frac{1}{4}} = 15 \left(\frac{W}{L}\right)^{3/4} \left(\frac{UD}{\nu}\right)^{\frac{1}{4}}$$
(24)

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$$\frac{\tau_s}{T_{conv}} \sim 170 \left(\frac{W^4}{L^3 D}\right)^{\frac{1}{2}} = 170 \left(\frac{W}{L}\right)^{\frac{3}{2}} \left(\frac{W}{D}\right)^{\frac{1}{2}}$$
(25)

⁶¹⁹ Using the approximate nondimensional relationships, the model parameters are plotted in ⁶²⁰ figures 10(a) and 10(b). Each plot has symbols for cases that vary L, W, D, and U compared ⁶²¹ to the base case. Cases 6 and 7 (as shown in table 1) were considered outliers. For these cases ⁶²² L is varied such that the aspect ratio $W/L \sim 1$. Above an aspect ratio of one, the overall ⁶²³ flow structure has been shown to change to a multiple eddy configuration. This transition to ⁶²⁴ another type of flow field may not follow the same trends as lower aspect ratio dead zones. ⁶²⁵ These cases were not used when determining the exponents.

The non-dimensional primary region time scale is cast as an effective Reynolds number 626 $(\frac{W^3D}{L^3}\frac{U}{\nu})$, with the length scale given as W^3D/L^3 . This relation can also be thought of as 627 a combinations of dependence on the geometry, W/L, and flow, Re_D , conditions. As seen 628 from figure 10(a), the non-dimensional primary region time scale increases with increase 629 in the aspect ratio and the Reynolds number based on the depth. It should be noted 630 that this time scale is normalized by the normalized by the flow time scale L/U. The 631 primary zone time scale decreases with increasing velocity, however, the ratio of time scales 632 increases with increasing Re_D . This result is also consistent with the predictive relationship 633 developed by Jackson et al. (2013) using laboratory-scale experiments on isolated dead-zones 634 in idealized semi-circular configurations. While this trend in the present work is empircally 635 derived, its form can be attributed to physical phenomenon. It is understandable that the 636 aspect ratio has a large influence as experiments have shown that it largely determines the 637 shape and quantity of eddies in the dead zone. The time scale ratio weakly depends on D. 638 This result is consistent with Constantinescu et al. (2009) and Hinterberger et al. (2007) 639 who showed this shallow flow to have weak dependence on the depth. Uittewaal et al. (2001) 640 and Weitbrecht et al. (2008) also showed exchange velocities to be roughly proportional to 641

U. Equation 24 implies that the exchange velocity depends on $U^{0.8}$.

⁶⁴³ When analyzing the secondary region time scale, the Reynolds number had a very small ⁶⁴⁴ exponent meaning that the quantity does not significantly depend on U and only geometric ⁶⁴⁵ ratios were considered. The secondary time scale ratio, as shown in equation 25, scales with ⁶⁴⁶ geometry only. A lack of dependence on U may be attributed to the small average velocities ⁶⁴⁷ within the secondary region and small turbulent diffusion across the region that determines ⁶⁴⁸ the time scale. Similar to τ_p , the secondary time scale is heavily dependent on the aspect ⁶⁴⁹ ratio and slightly dependent on the depth.

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SUMMARY AND CONCLUSIONS

Parametric studies varying the length, depth, width, and the averaged free-stream ve-651 locity were performed on idealized dead zones with rectangular cavity using three dimen-652 sional Reynolds averaged Navier Stokes simulations based on the experimentally validated 653 $k-\omega$ model. The main purpose of this fundamental numerical study was to identify scales 654 that are important to characterize the residence times in lateral storage zones occurring in 655 small streams. In this study, seventeen cases were investigated wherein the aspect ratio, 656 $0.4 \leq W/L \leq 1.1$, and Reynolds number based on the width, $5000 \leq Re_D \leq 20300$, were 657 varied over a range typically observed in small streams. For this range, the main flowfield is 658 characterized by an open cavity flow consisting of a mixing layer that spans the entire length 659 of the dead zone and a large main recirculation region within the dead zone. 660

In addition to showing good validation with available experimental data, our main con tributions of the present work are:

663 664 1. correlating the hydraulic residence time (the Langmuir time scale) to the rotation time scale within the dead zone, a quantity that can be easily measured in the field,

developing a new scaling based on the momentum thickness of the upstream boundary
 layer that makes the entrainment coefficient on the order of 1, instead of traditional
 values of 0.01 with large variability,

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3. indicating an existence of two time scales within the dead zone for the conditions considered (subcritical isolated dead zone for $0.4 \le W/L \le 1$),

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 developing a two-zone model with parameters calibrated to predict residence time scales through power law correlations involving the dead zone geometric quantities and flow Reynolds number.

Based on the flow features observed, it was hypothesized that the hydraulic residence 673 time (or the Langmuir time scale) may depend on the average rotation rate within the 674 dead zone, the geometric scales, and the characteristics of the upstream boundary layer that 675 drives the flow and mixing layer over the dead zone. It was shown that the Langmuir time 676 scale is inversely proportional to the average rotation rate (or average vorticity) within the 677 dead zone. The entrainment coefficient (k_e) , used to relate the exchange velocity to the 678 average free-stream velocity was shown to be on the order of θ/W , the ratio of the upstream 679 boundary layer momentum thickeness (θ) to the width (W) of the dead zone. 680

For a perfectly mixed dead zone, the Langmuir time scale completely describes the resi-681 dence time of the dead zone. However, the numerical simulations show that the dead zone 682 is not perfectly mixed. The core region of the main recirculation region retains scalar longer 683 than the perimeter region. This nonuniformity indicates the presence of multiple time scales 684 within the dead zone that can be approximated by a two region model, a primary perimeter 685 region that interacts with the mixing layer and exchanges scalar with the free-stream di-686 rectly and a secondary core region that interacts with the primary region. The regions were 687 approximated as continuously stirred tank reactors with mass transport between them. The 688 resultant two-region model involved three parameters, the primary region time scale, the 689 secondary region time scale, and a scaling factor approximately proportional to the ratio of 690 the primary region volume to the dead zone volume. These parameters were obtained from 691 the RANS data and using SNOPT optimization procedure that fits the model to the RANS 692 concentration curves. The fitting error was less than 2%. 693

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Fitting the two region model to the RANS results showed that the primary region time

scale is directly proportional to the Langmuir time scale, indicating that the primary region 695 is well mixed and also dominated by mixing due to rapid rotation as well as turbulent 696 diffusion. The secondary region time scale was generally two to four times larger than the 697 Langmuir time scale and determines the late time behavior of the dead zone. The larger 698 secondary region time scale is characteristic of the lower turbulent diffusivity within the core 699 region. This comparison also suggests that time scale determined using field tracer tests with 700 concentration measurements taken uniformly over the dead zone can result in an apparently 701 larger Langmuir time scale owing to the slower mixing processes within the secondary region. 702 This observation was consistent with the field measurements on natural dead zones as noted 703 by Jackson et al. (2012). 704

Additional power law relationships were formed to correlate the three model parameters 705 to the basic geometric and flow parameters. The trends for the primary and secondary 706 time scales collapsed and would therefore allow the time scales to be predicted from basic 707 geometric and flow measurements of a dead zone. The primary time scale was found to be 708 well correlated with the aspect ratio, $(W/L)^{3/4}$, and Reynolds number based on the depth, 709 $(UD/\nu)^{1/4}$. An effective length scale, W^3D/L^3 , was defined to describe the primary region 710 time scale suggesting dependence on the aspect ratio as well as the depth of the dead zone. 711 The secondary region time scale was found to be dependent on only geometric parameters. 712 A lack of dependence on U may be attributed to the small average velocities within the 713 secondary region and small turbulent diffusion. The average value for the weighting factor 714 was found to be 0.55 with a standard deviation of 0.17, indicating that the dead zone volume 715 is almost equally split between the primary and secondary regions. 716

The predictive capability of these results is limited to the range of parameters studied wherein the main flowfield is characterized by an open cavity flow consisting of a mixing layer that spans the entire length of the dead zone and a large main recirculation region within the dead zone. Such conditions were obtained for shallow sub-critical dead zones (0.16 < Fr < 0.32) with aspect ratios $0.3 \le W/L \le 1$ over relatively low Reynolds numbers (5000 \le $Re_D \leq 20300$) based on the stream depth. For these conditions, additional fundamental work involving flume studies as well as high-fidelity large-eddy simulation on idealized, isolated dead zones are needed to corroborate the present findings.

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727 APPENDIX I. NOTATION

- 728 The following symbols are used in this paper:
- 729 A = Planform dead zone area
- $C = \text{Scalar concentration where }_{0}=\text{initial, }_{DZ}=\text{dead zone, }_{mc}=\text{main channel, }_{p}=\text{primary re$ $gion, and }_{s}=\text{secondary region}$
- $_{732}$ $\Delta C =$ Concentration difference between the dead zone and the main channel
- $_{733}$ Γ = Circulation calculated around a closed loop
- $_{734}$ D = Dead zone depth
- 735 D_T = Turbulent scalar diffusivity
- $_{736}$ E = Entrainment velocity
- 737 θ = Momentum thickness
- 738 Fr = Froude number
- 739 $k_e =$ Entrainment coefficient
- $_{740}$ $k_p =$ Eigenvector for the primary region term
- $_{741}$ $k_s =$ Eigenvector for the secondary region term
- $k_W = T$ wo region model weighting factor
- 743 k = Turbulent kinetic energy
- $_{744}$ l = Closed path length variable for the calculation of circulation
- $_{745}$ L = Dead zone length in the streamwise direction
- $_{746}$ M = Mass of scalar in the dead zone
- 747 ν = Kinematic viscosity
- ⁷⁴⁸ ν_T = Turbulent diffusivity of the fluid
- 749 ω = Turbulent dissipation rate
- 750 $\omega_v =$ Vorticity
- $_{751}$ Ω = Average rotation rate in the dead zone
- $_{752}$ P = Fluid pressure
- $_{753}$ Q = Volumetric flow rate where $_{pm}$ =flow between the primary region and main channel and $_{754}$ $_{ps}$ =flow between the primary and secondary regions
- $Re_D = Reynolds$ number based on the dead zone depth
- 756 ρ = Fluid density
- 757 Sc = Scalar Schmidt number
- 758 Sc_T = Turbulent scalar Schmidt number
- 759 t = Time
- $T = Dead zone time scale where <math>_0 = asymptotic time scale, avg = average time scale, conv = convective time scale, avg = average time scale, time scale, avg = av$
- time scale, and $_{rot}$ =rotation time scale
- $\tau_{ij} = \text{Reynolds stress tensor}$
- $\begin{array}{ll} \tau & \text{Dead zone time scale where }_{L} = \text{Langmuir time scale, }_{p} = \text{primary region time scale, }_{s} = \text{secondary} \\ \text{region time scale, }_{pm} = \text{primary region to main channel time scale, }_{ps} = \text{primary region to} \end{array}$
- secondary region time scale, and $_{sp}$ =secondary region to primary region time scale u_i = Fluid velocity vector
- u_0 Velocity outside the boundary layer
- $_{768}$ U = Average main channel velocity
- 769 U_m = Mixing layer characteristic velocity

- V = Dead zone volume where _p=primary region volume and _s=secondary region volume 770
- W = Dead zone width 771
- 772 x_i = Position vector 773 ΔX^+ = Streamwise position in wall units
- ΔY^+ = Depth position in wall units 774
- $\Delta Z^+ =$ Spanwise position in wall units 775

776 APPENDIX II. REFERENCES

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000	T	is of parametric study cases and time scale results.

Case	<i>W</i> [m]	L [m]	D [m]	$U\left[\frac{\mathrm{m}}{\mathrm{s}}\right]$	$ au_L$	$ au_p$	τ_s	k_W	Fr
Base	0.5	1.25	0.046	0.221	397.2	457.4	1086.3	0.669	0.32
2	0.5	1.45	0.046	0.221	350.1	372.7	808.5	0.350	0.32
3	0.5	1.05	0.046	0.221	426.6	408.0	1148.0	0.637	0.32
4	0.5	0.85	0.046	0.221	454.4	410.6	1275.1	0.691	0.32
5	0.5	0.65	0.046	0.221	438.1	414.5	1331.9	0.747	0.32
6	0.5	0.55	0.046	0.221	447.1	403.3	1115.3	0.745	0.32
7	0.5	0.45	0.046	0.221	498.4	347.7	711.4	0.520	0.32
8	0.5	1.25	0.046	0.248	349.3	402.1	909.1	0.664	0.32
9	0.5	1.25	0.046	0.193	429.4	502.8	1262.1	0.686	0.287
10	0.5	1.25	0.046	0.165	484.8	584.4	1449.0	0.645	0.245
11	0.5	1.25	0.046	0.110	671.3	593.6	1643.6	0.291	0.163
12	1.25	1.25	0.046	0.221	819.3	838.2	4767.9	0.549	0.32
13	1	1.25	0.046	0.221	667.6	724.3	4123.8	0.594	0.32
14	0.75	1.25	0.046	0.221	516.6	608.0	3284.0	0.674	0.32
15	0.5	1.25	0.092	0.221	494.1	470.7	584.5	0.250	0.23
16	0.5	1.25	0.063	0.221	478.0	453.2	612.8	0.250	0.28
17	0.5	1.25	0.023	0.221	149.7	372.1	1243.4	0.428	0.46

 TABLE 1.
 List of parametric study cases and time scale results.

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FIG. 1. Dead zones types, flow features and geometric parameters: (a) planview schematic of a typical dead zone showing the mixing layer and recirculation regions, (b) a photograph of natural dead zone (courtesy T. R. Jackson, unpublished.), (c) planview showing the definitions of ideal dead zone parameters.



FIG. 2. Streamlines at the free surface in a dead zone after the shear layer is fully developed for different W/L corresponding to the experiments by Weitbrecht *et al.* (2008).



FIG. 3. Spanwise profiles: (a) Streamwise velocity profile corresponding to the x = 24, (b) turbulent kinetic energy corresponding to the x = 25.



FIG. 4. Comparison of predicted Langmuir time scale with experimental results from Uijttewaal *et al.* (2001) and Weitbrecht *et al.* (2008) for series of dead zones with different aspect ratios.



FIG. 5. The Langmuir time scale, τ_L versus W/U for all cases. Inverse slope is equal to the entrainment coefficient ($1/k_e$), R^2 for the fit is 0.72.



FIG. 6. The Langmuir time scale versus the rotation time scale for all cases: (a) τ_L versus $1/\overline{\omega}_v$ (R^2 for fit is 0.92), (b) τ_L versus $W/\theta\overline{\omega}_v$ (R^2 for fit is 0.74).



FIG. 7. Flowfield and passive scalar in case # 14 W/L = 0.6: (a) streamlines, (b) passive scalar plot at late times showing non-uniform mixing within the dead zone. Schematic of two-region model is also shown.



FIG. 8. Temporal evolution of the passive scalar concentration for different W/L on a semi-log axis. Time is normalized by the primary zone time scale: (a) different cases, (b) linear fit for the baseline case.



FIG. 9. Comparison of the Langmuir time scale, τ_L , the primary region time scale, τ_p , and the rotational time scale, $T_{rot} = 2/\overline{\omega}_v$: (a) τ_L versus τ_p (R^2 for fit is 0.68), (b) τ_p versus $1/\overline{\omega}_v (=T_{rot}/2)$ (R^2 for fit is 0.73).



FIG. 10. Power law relation for non-dimensionalized primary and secondary time scales with the geometric parameters and Reynolds number. (a) τ_p/T_{conv} (R^2 for fit is 0.95), (b) τ_s/T_{conv} (R^2 for fit is 0.73).