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## Reaction enhancement in an unsteady obstacle wake: Implications for broadcast spawning and other mixing-limited processes in marine environments

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#### ABSTRACT

Structured wakes behind flow obstacles are shown to be regions that enhance mixing and reactions between initially distant scalars, with implications for a wide range of mixing-limited biogeochemical processes in marine systems (e.g., broadcast spawning, phytoplankton-nutrient interactions). Reaction of initially distant reactive scalars in the structured laminar wake of a round obstacle is quantified using direct numerical simulations of the 2D Navier–Stokes and reactive transport equations with Reynolds number of 100 and Schmidt number of 1. Scalars are released upstream of the obstacle, initially separated by ambient fluid that acts as a barrier to mixing and reaction. Reaction is computed using second-order kinetics in the low–Damkholer limit. Reaction enhancement is quantified by comparing the obstacle-wake reactions to those in a similar flow but without the obstacle. Integrated reaction rates are shown to be orders of magnitude larger in the obstacle wake for cases with significant initial separation between the scalars. The role of unsteady processes in the reaction enhancement is also investigated by quantifying the scalar covariance in different regions of the wake.

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#### 1. Introduction

Fluid physics controls a wide range of biogeochemical processes in aquatic environments. In particular, fluid stirring serves to sharpen spatial gradients in transported scalars (e.g., chemicals, nutrients, microorganisms, gametes), enhancing diffusive mixing that promotes chemical reactions and other scalar interactions including nutrient uptake, respiration, and fertilization. In the absence of mechanical stirring, scalar mixing is accomplished only by molecular diffusion or microorganism motility, processes that can greatly limit interactions between initially distant scalar fields.

Mixing-limited problems abound in natural and engineered aquatic systems. Physical stirring controls phytoplankton–nutrient interactions (Philippart et al., 2000), phytoplankton–zooplankton interactions (Fasham et al., 1990), interactions between nutrients and food-web structure (Polis et al., 1997), and nutrient uptake and chemotaxis by bacteria (Taylor and Stocker, 2012). In engineered systems, stirring and mixing are critical to wastewater treatment (Bagtzoglou et al., 2006) and disinfection (Liu and Ducoste, 2006).

A particularly vivid example of a mixing-limited process in marine biology is broadcast spawning, the reproductive strategy used by a range of benthic invertebrates (Crimaldi and Zimmer, 2014). Most benthic invertebrates spawn their gametes into the ambient flow, and

\* Corresponding author. *E-mail address:* crimaldi@colorado.edu (J.P. Crimaldi). male and female adults are typically separated by some distance on the seabed, successful fertilization relies on structured stirring to bridge the initial separation between sperm and eggs. The resulting fertilization is typically modeled as a second-order reaction. Stirring by the flow, however, has competing effects; while it can promote gamete aggregation, it can also act to dilute gamete concentrations. The details of physical-biological coupling in this process are still not understood. The exact contributions of larger-scale (stirring of gamete plumes) and smaller-scale (sperm-egg encounters) processes to fertilization success have not been established for even a single species. However, studies suggest that structured stirring by single vortices may enhance fertilization rates (Crimaldi and Browning, 2004; Crimaldi et al., 2008). It is likely that collections of vortices in obstacle wakes could induce similar, or greater, enhancements. Wake-producing obstacles could include (in decreasing scales) islands, reef structures, coral heads, coral branches, and various roughness elements on the seabed. Turbulence is ubiquitous in natural systems, and is typically cited as

fertilization occurs externally to female reproductive tracts. Because

Turbulence is ubiquitous in natural systems, and is typically cited as the key mechanism for promoting stirring, mixing, and reactions of biogeochemical agents. However, laminar flows can also be effective in this regard, and these laminar flows control biogeochemical processes at low Reynolds number, the regime of all aquatic processes at sufficiently small scales. In particular, a large body of literature exists on the topic of stirring, mixing, and reactions by laminar chaotic flows (Ottino, 1989; Muzzio and Liu, 1996; Károlyi et al., 1999; Tél et al., 2000; Szalai et al., 2003; Tél et al., 2005).

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Reefs and islands are common obstacles to incident flows in marine systems (albeit at relatively large scales and Reynolds numbers). Mixing in island wakes is associated with increased particle retention and nitrate concentrations (Coutis and Middleton, 2002; Hasegawa et al., 2004; Venchiarutti et al., 2008), phytoplankton blooms (Heywood et al., 1990; Signorini et al., 1999; Sandulescu et al., 2007; Hasegawa et al., 2008, 2009) and aggregations of coral gametes and larvae (Wolanski et al., 1989; Willis and Oliver, 1990). At the other end of the physical scale spectrum, the importance of obstacle wakes has been shown for benthic invertebrate sensory appendages (Koehl et al., 2001; Mead et al., 2003), and for swimming microorganisms (Yen and Strickler, 1996; Guasto et al., 2012). Despite the large range of studies about the importance of obstacle wakes on ecological function, very little is known about the quantitative reaction enhancement between initially distant scalars. To address this shortcoming, we consider an idealized scenario that can serve as a process-level model for a host of problems in marine science.

In the present study, we consider stirring, mixing, and reaction of a pair of initially distant scalars (e.g., egg and sperm, plankton and nutrients, etc.) by one of the most basic and fundamental flows: the structured laminar wake behind an obstacle. We consider the specific case for a 2D flow around a round obstacle at Reynolds number 100, but many of the ideas that result from the study have general implications for similar flows around obstacles of other shapes, for other Reynolds numbers, and in 3D flows. The goal of the study is to show that the structured obstacle wake serves as an effective reactor vessel that enhances mixing and reactions between two initially distant scalars, and to quantify this reaction enhancement relative to a comparable flow without the obstacle.

#### 2. Problem Formulation

We consider viscous 2D flow with density  $\rho$  and kinematic viscosity  $\nu$  around a round obstacle with diameter  $\phi$  as shown in Fig. 1.

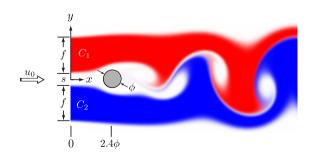
The incoming flow is steady, laminar and uniform with speed  $u_0$ , and a quasi-steady periodic wake develops downstream of the obstacle. The viscous flow field  $\mathbf{u} = [u, v]$  is governed by the incompressible Navier–Stokes equations

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + R e_{\phi}^{-1} \nabla^2 \mathbf{u}, \tag{1}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = \boldsymbol{0}, \tag{2}$$

where length, time, velocity, and pressure have been scaled by  $\phi$ ,  $\phi/u_0$ ,  $u_0$ , and  $\rho u_0^2$ , respectively. The character of the resulting wake is parameterized solely by the Reynolds number

$$Re_{\phi} = \frac{u_0\phi}{\nu}.$$
 (3)



**Fig. 1.** Schematic of the flow and scalar release conditions. Steady laminar flow with speed  $u_0$  forms an unsteady wake behind a round obstacle with diameter  $\phi$ . Scalars  $C_1$  and  $C_2$  are released upstream of the round obstacle and are stirred by the wake. Scalar filaments have initial width *f* and lateral separation *s*.

The flow is subject to boundary conditions  $\mathbf{u} = (1, 0)$  for  $x \to -\infty$ , and  $\mathbf{u} = \mathbf{0}$  on the obstacle boundary.

The flow transports two reactive scalar filaments with initial width f and initial separation s. Filament concentrations are normalized by the source concentration  $C_0$ , with the resulting non-dimensional concentration fields denoted  $C_1(\mathbf{x}, t)$  and  $C_2(\mathbf{x}, t)$ . The concentration fields are governed by a coupled pair of 2D reactive transport equations

$$Re_{\phi}Sc(\partial_{t}C_{1} + \mathbf{u} \cdot \nabla C_{1}) = \nabla^{2}C_{1} - DaR, \qquad (4)$$

$$Re_{\phi}Sc(\partial_{t}C_{2} + \mathbf{u} \cdot \nabla C_{2}) = \nabla^{2}C_{2} - DaR,$$
(5)

where velocity is still scaled by  $u_0$ , but length and time are now scaled by *s* and  $s/u_0$ , respectively. The reaction rate *R* is scaled by  $kC_0^2$ , where *k* is the coefficient for the second-order reaction kinetics, giving

$$R = C_1 C_2. \tag{6}$$

The Schmidt number,

$$Sc = \frac{\nu}{D},$$
 (7)

is a ratio of the diffusivities of momentum and mass, and the Damköhler number,

$$Da = \frac{s^2 k C_0}{D},\tag{8}$$

is defined here as a ratio of diffusive and reaction time-scales (small *Da* corresponds to reactions that proceed slowly relative to diffusion). The scalar boundary conditions are

$$C_{1}(x = 0) = \begin{cases} 1 & \frac{1}{2} < y < \left(\frac{1}{2} + f/s\right) \\ 0 & \text{otherwise} \end{cases},$$
(9)

$$C_2(x=0) = \begin{cases} 1 & \left(-\frac{1}{2} - f/s\right) < y < -\frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$
(10)

Numerical simulations of reactive flow around the round obstacle were performed via finite-element discretization to the Navier-Stokes equations (Eqs. (1)-(3)) and the reactive transport equations (Eqs. (4)–(10)) for  $Re_{\phi} = 100$ , Sc = 1, and Da = 0.01. The COMSOL Multiphysics package was used to generate the finite-element mesh and solve the resulting system of equations with the direct PARDISO solver (Schenk and Gärtner, 2004); details are given in (Crimaldi and Kawakami, 2013). Time-stepping was adaptive, and mesh refinement was performed to ensure solution convergence. For the Navier-Stokes equations, the inlet boundary condition was uniform normal flow  $\mathbf{u} =$  $-u_0$ **n**, and the outflow boundary condition was zero viscous stress  $\nu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} = \mathbf{0}$  with a Dirichlet condition on pressure  $p = p_0$ . The side walls were slip boundaries subject to impermeability  $\mathbf{u} \cdot \mathbf{n} = \mathbf{0}$  and zero stress  $\mathbf{t} \cdot (-p\mathbf{I} + \nu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = \mathbf{0}$ , and the obstacle surface was impermeable no-slip  $\mathbf{u} = \mathbf{0}$ . The initial condition was  $\mathbf{u} = \mathbf{0}$ , and the simulation was run until a guasi-steady-state was achieved, as determined by ensuring periodicity within the domain. The resulting vortex shedding frequency  $\omega$  is often expressed nondimensionally as the Strouhal number, given by  $St = \omega \phi/u_0$ ; for the present study we obtained St = 0.18, which is within the range of previously calculated values (Deshmukh and Vlachos, 2005) at  $Re_{\phi} = 100$ .

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