



**AFRL-AFOSR-UK-TR-2021-0015**

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Fundamentals of Molecular Communications in Complex Environments

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**06/24/2021**  
**Final Technical Report**

**DISTRIBUTION A: Distribution approved for public release.**

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**REPORT DOCUMENTATION PAGE**

Form Approved  
OMB No. 0704-0188

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<b>1. REPORT DATE (DD-MM-YYYY)</b> 24-06-2021		<b>2. REPORT TYPE</b> Final		<b>3. DATES COVERED (From - To)</b> 01 Feb 2017 - 31 Jan 2021	
<b>4. TITLE AND SUBTITLE</b> Fundamentals of Molecular Communications in Complex Environments				<b>5a. CONTRACT NUMBER</b>	
				<b>5b. GRANT NUMBER</b> FA9550-17-1-0056	
				<b>5c. PROGRAM ELEMENT NUMBER</b> 61102F	
<b>6. AUTHOR(S)</b> Weisi Guo				<b>5d. PROJECT NUMBER</b>	
				<b>5e. TASK NUMBER</b>	
				<b>5f. WORK UNIT NUMBER</b>	
<b>7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)</b> UNIVERSITY OF WARWICK UNIVERSITY HOUSE THE UNIVERSITY OF WARWICK COVENTRY, WEST MIDLANDS CV4 8UW GBR				<b>8. PERFORMING ORGANIZATION REPORT NUMBER</b>	
<b>9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)</b> EOARD UNIT 4515 APO AE 09421-4515				<b>10. SPONSOR/MONITOR'S ACRONYM(S)</b> AFRL/AFOSR IOE	
				<b>11. SPONSOR/MONITOR'S REPORT NUMBER(S)</b> AFRL-AFOSR-UK-TR-2021-0015	
<b>12. DISTRIBUTION/AVAILABILITY STATEMENT</b> A Distribution Unlimited: PB Public Release					
<b>13. SUPPLEMENTARY NOTES</b>					
<b>14. ABSTRACT</b> In this project, the PI looked into micro- and macro-scale molecular communication as a way to communicate in environments not suitable to wave signals. In particular they were interested in the information capacity of molecular signalling pathways in both micro-scale diffusion and macro-scale turbulent channels. The general approach is to understand how information can be embedded in the structure of molecular "puffs" and how mutual information between transmitter and receiver is degraded in different fluid dynamic channels. The methods combined a wide variety of experimental set-ups including planar laser-induced fluorescence (PLIF) and particle image velocimetry (PIV) methods - to extract the stochastic distribution of molecular signals over space and time. The team then use these channel statistics to inform the development of new modulation coding methods, as well as the achievable mutual information of the channels. Combined together, this led to 6 IEEE journal publications, 2 IEEE flagship conference papers. This works were submitted as evidence to emerging IEEE standards on nano-communications P1906.1.					
<b>15. SUBJECT TERMS</b>					
<b>16. SECURITY CLASSIFICATION OF:</b>			<b>17. LIMITATION OF ABSTRACT</b>	<b>18. NUMBER OF PAGES</b>	<b>19a. NAME OF RESPONSIBLE PERSON</b>
<b>a. REPORT</b>	<b>b. ABSTRACT</b>	<b>c. THIS PAGE</b>			NANDINI IYER
U	U	U	SAR	14	<b>19b. TELEPHONE NUMBER (Include area code)</b> 314-235-6161



JANUARY 5, 2021

# FINAL REPORT

## 2017-21 (YEAR 1-4)

Grant Number: FA9550-17-1-0056

Research Title: Fundamentals of Molecular Communications in Complex Environments

PI Name: Dr. Weisi GUO

Period of Performance: Jan 2017-2021

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## Summary

In the PhD project, we looked into micro- and macro-scale molecular communication as a way to communicate in environments not suitable to wave signals. In particular we were interested in the information capacity of molecular signalling pathways in both micro-scale diffusion and macro-scale turbulent channels. Our general approach is to understand how information can be embedded in the structure of molecular "puffs" and how mutual information between transmitter and receiver is degraded in different fluid dynamic channels. Our methods combined a wide variety of experimental set-ups including planar laser-induced fluorescence (PLIF) and particle image velocimetry (PIV) methods - to extract the stochastic distribution of molecular signals over space and time.

We then use these channel statistics to inform the development of new modulation coding methods, as well as the achievable mutual information of the channels. Combined together, this led to 6 IEEE journal publications, 2 IEEE flagship conference papers. This works were submitted as evidence to emerging IEEE standards on nano-communications P1906.1.

## Introduction

The aim is to understand the fundamental advantages and limitations of molecular communications in complex environments and exploit its potential. Despite the abundant use of molecular signalling in nature, we humans lack knowledge in this area and as such have not exploited its potential. Molecular communication has gained significant research attention in recent years, providing an alternative and attractive way to communicate at small-scales, as well as in challenging propagation environments. Its applications include targeted drug delivery and surgery scenarios as well as other electromagnetically hostile environments. In the foreseeable future, the demand for small devices that can coordinate and communicate with each other to complete a precision task will grow. In nano-medicine alone, the market for targeted drug-delivery [1] is estimated to be over \$520 billion by 2019 with a 16% CAGR. This proposal will focus on understanding the performance of molecular communications in complex diffusion environments that are relevant to a number of envisaged application scenarios. We are part of the first team to have built a molecular communication test-bed [4] and tested it in hostile environments [2,3,5]. Novel signal processing [7], error correction coding [8] have been devised to exploit its advantages. In this project, a combination of theory, simulation, and experimentation methodologies will be push the research further into complex propagation domains and seek to develop new nano-scale communication protocols.

## Methods, Assumptions and Procedures

### Channel Model and Assumptions for Diffusion Channels

The initial 12-months of research focused on modeling the basic diffusion-advection channel in a general way, via an *effective diffusion equation*, where the channel impulse response  $\phi(t,d)$  is given by the solution to Fick's 2<sup>nd</sup> Law in a 3-dimensional environment:

$$\phi(t, d) = \frac{1}{\sqrt{4Dt^3}} e^{(d-vt)^2/4Dt}$$

where the parameter  $D$  is an effective diffusivity typically used to explain complex *viscous diffusion* phenomenon where the resultant effect has a similar profile to diffusion. This is commonly an empirical value determined through experimentation. The other parameters are time ( $t$ ), distance ( $d$ ), and flow velocity ( $v$ ). This is also known as the first hitting distribution. Other forms of this equation include the first passage distribution, which incorporates an absorbing receiver of finite size. Details of these equations and usage in molecular communications can be found in my paper [9].

How accurate this channel model assumption is in different fluid environments (e.g. different Reynolds numbers, fluid types, and obstacle fields) remains to be investigated in the 2<sup>nd</sup> year (2018). For now, we assume the  $D$  parameter is isotropic and sufficient to cover all forms of complexities, which has been used for oceanic modeling.

### Channel Model and Assumptions for Turbulent Channels

The second year of research, we significantly updated our channel model to fully capture the complex fluid dynamic effects of turbulence, with a Reynolds Averaged Navier Stokes equation, which is a significant improvement over simple diffusion-advection dynamics:

$$c\bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = c\bar{f}_i + \frac{\partial}{\partial x_j} \left[ -\bar{p}\delta_{ij} + \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \overline{cu'_i u'_j} \right]$$

where  $c$  represents concentration and depends on a variety of parameters (velocity  $u$ , pressure  $p$ , viscosity). Details of these equations and usage in molecular communications can be found in [9].

### Analytical Method and Procedures

The primary analytical method is using COMSOL multiphysics simulator to model the RANS equation and benchmarked against our own or existing literature's experimental results. We also set up a fluid dynamic test environment below, with a 20m fluid flume fitted with 2D PIV particle tracing and obstacle fields for continuous experimental validation and testing – see Fig. 1. The details are outlined in our paper [10].

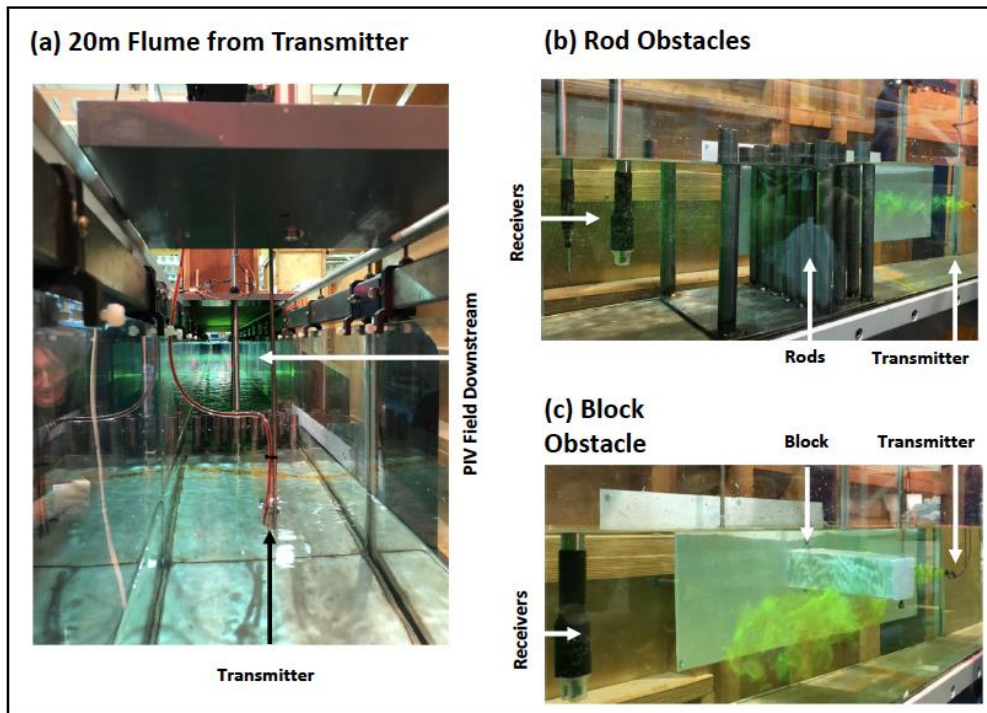


Figure 1: Flow based molecular communication test facility with obstacles and PIV particle tracing.

## Mobile Channel Characterization

The initial work characterized the transposition error probability in mobile channels. Unlike radio and acoustic communications, there is a danger in molecular communications that the transceivers can move faster than the molecular information. This can lead to information transmitted later to arrive earlier, causing bit transposition error. Our first piece of work characterized the probability of this event [P2]. In this work, we assume that there are 2 random walk processes (characterized by diffusivity values  $D_p$  for information and  $D_{\text{total}}$  for mobility), one by the information and one by the distance between the transmitter and receiver. As such, this double random walk process leads to an information leads to a response delay  $t_n$  for the  $n$ -th bit, given by the PDF in Fig. 2a, where  $\text{erf}(\cdot)$  is the error function and  $R$  is the mobile distance between receiver and transmitter.

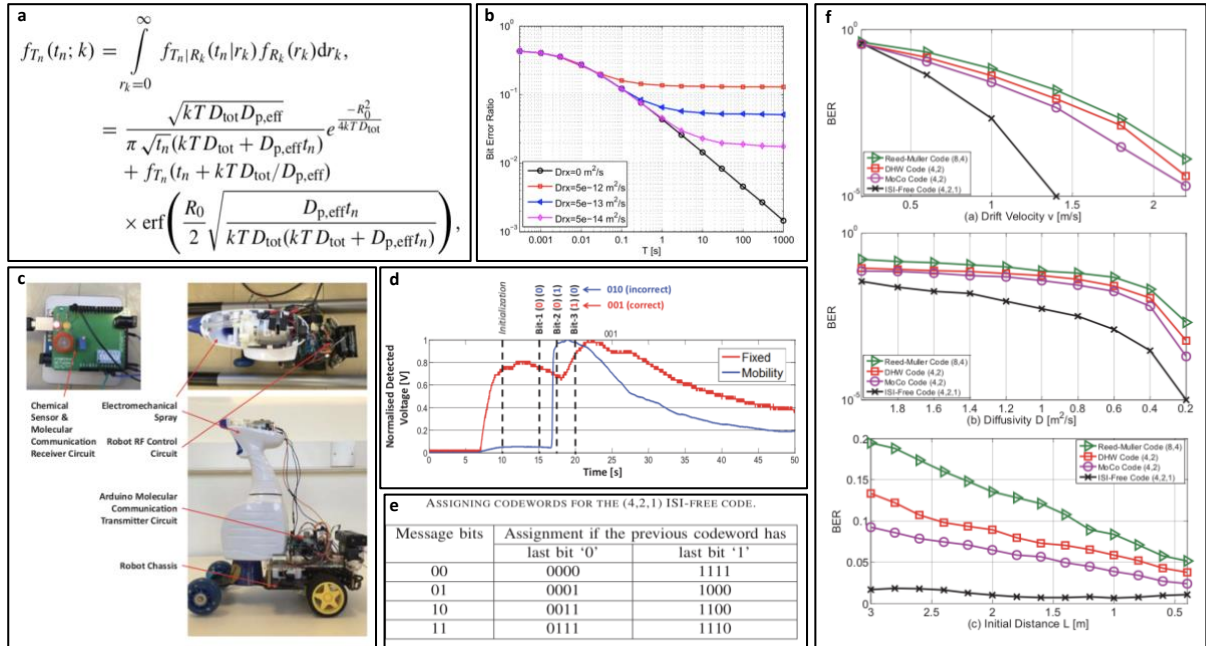


Figure 2: Transposition PDF and transposition bit error rate performance against different mobility speeds.

In Fig. 2b, we show that as the random walk speed of the transmitter/receiver increases, the error rate curve saturates against increased bit period ( $T$ ), indicating that there is no clear way to improve the reliability of the channel and that the performance of mobile molecular communication channels is fundamentally limited by mobility speed in a random movement scenario. Detailed results can be found in [P2].

### Coding over a Mobile Channel

In order to improve upon the error performance, we applied basic transposition error combating forward error correction (FEC) codes. Here, we implement ISI-free code [14] on a mobile molecular communication robot – see Fig. 2c-e. We show that the robot suffers from transposition error, and standard Reed-Muller FEC codes [13] which combat additive noise errors is insufficient – see Fig. 2f. The application of Distinct Hamming Weight (DHW), MoCo, and ISI-free codes can significantly improve performance, all of which are outlined in [P3] and [9]. Detailed results can be found in [P3].

## Large-Scale Communication Performance

Thus far, we have examined the performance of point-to-point communications. In multiple access systems, whereby a large number of  $K$  transmitters are simultaneously transmitting at different time intervals, they will all interfere with each other, as shown in Fig. 3a. We apply stochastic geometry analysis in a 3-dimensional space. First, we derive analytical expressions for signal strength (see Fig. 2b) and signal-to-interference ratio, both of which are too complex to show here and can be found in [P4] and [P5]. We then derive the single bit error probability for both passive and absorbing receivers – see Fig. 2c/d evaluated at different transmitter densities. The analytical results (lines) are all validated using Monte-Carlo simulations (symbols).

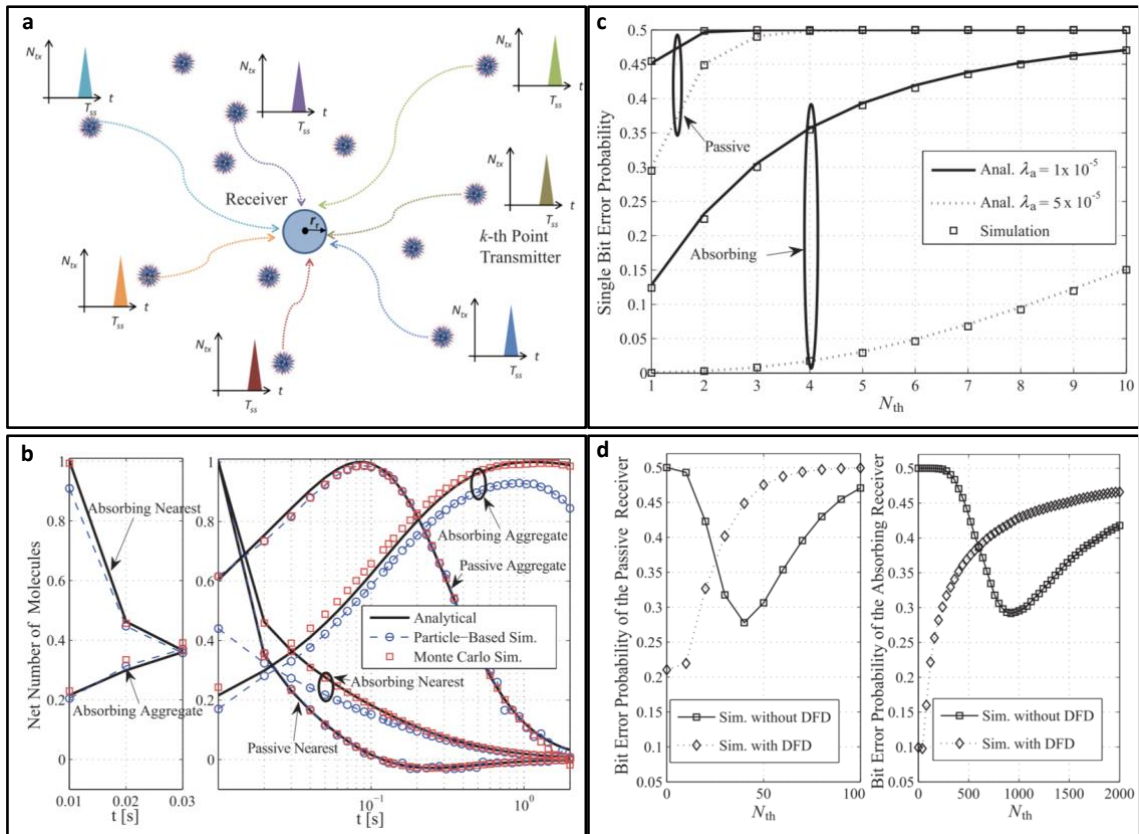


Figure 3: Simultaneous large-scale molecular communications by  $K$  transmitters.

Detailed results can be found in [P4] and [P5].

# Self-Propelling Vortex Structures for Chemical Information Delivery

## Introduction & Motivation

Molecular signal coherence in fluid dynamic channels is severely hindered by mass, momentum, and turbulent diffusive forces. The combination of such forces causes long molecular tails, which results in severe inter-symbol-interference (ISI) and limits the achievable symbol rate. Here, we propose to modulate information symbols into stable vortex ring structures to minimize ISI. Each vortex ring can propagate approximately 100x the diameter of the transmission nozzle without losing its compact shape. First, we show that the ISI from sequential transmissions is minimal and reduces rapidly with distance after transmission. This is the opposite effect to conventional molecular puffs undergoing advection-diffusion, whereby ISI increases with distance. Second, we show that by maintaining a coherent signal structure, the signal-to-interference (SIR) ratio is 211x higher over conventional chemical puffs. Also, we demonstrate the vortex ring using a proof-of-concept prototype. The results point towards a promising pathway for higher capacity channels. The details are described in our paper [11, P6].

## Vortex Ring Generation

Turbulence is not only inherently very difficult to model, but it also doesn't directly help us understand the communication capacity of the channel. Yet, we can take advantage of a certain structure called a vortex ring, that propagates well in turbulent fluid channels. The vortex ring retains spatial structure through its rotational momentum and has a sharper concentration time profile than a standard puff. This has the potential to significantly reduce inter-symbol-interference (ISI) from sequential transmissions and as such allow us to transmit at a higher symbol rate. The vortex ring core is a torus shaped fluid or gas structure, that retains shape (e.g., mitigates dispersion) for long propagation distances (typically 50x nozzle diameter). Each vortex ring is a region, where the molecules mostly spin around an axis in a closed loop. Finally, it should be noted that one of the possible applications of the vortex rings is the Line-of-sight (LOS) communication.

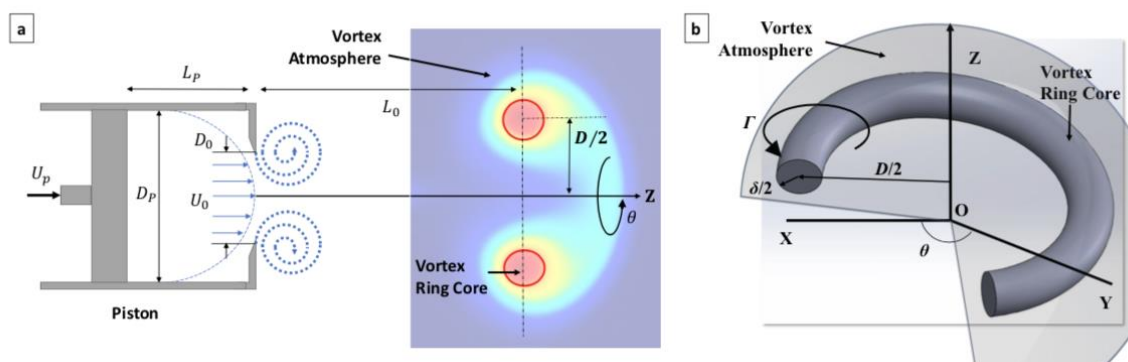


Figure 4: (a) illustration of transmitter piston to generate a vortex ring, (b) illustration of vortex ring core and orientation coordinates.

## Vortex Ring Propagation

A vortex ring is a bounded region of vorticity in which the vortex lines form closed loops. Vortex rings which are circular and stable and can retain molecular information in a self-sustained structure. It is worth noting that the vortex core can become wavy (Widnall instability) at some point during its existence depending on conditions. The general properties of every vortex ring can be observed in Fig. 2, where the vortex ring core has diameter of  $D$  (approximately 1.3x the nozzle diameter  $D_0$ ) and the bulk of vorticity in the region has diameter of  $d$ . There is also a small atmosphere surrounding the core.

For a single symbol, the resulting SIR is as follows - see Fig.3 (left): (1) Vortex Ring: +51.5dB, and (2) Puff: +9.5dB. We can see approximately a 211x improvement when the vortex ring is compared to the puff. As shown in Fig.3 (right), we can see that SIR as a function of transmission distance for a standard puff (SIR decays with distance) and a vortex ring (SIR increases with distance). A snapshot of the 3D profile and a demonstration is shown in Fig.4.

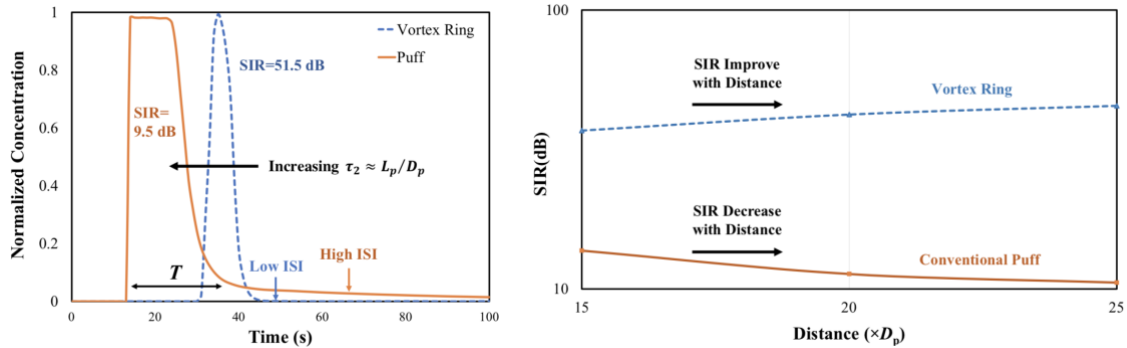


Figure 5: SNR Improvement compared to puff (left) and with distance (right).

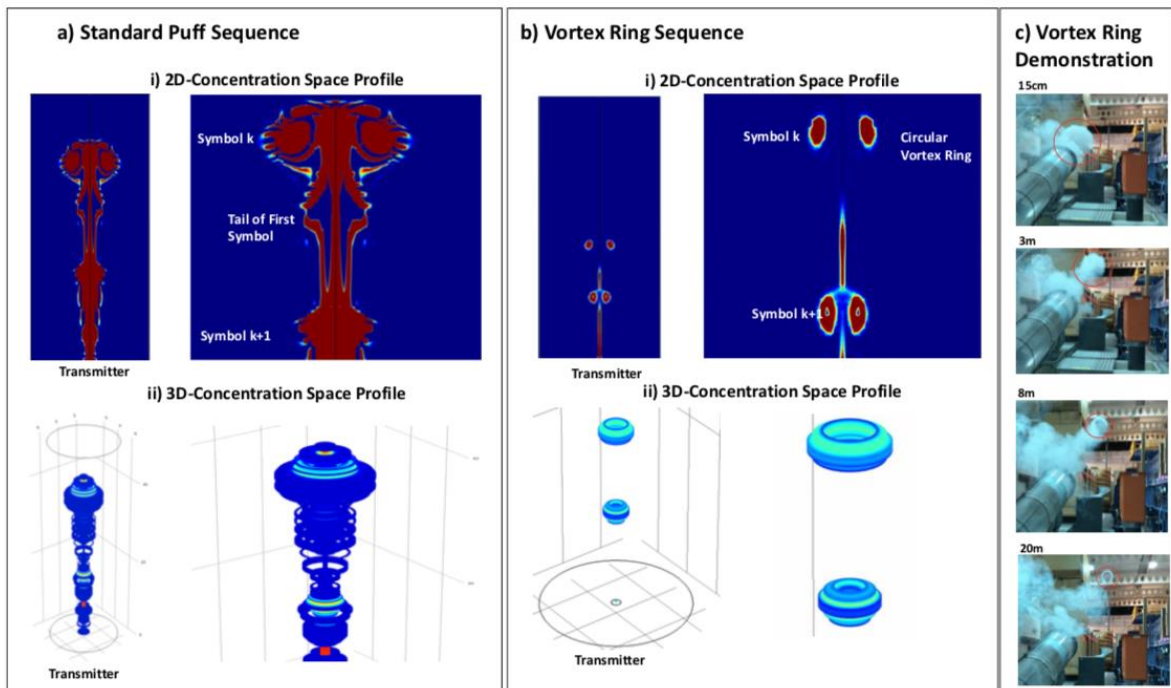


Figure 6: 3D puff (a) and vortex ring (b) sequential information structures; and a demonstration in air (c).

# Mutual Information and Noise Distributions

## Introduction & Motivation

Information embedded in the fluid dynamic properties undergo stochastic behaviour when propagating from transmitter (Tx) to receiver (Rx). This is due to the high dimensionality and continuous dynamic forces of the environment, which erodes the achievable mutual information. Quantifying the statistical noise distribution and mutual information with respect to the key fluid dynamic parameters is important to molecular communication. Significant research has been conducted and a review of channel models and associated physical layer techniques. Experimentation is essential to capture realistic variational behaviour in fluid dynamics. Early experimental work started with tabletop prototypes characterizing experimental throughput and noise process with crude chemical sensors, which has now advanced to encoding in chemical mixtures with mass spectrometer demodulation. This coincides with parallel work in replicating pheromone signals. In our attempts to understand and improve the achievable mutual information in macro-scale fluid dynamic channels with complex forces, recent work (2018-19) has characterized the evolving information structure in turbulence, tracked info-molecules using fluorescence, characterized the linearity of sequential pulse combining and generated self-propagating structures to increase symbol rate and transmission range. We contribute to this growing area of experimental research by 1) Experimentally quantifying additive and transposition noise in macro-scale environments, under the heterogeneous forces of shear stress, eddies, and diffusion advection; 2) Finding the corresponding mutual information and optimal transmission strategy; 3) Detailing the experimental procedure with planar laser induced fluorescence (PLIF) approach to benefit future researchers.

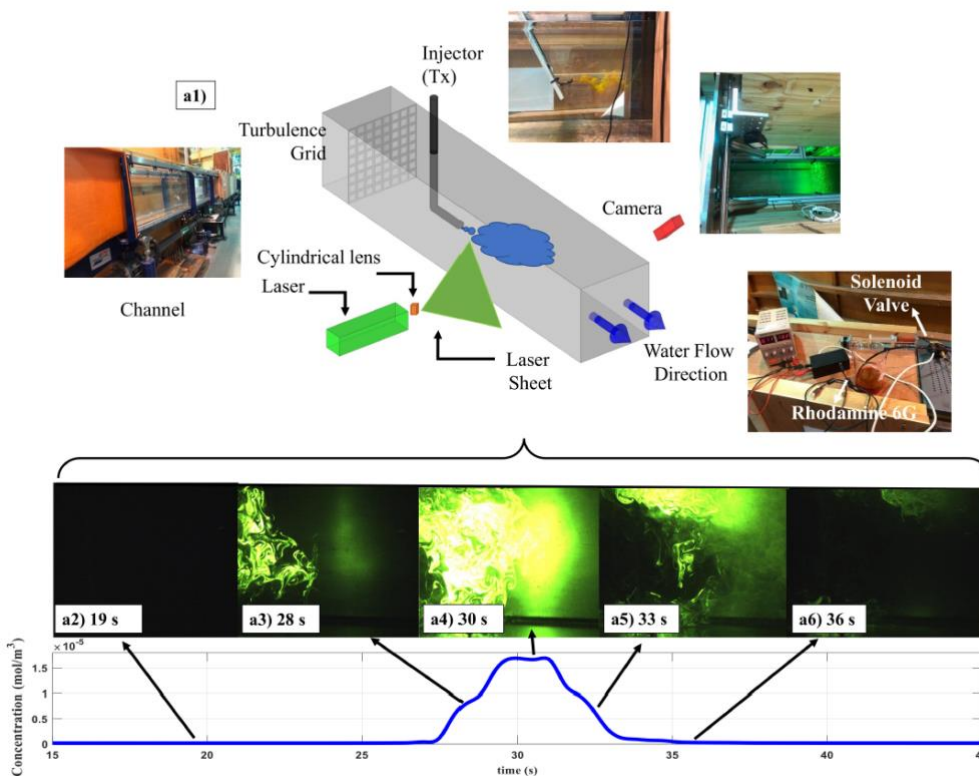


Figure 7: Schematic of the experimental setup

## Experimental setup

A schematic of the experimental setup including the injector (transmitter), laser and camera is shown in Fig.8. The channel is 15 m long and 300 mm wide and 380 mm deep. All channel walls are made of

glass enabling convenient optical purposes. The velocity of the water flow is controlled by a pump with a fixed flow rate which is placed between the inlet and outlet of the water flume. To maintain a constant head in the flume, there is a board at the outlet of the flume and by adjusting the angle of the board, we can set the water height across the flume. After eight injections, the water in the whole loop was replaced by the fresh water to avoid detecting of the material from previous injection. Turbulence was generated by means of a stainless turbulence grid mounted inside the flume half a meter upstream of the injector. Puffs of fluorescent tracer liquid were released from a cylindrical pipe with the inner diameter of  $D = 5$  mm and the distance between the channel entrance and the pipe is 2.6 m. This pipe is connected to a solenoid valve, and it is controlled by a computer program. For examining the steady flow regime, we removed the turbulence grid and decreased the pump flow rate. The water channel velocity for the steady flow case is 0.086 m/s and for the turbulence case is 0.26 m/s. Also, the injection velocity for both of the regimes is the same and it is 1 cm/s.

Planar laser-induced fluorescence (PLIF) is a spectroscopic method that measures the concentration in turbulent mixing and shear flows such as plume and jet flows, which are representative of natural environments. In this method, the fluorescence dye traces the pathway of the information particles in the water channel, and it captures the various dynamics of the fluid flow like eddies, vorticities, velocity fluctuations, shear layers, etc. After ejection of the dye at the transmitter, the dye travels through the channel and when it arrives at the laser sheet (which is the receiver), the dye particles will be excited. Then, the fluorescence dye will de-energise and at this stage, the fluorescing photons are emitted from the dye molecules at the laser plane. The fluoresced light intensity depends on several factors including local dye concentration, photo bleaching, temperature and pH dependence, and laser saturation. By capturing the photons using a high-speed camera, the intensity of the images is obtained, and this intensity is correlated to the dye concentration using a calibration technique.

## Mutual Information

In this section the mutual information for steady flow case is derived. It is assumed that no molecular information is transmitted if bit 0 is sent with the probability  $p_0$ . Bit 1 is sent with the probability of  $p_1$ . The threshold for signal detection is  $C_{th}$ . We also assume that the total concentration of the inter-symbol interference (ISI) follows a Gaussian distribution with mean  $\mu_l$ , and standard deviation. This is reasonable because  $n_2$  follows a Gaussian distribution, and the total concentration of the ISI is a linear combination of each ISI component. We have

$$\begin{aligned} P(1|0) &= \int_{C_{th}}^{\infty} \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left[-\frac{(r - \mu_l)^2}{2\sigma_1^2}\right] dr \\ &= 1 - Q\left(\frac{C_{th} - \mu_l}{\sigma_1}\right), \\ P(0|1) &= \int_{-\infty}^{C_{th}} \frac{1}{\sqrt{2\pi}\sigma_2} \exp\left[-\frac{(r - c_{peak})^2}{2\sigma_2^2}\right] dr \\ &= Q\left(\frac{c_{peak} - C_{th}}{\sigma_2}\right), \end{aligned}$$

where  $Q(\cdot)$  is the Q function. The joint probability  $p(x, y)$  ( $x \in \{0, 1\}$ ,  $y \in \{0, 1\}$ ) represents the probability that the symbol  $x$  is transmitted and the symbol  $y$  is detected, and is derived as

$$\begin{aligned} p(0, 0) &= p_0(1 - P(1|0)), \\ p(0, 1) &= p_0P(1|0), \\ p(1, 0) &= p_1P(0|1), \\ p(1, 1) &= p_1(1 - P(0|1)). \end{aligned}$$

The mutual information can be expressed as

$$I(X; Y)|_{n_1} = \sum_{y \in Y} \sum_{x \in X} p(x, y) \log \frac{p(x, y)}{p(x)p(y)},$$

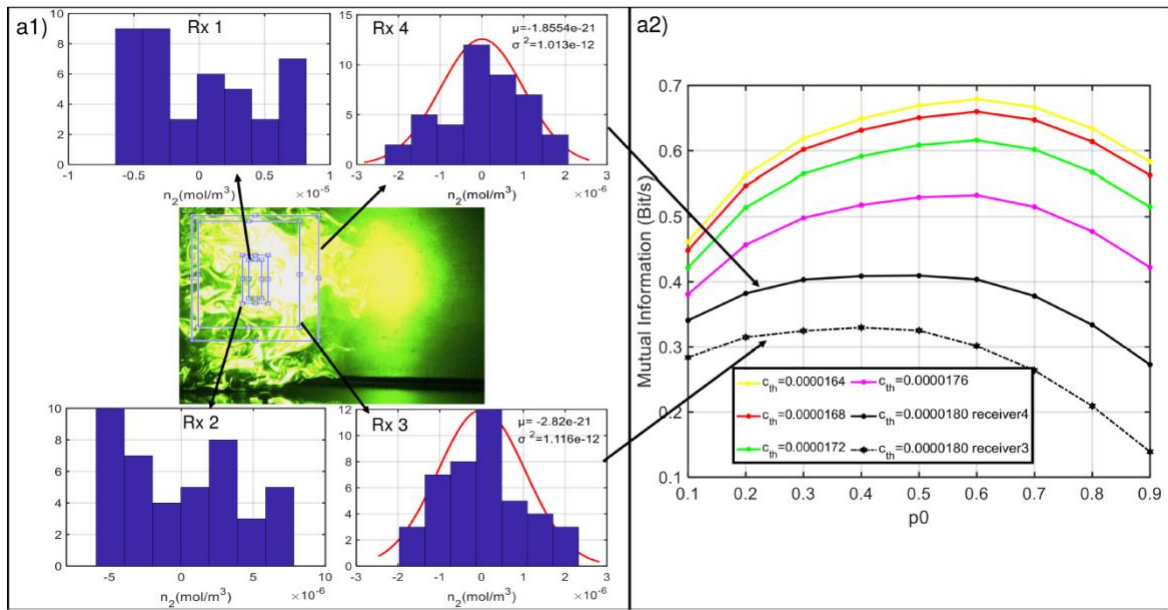


Figure 8: a1) Different receiver size and their corresponding histogram

As it is proven that  $n_1$  can be approximated as a Gaussian distributed random variable with mean  $\mu_1$  and standard deviation whose probability density function (PDF) is Gaussian distributed, the expected mutual information by concurrently considering both  $n_1$  and  $n_2$  can be expressed as

$$I(X;Y) = \int f(n_1)I(X;Y)|_{n_1} dn_1.$$

## Conclusions

In the project we built the evidence base to understand the fundamental advantages and limitations of molecular communications in complex environments and exploit its potential. Despite the abundant use of molecular signalling in nature, we humans lack knowledge in this area and as such have not exploited its potential. Molecular communication has gained significant research attention in recent years, providing an alternative and attractive way to communicate at small-scales, as well as in challenging propagation environments. Its applications include targeted drug delivery and surgery scenarios as well as other electromagnetically hostile environments.

We looked into micro- and macro-scale molecular communication as a way to communicate in environments not suitable to wave signals. In particular we were interested in the information capacity of molecular signalling pathways in both micro-scale diffusion and macro-scale turbulent channels. Our general approach is to understand how information can be embedded in the structure of molecular "puffs" and how mutual information between transmitter and receiver is degraded in different fluid dynamic channels. Our methods combined a wide variety of experimental set-ups including planar laser-induced fluorescence (PLIF) and particle image velocimetry (PIV) methods - to extract the stochastic distribution of molecular signals over space and time.

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## List of Relevant Publications and Grants

- [P1] "Molecular Channel Fading due to Diffusivity Fluctuations,"  
S. Qiu, T. Asyhari, **W. Guo**, S. Wang, B. Li, C. Zhao, M. Leeson  
IEEE Communications Letters, vol.21(3), pp.676-679, Mar 2017, IF 2.1 [[Link](#)]
- [P2] "Transposition Errors in Diffusion-Based Mobile Molecular Communication,"  
W. Haselmayr, S. Aejaz, A. Asyhari, A. Springer, **W. Guo**  
IEEE Communications Letters, vol.21(9), pp.1973-1976, May 2017, IF 2.1 [[Link](#)]
- [P3] "Mobile Molecular Communications: Positional-Distance Codes,"  
S. Qiu, T. Asyhari, **W. Guo**  
IEEE International Workshop on Signal Processing Advances in Wireless Communications (SPAWC), UK, Jul 2016 [[Link](#)]
- [P4] "Analyzing Large-Scale Multiuser Molecular Communication via 3D Stochastic Geometry,"  
Y. Deng, A. Noel, **W. Guo**, A. Nallanathan, M. ElKashlan  
IEEE Transactions on Molecular, Biological and Multiscale Communications, vol.3(2), pp.122-133,  
Sep 2017 [[arXiv](#)] [[Link](#)]
- [P5] "Stochastic Geometry Model for Large-Scale Molecular Communication Systems,"  
Y. Deng, A. Noel, **W. Guo**, A. Nallanathan, M. ElKashlan  
IEEE Global Communications Conference (GLOBECOM), USA, Dec 2016 [[Link](#)]  
[**IEEE Flagship Conference**]
- [P6] "Towards High-Capacity Molecular Communications using Sequential Vortex Rings," **M. Abbaszadeh, P. Thomas, W. Guo**, IEEE Transactions on Molecular, Biological and Multiscale Communications, to appear, Dec 2018

[P7] "Experimental Molecular Communications in Obstacle Rich Fluids," I. Atthanayake, S. Esfahani, P. Denissenko, I. Guymer, **P. Thomas, W. Guo**, ACM/IEEE International Conference on Nanoscale Computing and Communication (NanoCom), Iceland, Sep 2018

Mo-IoNT - Molecular Internet-of-Nano-Things, **EC H2020, PI** (Scientist in Charge), 792799, [Link](#), 2018-20, €195k

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- [4] "Tabletop Molecular Communication: Text Messages through Chemical Signals," N. Farsad and **W. Guo** and A. Eckford, PLOS ONE, 2013
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- [7] "Mobile Molecular Communications: Positional-Distance Codes," S. Qiu, T. Asyhari, **W. Guo** IEEE International Workshop on Signal Processing Advances in Wireless Communications (SPAWC), UK, Jul 2016
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