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Molecular Physical Layer for 6G in Wave-Denied Environments

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***Abstract*—The 6th Generation (6G) of wireless systems are likely to operate in environments and scales that wireless services have not penetrated effectively into. Many of these environments are not suitable for efficient data-bearing wave propagation. Molecular signals have the potential to deliver information by exploiting both new modulation mechanisms via chemical encoding and new multi-scale propagation physics. Whilst the fusion of biophysical models and communication theory has rapidly advanced the *molecular communication* field, there is a lack of real-world macro-scale applications. Here, we introduce application areas in: 1) defence and securities - ranging from underwater search and rescue to covert communications; and 2) cyber-physical systems - using molecular signals for health monitoring in underground networked systems. These engineering applications not only demand new wireless communication technologies ranging from DNA encoding to molecular graph signal processing, but also demonstrate the potential for molecular communication to contribute in traditional yet challenging engineering areas. Together, it is increasingly believed that molecular communication can be a new physical layer for 6G, accessing and extracting data from extreme wave-denied environments.**

***Index Terms*—molecular communication; defence; security; Internet-of-Things; cyber-physical systems; 6G;**

I. INTRODUCTION

As 5G and Beyond rolls out around the world, researchers and industry are already actively pursuing fundamentally new technologies for 6G's air interface - to connect new devices in new challenging environments. There are extreme environments that simply don't permit the use of wave-based wireless systems. These environments are often embedded (e.g. with lossy channel in fluids etc.), hostile (e.g. with jamming and eavesdroppers), and small (e.g. requires nanotechnology). Examples include coordinating robots in underground search & rescue, covert messaging in hostile territory, and health monitoring in embedded pipe networks and human body. Therefore, a new physical layer for 6G wireless is needed - this is recognised publicly by leading industrial leaders in telecommunications, underground critical infrastructure protection, and defence & securities.

In response to these emerging challenges, the research community have been developing new information carriers. Many key foresight papers have already proposed that molecular communication can enable a new generation of **human** in-body nano-network, such as in vivo connectivity for targeted drug delivery and healthcare applications under the umbrella of Internet-of-Nano-Things [1]. However, very few macro-scale engineered **machine** applications have been proposed and we set out to do this and demonstrate the capabilities and limitations of molecular communication.

Abundant in nature, absent in engineered systems; molecular communication (MC) is a rapidly advancing technology that has the potential to communicate in wave-denied environments. We have yet to realise its full potential in engineering. Originally proposed as a bio-inspired parallel to cell signaling, MC has been proposed for a wide range of biomedical applications ranging from targeted drug delivery [1] to opto-genetics. Whilst significant advances have been made to explore the synergy between established radio communication techniques (e.g. MIMO, cognitive, system building blocks) [**?**] and emerging MC systems, we must remember that the underlying physics of MC is not well understood and experimental evidence to support models are still primitive. Therefore, it is important to begin with challenges that motivates us to understand the underlying information theory and physical layer of MC through well motivated experimentation. This is particularly missing in the macro-scale engineering and engineered systems, there is a lack of application areas for MC. Macro-scale MC has seen a steady rise in prototyping due to its relatively low cost compared to micro-scale equivalents.

Our intention for this paper is to first review the rapid recent advances in macro-scale molecular communication (MC), specifically focused on: 1) encoding and decoding information using chemical and biological macro-molecules, and 2) turbulent channel modeling using computational fluid dynamics (CFD). This already sets the review apart from other reviews, which predominantly focus on nano-/micro-scale applications with diffusion-advection channels.

We then review recent and ongoing work in the application areas of defence and securities (Section III) and cyber-physical systems (Section IV). This is largely an overview of 5 years of experimental work (see Figure1) at University of Warwick in collaboration with BUPT and Tongji University - made possible through 4 collaborative research grants. We also review work conducted across the world in these areas as well and show a growing recognition that MC can find diverse applications. We show the reader that there are application areas that demand innovative and fundamentally new molecular wireless communication design, intermixed with fluid

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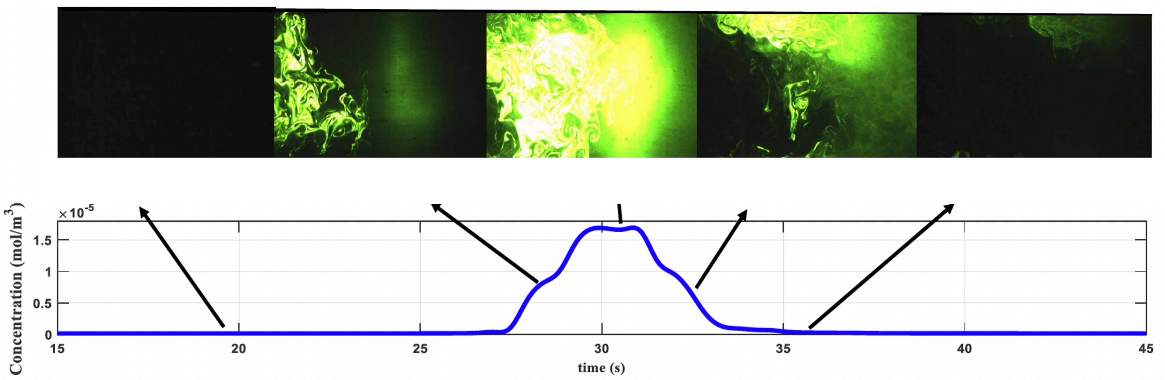

Fig. 1. Molecular Communication Lab Transforming Fluid Dynamic Knowledge into Communication Theory: PLIF data extraction: concentration data informs noise characterisation and mutual information analysis (see [3]).

dynamics and other traditional engineering areas. In Section V we argue that these macro-scale opportunities can join with the nano-scale healthcare applications to form a new 6G physical layer.

II. Advances in Macro-Scale Molecular Communication

We first detail a work stream in experimentation and analysis, which we show in Figure 1(left). We first illustrate channels which can not only enable MC, but also quantify the propagation of MC information (e.g. how information disperses or mixes with ambience). This can be enabled by a range of techniques (explained later) which ignite the molecular information bearers and are captured with a high speed camera for post-analysis for quantifying propagation and noise models. As shown in Figure 1(right), that analysis enables us to quantify the mutual information achievable across the 3D channel under realistic fluid dynamic conditions (e.g. beyond mass diffusion and advection forces) [3]. The key difference in our work compared to measurement/sensing work in fluid dynamics research is that we are attempting to encode and decode continuous streams of information, whereas other areas are just sensing a constant signal (e.g., a pollutant or heartbeat). In that respect, we are interested different attributes of signals which may serve as more stable and hence better features for encoding data or need novel mechanisms to combat the challenge.

A. Channel Modelling in Turbulence

Existing research at the nano-/micro-scale channels have predominantly used mass diffusion-advection channel models, assuming operating at low Reynolds number. This is appropriate for many of the nano-scale and biological environments (e.g. capillaries and cell membranes) and leads to tractable additive Gaussian concentration and inverse-Gaussian timing models. However, at the macro-scale and for low viscosity fluids, we enter the high Reynolds number regime where there are additional continuous forces (sheer forces, turbulence and momentum diffusion [4]). As such, it is imperative to develop understanding of more realistic models by solving Navier-Stokes (NS) equations with turbulence [5] - typically with finite-element (FE) simulation using either open source solvers or commercial packages such as COMSOL.

1) From Theory to Practice: Our experimental platform is one of the first in the world to use Particle Image Velocimetry (PIV) or Planar Laser-Induced Fluorescence (PLIF) to track molecular information and inferring the achievable mutual information (MI) in a turbulent channel [3]. The PIV or PLIF system can be useful for understanding how information propagates in real world (e.g. underwater rivers and oceans - see applications later in paper), given that the dimensionless number match between the scenario and experimentation. The receiver is either: (1) high speed camera - images are analysed for luminescence strength as a proxy for concentration, or (2) submersible optical fluorometer. Various obstacles are installed to mimic real-world environments. Using the measurement data from repetitive transmissions, we quantify the noise distribution and maximize the achievable MI of the channel. We do so by configuring the input distribution and observing the noise at the output and identifying the MI as defined in [3]. In order to calculate MI, one of the challenges is gathering repeated experimental data to quantify the noise distribution, which can be slow in real-time experiments. Other similar work have optimised the modulation strategy, which can also improve MI preservation in turbulent channels [4].

2) Fundamental Transmission Limits: There exist established fundamental limits to how far a coherent MC signal can travel before it *fully mixes* into the atmosphere, making individual and sequential signal symbols indistinguishable. Here, coherence is defined as when the signal structure transmitted can still be recognised at the receiver (e.g., mutual information > 0). The underlying relevant processes are governed by the complexities of fluid turbulence with its associated classic energy cascade. Turbulent flows comprise eddies of different length scale. Energy is cascaded from the largest scales of motion to successively smaller scales until it gets dissipated, due to the action of viscosity, at a smallest length scale referred to as the Komogorov micro-scale. Experimental studies addressing issues linked to the fundamental limits of macro-scale molecular communication in the context of this turbulence framework were conducted in [4] and [3]. We have investigated underwater, buoyancy-

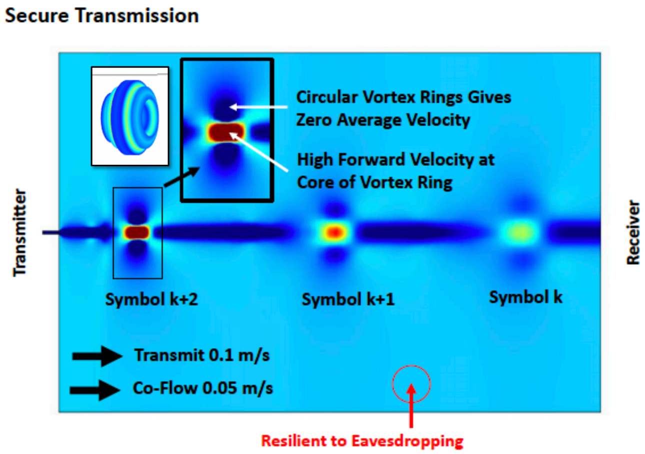

Fig. 2. Secure Molecular Vortex Rings [6].

driven vertical macro-scale molecular communication that is of potential relevance to submarine communication. Information was coded onto sequential molecular plumes. The information capacity loss, due to turbulent entrainment of ambient water into the molecular plumes, was addresses by adopting the entrainment assumption. This leads to a Gaussian cross-plume velocity profile, which has interpretable attributes such as bore-sight strength and size of transmit antenna. That is to say the forward velocity, which we know is important for symbol coherence, is reduced laterally by how far one detects outside the bore-sight.

3) Breaking the Limits using Vortex Rings: Whilst there are fundamental limits to how far a MC signal puff can travel before it mixes with the atmosphere and the momentum and signal structure is lost (see Fig.2), we can break this limit using self-propagating structures. In order to break the barriers posed by mass, momentum, and turbulent diffusive forces, we propose to modulate information symbols into stable vortex ring structures to maximize the transmission range and minimize ISI (see Fig.2). Each vortex ring can propagate approximately $100\times$ the diameter of the transmission nozzle without losing its compact shape. In [6], we show that the ISI from sequential vortex ring 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. Furthermore, we show that by maintaining a coherent signal structure, the signal-to-inference (SIR) ratio is 2 orders of magnitude higher over conventional puffs. The results point towards a promising pathway for higher capacity channels.

B. Encoding Information

As discussed previously, macro-scale MC signals transverse over significantly longer distances than their nano-/micro-scale MC by 7 to 10 orders of magnitude. The forces which affect macro-scale MC signals are significantly more dynamic, higher dimensional (e.g. many coupled forces), and are subject to a variety of external perturbations. The channel model is reviewed in detail later in this section. As such, the traditional modulation methods of concentration shift-keying (CSK) and timing shift keying are fundamentally unreliable - details of which we explain below in the fundamental limits part. Whilst aforementioned techniques such as vortex rings [6] can improve the coherence of the pulse shape in turbulent channels, the encoding limitations (e.g. reliance on timing or concentration features) must be overcome through biochemical modulation. The demand to mimic nature and use a form of biochemical shift-keying is critical to macro-scale MC reliability.

1) Chemical Encoding & Decoding: Transmission of chemically coded information via an odour stream was first demonstrated by Taylor et al., in 2015 [2] for a wide range of volatile organic compounds (VOCs) via a programmable generator capable of producing a very large number of chemical combinations. This demonstrated, for the first time, scalable chemical encoding in molecular communications. Information can either be modulated on to the chemical structure, or when coupled with traditional CSK modulation, a form of ”chemical bandwidth” is created (number of independent chemical signatures that can be encoded iwithout mutual chemical interference). The fundamental technologies at the transmitter side include a mixing chamber for different VOCs, which is then carried on an inert gas stream (carrier channel) enables smoother propagation. The receiver is a mass spectrometer that can translate complex chemical spectrum data back into the digital message.

In terms of the selection of chemical compounds, carbohydrates have distinct advantages in that they are the class of biological macro molecule with probably the greatest potential for complexity and therefore for storing information. Monosaccharides typically contain 3 to 6 carbons, and many can exist as both ringed and straight-chained molecules. Monosaccharides can vary in relatively subtle ways, which makes them very difficult to tell apart chemically as well as by mass, but modern technology have made it possible to map their sites and structures. Unlike DNA and peptides (see below), they can polymerise in more than one dimension as glycosidic linkages can be formed between multiple sites of monosaccharides, making a specific polysaccharide structure extremely difficult to synthesise chemically robustly. However, unlike DNA or peptides, they do not require a template to be produced biologically. Other selection criteria in research include mimicking the biological signature and designing chemical reactions to prolong the lifetime of the signal in propagation. In the latter case, researchers at Catania have advanced this area by using: (1) fluorescent molecules switched by pH-driven hydrolysis exploits the reactivity of the chemical messenger to achieve a stable signal at the receiver [7], and (2) carbon nano-particles to achieve low drag molecular propagation for sharper signals.

2) Biochemical DNA Encoding & Decoding: DNA storage have been shown to offer significant advantages over electrical and magnetic storage in terms of cost efficiency for either large file sizes or long term storage. Current technology can achieve Mbits of reliable information storage with less than 1% error and can persist for 50 years. Research conducted at the University of Cambridge by Keyser [8] and Akan et al. [9], has been developing the experimentation and theoretical foundation for

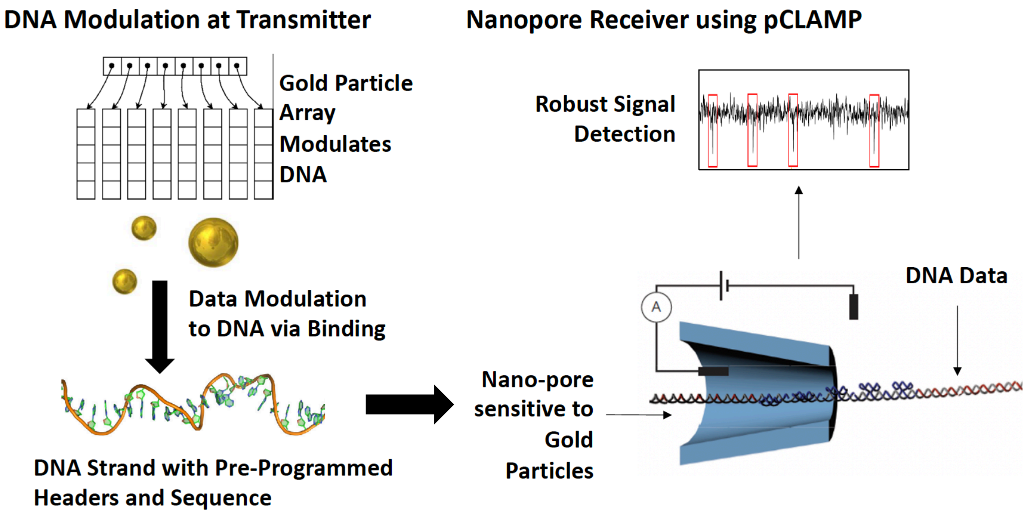

Fig. 3. DNA encoding using gold particles as conducting modulation bits at transmitter, which can be read as a DNA ”bar code” at receiver.

encoding information in biological macro-molecules, or DNA strands. Transmission of digital information can be achieved in a number of ways:

- Direct encoding: information can be directly expressed into DNA strands, with (1) redundancies expressed via overlapping segments and parity check for error correction, and (2) indexing to enable strands to avoid block level transposition errors. RNA, whilst a potential candidate, is less stable than DNA so not the best choice in this context. There are also carbohydrate chain examples, which can be configured to have recognisable header data, as well as stable storage data chemicals.
- Electrical encoding: information can be modulated through highly conductive particles attached to the DNA strand - see Figure3. A nanopore can read the DNA as a OOK modulated barcode [8]. This can enable high capacity molecular communication [9].

One critical challenge highlighted in Figure3 is the need for blind signal processing, whereby a number of complex processes can cause signal distortion in the channel: (1) the fluid dynamic channel is non-reversible (e.g., a reverse pilot signal cannot estimate the channel properties), (2) DNA strands may structurally wrap itself during transport causing decoding issues, (3) physical encoding can fail at transmitter. As such, it is necessary to develop blind signal processing techniques that either use high-dimension feature embedding [10] with transformed space/coordinate methods, and stochastic resonance [11] methods.

Another challenge in real-world deployment is that DNA is rarely, if ever sent in nature as a form of information carrier, because it cannot survive in a bacteria rich environment. Physical protection, a synthetic wrapper or cells will be necessary for their replication, but of course these hosts are not free from mutations (other engineered encapsulation approaches are being tested). However, there is recent evidence that mentions stable storage in bacterial cells. In many of these cases, some of our discussion is based on what biology can achieve, whilst what we want to highlight is what engineering systems can be built to achieve this, e.g., these systems can interact and integrate in a real engineering environment.

III. DEFENCE & SECURITIES APPLICATIONS

A. *Search & Rescue in Deep Ocean*

One key application for molecular communication is deep ocean long distance localization for search and rescue applications. This hidden transmitter and missing receiver (HTMR) problem was first articulated in [12], inspired by the MH370 disaster and other submarine disasters. Compared with acoustic wave-based signals from the black box, molecular information does not lose energy as rapidly with distance. It can be seen that acoustic wave energy not only decay more rapidly with distance, but also aggressively with frequency. There are several challenges in ocean scale MC:

- Vertical communication with dynamic mixing: we may wish to communicate vertically through layers of ocean with varying densities and viscosity values due to differential heating from the sun and stratified gravity currents. As discussed previously, the entrainment process tells us that the degree to which the signal will be mixed into the ocean and limit to the achievable capacity. We also know that if the receiver is misaligned with the transmitter, then the concentration will diminish due to the Morton entrainment process.
- Localization in stochastic gradients: the challenge is that the ocean currents generate stochastic drifts that leads to a *rough and time-varying gradient ascent localization problem*. As such, we developed a Rosenbrock gradient ascent algorithm, whereby a wait function and an adaptive sampling process are used to overcome stochastic changes in the molecular signal gradient in ocean environments. We are able to achieve long range detection of DNA encoded messages using the methods discussed previously in [8].

Despite these challenges, we believe MC still presents interesting opportunities for delay-tolerant low data rate messaging in ocean spaces, especially when the range of acoustic and optical systems remains low and prone to detection.

B. *Covert Messaging*

Wireless messaging in complex environments such as mazes and tunnel networks is prevalent in defence and security environments. Unmanned Autonomous Systems (UAS) scouting enemy tunnel networks and rescuing under rubble in post earthquake scenarios are some examples, where EM and acoustic waves would suffer heavy absorption and diffraction loss. Molecular signals have been demonstrated to be able to robustly transverse complex tunnel / pipe networks, as well as overcome complex obstacles without any loss to signal shape.

Covert messaging is crucial for a number of security and military applications. In hostile environments, the airwaves are fully jammed or monitored, risking interception. Biological messages represents a technology leap, where we can send highly directional messages via invisible vortex rings [6], whereby self-sustaining structures loaded with molecular information can travel long distances whilst being immune to electromagnetic and acoustic interference or eavesdropping (see Fig.2). Another potential advantage of MC is the ability to detect and localize eavesdroppers. In traditional wave based systems, silent eavesdroppers are notoriously difficult to detect and localize. The energy absorbed by eavesdroppers are only detectable from reflected rays in a multi-path environment, and pales compared to the absorption loss from the environment. Conversely, in molecular communications, the data bearing molecules undergo diffusion via random walk propagation, which means that there is a finite probability to travel in an opposite direction without reflection. This property is exploited to detect the silent eavesdropper [13]. This yields an extra layer of security compared to traditional wireless communication.

IV. CYBER-PHYSICAL SYSTEM (CPS) APPLICATIONS

In CPS applications, we primarily discuss two extreme environments that present challenges to conventional EM and acoustic wireless signals. First, in infrastructure health monitoring, ageing infrastructure is a large-scale challenge for many developed countries. Second, in industrial chemical plants, the environment can be hostile to wave based signals due to the excessive heat and radiation noise.

A. *Monitoring Water Distribution Networks (WDN)*

WDN can suffer from a number of critical failures ranging from burst pipes, pressure loss, and contamination. Whilst low-frequency ground-penetrating waves can provide intelligence, detailed data collection require embedded sensors inside the WDN pipes. The key challenge is to extract data out from inside WDN and other similar pipe networks (e.g. natural gas, oil, sewage). WDN tend to be extremely large (millions of junctions stretching over 100,000km). The problem is illustrated in Fig.4, where a contamination occurs at a given node in the WDN. The contaminants quickly spread around the WDN, with varying levels and dynamic response signals.

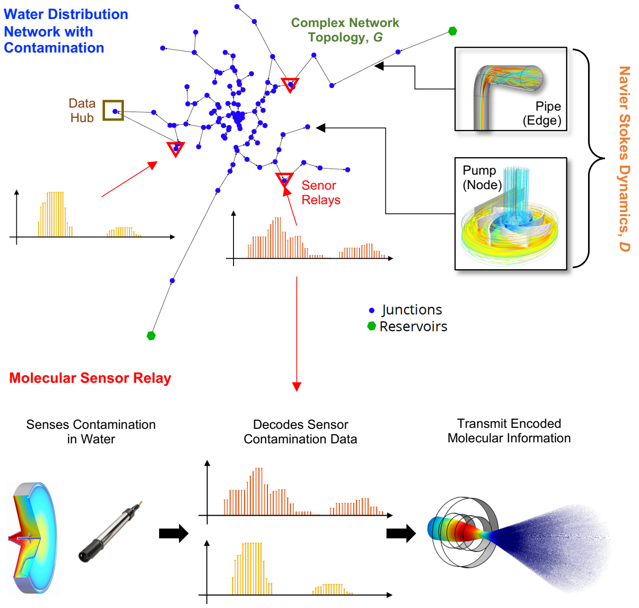

Fig. 4. Monitoring Contamination in Water Distribution Network (WDN) using Molecular Relay Communication. Macro-scale simulations using EPANET2 and micro-simulations using COMSOL with CFD and particle tracing modules.

1) *Relay Network with Navier-Stokes Dynamics:*

MC offers the opportunity to send artificial molecular signals from a number of sensors to a single data hub (see Fig.4 - Relay Channel). This can be formulated into a familiar relay channel, where (see Fig.4):

- The *WDN dynamics* is the *multi-path channel*, where time varying demands and multiple network paths give rise to multiple signals;
- The *contaminant* starts at the *source*;
- The *data hub* is the *destination*, but cannot alone decode the attributes of the source pollutant due to it being too far away and the multi-path loss through the WDN;
- The *MC devices* are the *relays* distributed strategically in the WDN, which can sense the source pollution and transmit an alternative harmless molecular signal to the data hub.

The multiple MC relay devices together enable the destination data hub to understand the pollution dynamics in the WDN.

2) *Relay Placement using Graph Fourier Transform (GFT) Operators:*

The relays should be strategically placed in accordance to the orthogonal components of the WDN (see Fig.4). There are two dimensions to consider in networks such as WDN: 1) the topology of the WDN, and 2) the Navier Stoke (NS) dynamics of water flow (reflected either through PDE function or flow data). As such, each junction node is not only connected to other nodes, but also have multi-dimensional dynamic signals (e.g. concentration, pressure, flow rate). Techniques such as compressed sensing (CS) and GFT operators can transform the WDN dynamics into a sparse matrix that have varying or static sample locations for MC relay deployment:

- Compressed Sensing (e.g. sequential PCA) can reveal the optimal smallest set of dynamic relay locations. However, the location of the relays change at each time step, and therefore a larger set of relays need to be deployed, switching on and off over time.
- Graph Fourier Transform can reveal the optimal smallest set of static relay locations. Whilst the placement is static, it is a larger set than CS at any given time instance.

Both CS and GFT approaches offer a pathway for strategically placed orthogonal relays to detect the contamination/pollution dynamics and transmit MC signals to the destination data hub for analysis (see Fig.4). After which, the relay data can recover the WDN condition at each node [14].

B. Embedded Sensing in Chemical Engineering

In chemical engineering, catalysis is an important step in many reactions. The catalyst bed is a porous medium that chemicals pass through and react with the catalyst bed. Often this is done at high temperature and pressure in the presence of high acoustic and electromagnetic noise. Understanding the rate of reaction, the status of the catalyst bed (depletion and structure), as well as the rate of chemicals passing through the bed is important. Existing methods in industrial sensing including using magnetic particles that can be guided and tracked. However, they do not cope well with complex structures such as porous media. Here, we propose to use molecular signals to both sense the porous media state, track the rate of reaction, and rate of flow. This is achieved by using a reaction-based porous media statistical breakthrough curve [15]. By sending sequential dynamic signals, it is possible to infer the statistical parameters of the porous media catalyst bed.

V. CONCLUSION AND DISCUSSION ON FUTURE 6G

6G and future wireless networks are likely to operate in extreme environments (in addition to current environments). These environments are likely to be extremely: (1) lossy (e.g. absorption), (2) adversarial (e.g. jamming and interception), and (3) incompatible (e.g. due to biological safety or size constraints) to radio-waves. As such, we are motivated to consider molecular communication systems. We divide the application areas across these 3 multi-scale sectors:

- **In-body:** Inside our body, molecular signals can act as coordination commands between sensors that perform synchronized detection and drug delivery (chrono drug delivery). These can achieve coordination between micro-robots at the local scale (microns) to piggy-backing on hormone pathways in blood streams (macro). This realizes the Internet-of-Nano-Things (IoNT) vision, which has already been well articulated [1].
- **Industry:** Complex physical systems that are embedded or exist in challenging environments (e.g. deep underground, deep ocean, high temperature and pressure, high noise, high toxicity), require new cyber-physical systems to monitor their health. When wave based communication fail, we have identified that molecular signals are likely to succeed. They would have to propagate through complex environments involving vast fluid networks, catalyst beds, and be at the mercy of complex biological and chemical reactions. Indeed, this has been proposed for sewage monitoring using molecular communication robots.
- **Defence:** The congested EM battle-space means that new methods of communication is sorely needed, ones that are: (1) immune to EM countermeasures, (2) resilient against eavesdroppers, and (3) can last or persist for long periods in hostile environments. DNA encoded messages living in bacteria satisfies these criteria, and research is underway to explore how this can be utilized on Autonomous Systems for delivering sensitive information.

In summary, the field of molecular communication has picked up pace in the last few years, thanks to the efforts made by the research community. We have worked for 10 years on molecular communications. We have seen how research projects around the world have advanced from simple transpositions of classical communication theory in a mass diffusion setting, towards addressing serious challenges in healthcare, industry, and defence - interfacing biophysics with information theory. Here, in this multi-disciplinary landscape, we find a demand for multi-disciplinary knowledge involving fluid dynamics, synthetic biology, and information theory.

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Jerome Charmet is an associate professor at the University of Warwick. His work is on microfluidics and in particular how to encode information through augmenting organic macro-molecules, including DNA. He received his PhD degree from the University of Cambridge and has worked for more than 10 years in industrial and academic positions.

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Peter Thomas is a full professor at the University of Warwick. He is the head of the Fluid Dynamics Research Centre and works on experimental fluid dynamics, tracking large-scale effects in oceans. His particular expertise lies in particle-laden flows, vortex rings, and granular media.

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