

Molecular Physical Layer for 6G in Wave-Denied Environments

Weisi Guo, Mahmoud Abbaszadeh, Lin Lin, Jerome Charmet, Peter Thomas, Zhuangkun Wei, Bin Li, and Chenglin Zhao

ABSTRACT

The sixth generation (6G) of wireless systems are likely to operate in environments and scales that wireless services have not penetrated effectively. 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. While 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 defense and security, ranging from underwater search and rescue to covert communications; and cyber-physical systems, such as 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 but 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.

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 do not permit the use of wave-based wireless systems. These environments are often embedded (e.g., with lossy channel in fluids), hostile (e.g. with jamming and eavesdroppers), and small (e.g. requiring nanotechnology). Examples include coordinating robots in underground search and rescue, covert messaging in hostile territory, and health monitoring in embedded pipe networks and the human body. Therefore, a new physical layer for 6G wireless is needed; this is recognized publicly by leading industrial leaders in telecommunications, underground critical infrastructure protection, and defence and security.

In response to these emerging challenges, the research community has 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-networks, such as in vivo connectivity for targeted drug delivery and healthcare applications under the umbrella of the 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 but 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 realize its full potential in engineering. Originally proposed as a bio-inspired parallel to cell signaling, MC has been proposed for a wide range of bio-medical applications ranging from targeted drug delivery [1] to opto-genetics. While significant advances have been made to explore the synergy between established radio communication techniques, such as multiple-input multiple-output (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 motivate 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, where 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 article is to first review the rapid recent advances in macro-scale MC, specifically focused on:

1. Encoding and decoding information using chemical and biological macro-molecules
2. Turbulent channel modeling using computational fluid dynamics (CFD)

This already sets this review apart from others, which predominantly focus on nano-/micro-scale applications with diffusion-advection channels.

We then review recent and ongoing work in the application areas of defense and security and cyber-physical systems. This is largely an overview of five years of experimental work (Fig. 1) at the University of Warwick in collaboration with

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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.

In that respect, we are interested in 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.

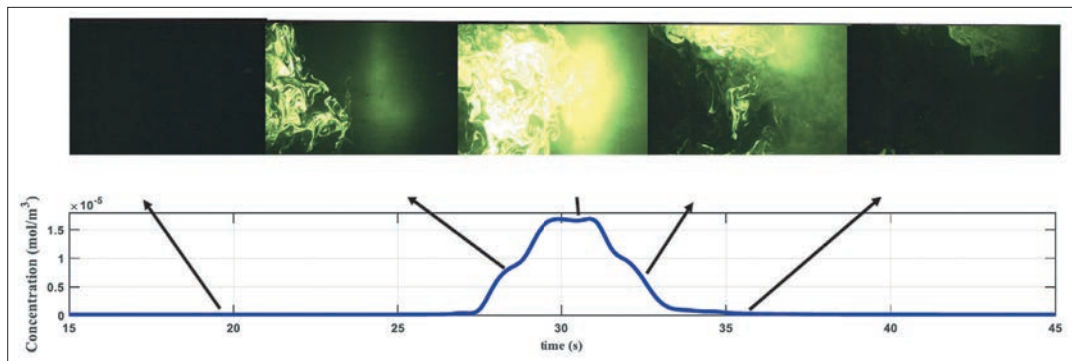


FIGURE 1. Molecular communication lab transforming fluid dynamic knowledge into communication theory; PLIF data extraction: concentration data informs noise characterization and mutual information analysis [3].

Beijing University of Posts and Telecommunications (BUPT) and Tongji University, made possible through four collaborative research grants. We also review work conducted across the world in these areas as well and show 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 dynamics and other traditional engineering areas. We argue that these macro-scale opportunities can join nano-scale healthcare applications to form a new 6G physical layer.

ADVANCES IN MACRO-SCALE MOLECULAR COMMUNICATION

We first detail a work stream in experimentation and analysis, which we show in Fig. 1 (left). We first illustrate channels that 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) that 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 Fig. 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 in different attributes of signals that may serve as more stable and hence better features for encoding data or need novel mechanisms to combat the challenge.

CHANNEL MODELING IN TURBULENCE

Existing research at the nano-/micro-scale channels have predominantly used mass diffusion-advection channel models, assuming operation at low Reynolds number. This is appropriate for many 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 (shear 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.

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 the real world (e.g., underwater rivers and oceans; see applications later in this article), given the dimensionless number match between the scenario and experimentation. The receiver is either:

1. High-speed camera: Images are analyzed for luminescence strength as a proxy for concentration.
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 works have optimized the modulation strategy, which can also improve MI preservation in turbulent channels [4].

Fundamental Transmission Limits: There are 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 recognized 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 scales. Energy is cascaded from the largest scales of motion to successively smaller scales until it is dissipated, due to the action of viscosity, at the smallest length scale, referred to as the Komogorov micro-scale. Experimental studies

addressing issues linked to the fundamental limits of macro-scale MC in the context of this turbulence framework were conducted in [3, 4]. We have investigated underwater, buoyancy-driven vertical macro-scale MC 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 addressed 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, the forward velocity, which we know is important for symbol coherence, is reduced laterally by how far one detects outside the bore-sight.

Breaking the Limits Using Vortex Rings: While there are fundamental limits to how far an MC signal puff can travel before it mixes with the atmosphere and the momentum and signal structure is lost (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 inter-symbol interference (ISI) (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-interference ratio (SIR) is two orders of magnitude higher over conventional puffs. The results point toward a promising pathway for higher-capacity channels.

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 that 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. While 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.

Chemical Encoding and Decoding: Transmission of chemically coded information via an odor 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

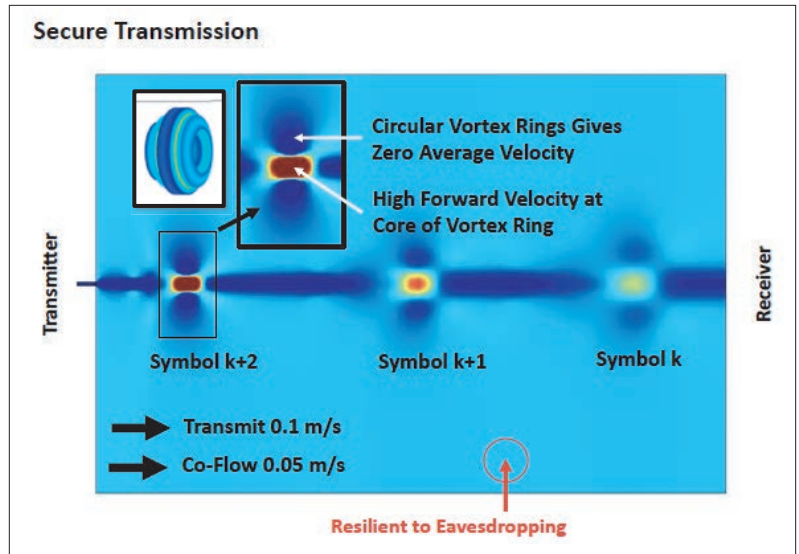


FIGURE 2. Secure molecular vortex rings [6].

the first time, scalable chemical encoding in MC. Information can be modulated onto 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 without 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), enabling 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 three to six 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 has made it possible to map their sites and structures. Unlike DNA and peptides (see below), they can polymerize in more than one dimension as glycosidic linkages can be formed between multiple sites of monosaccharides, making a specific polysaccharide structure extremely difficult to synthesize 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 to exploit the reactivity of the chemical messenger to achieve a stable signal at the receiver [7]
2. Carbon nano-particles to achieve low drag molecular propagation for sharper signals

Biochemical DNA Encoding and Decoding: DNA storage has been shown to offer significant

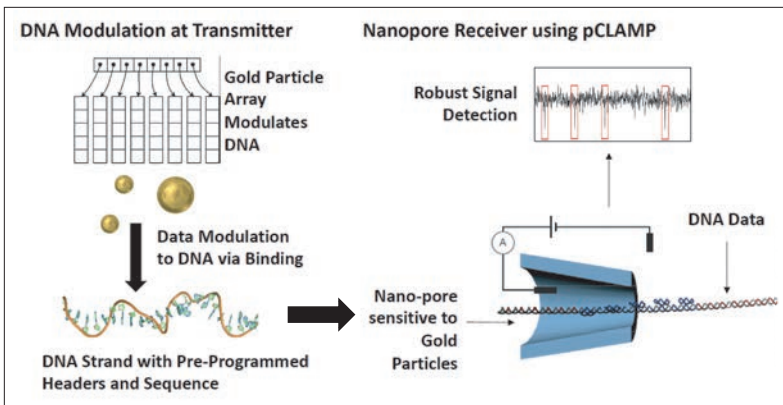


FIGURE 3. DNA encoding using gold particles as conducting modulation bits at the transmitter, which can be read as a DNA "bar code" at the receiver.

advantages over electrical and magnetic storage in terms of cost efficiency for either large file sizes or long-term storage. Current technology can achieve megabits of reliable information storage with less than 1 percent 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 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
 2. Indexing to enable strands to avoid block-level transposition errors
- RNA, while a potential candidate, is less stable than DNA and hence not the best choice in this context. There are also carbohydrate chain examples, which can be configured to have recognizable header data, as well as stable storage data chemicals.
- Electrical encoding: Information can be modulated through highly conductive particles attached to the DNA strand (Fig. 3). A nanopore can read the DNA as an on-off keying (OOK) modulated barcode [8]. This can enable high-capacity molecular communication [9].

One critical challenge highlighted in Fig. 3 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 themselves during transport, causing decoding issues.
3. Physical encoding can fail at the transmitter. As such, it is necessary to develop blind signal processing techniques that 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, while what we want to highlight is which engineering systems can be built to achieve this. For example, these systems can interact and integrate in a real engineering environment.

DEFENCE AND SECURITIES APPLICATIONS

SEARCH AND RESCUE IN DEEP OCEAN

One key application for MC 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 to 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 decays 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 the limit to the achievable capacity. We also know that if the receiver is misaligned with the transmitter, the concentration will diminish due to the Morton entrainment process.
- Localization in stochastic gradients: The challenge is that the ocean currents generate stochastic drifts, which 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.

COVERT MESSAGING

Wireless messaging in complex environments such as mazes and tunnel networks is prevalent in defence and security environments. Unmanned autonomous systems (UASs) scouting enemy tunnel networks and rescuing under rubble in post-earthquake scenarios are some examples, where electromagnetic (EM) and acoustic waves 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 represent 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 while being immune to EM and acoustic interference or eavesdropping (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 in comparison to the absorption loss from the environment. Conversely, in MC, the data bearing molecules undergo diffusion via random walk propagation, which means that there is a finite probability to travel in the 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.

CYBER-PHYSICAL SYSTEM APPLICATIONS

In cyber-physical system (CPS) applications, we primarily discuss two extreme environments that present challenges to conventional EM and acoustic wireless signals. First, in infrastructure health monitoring, aging 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 excessive heat and radiation noise.

MONITORING WATER DISTRIBUTION NETWORKS

Water distribution networks (WDNs) can suffer from a number of critical failures ranging from burst pipes, pressure loss, and contamination. While low-frequency ground-penetrating waves can provide intelligence, detailed data collection requires embedded sensors inside the WDN pipes. The key challenge is to extract data out from inside WDNs and other similar pipe networks (e.g., natural gas, oil, sewage). WDNs tend to be extremely large (millions of junctions stretching over 100,000 km). 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.

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 (relay channel, Fig. 4). This can be formulated into a familiar relay channel, where (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 its distance and the multi-path loss through the WDN.

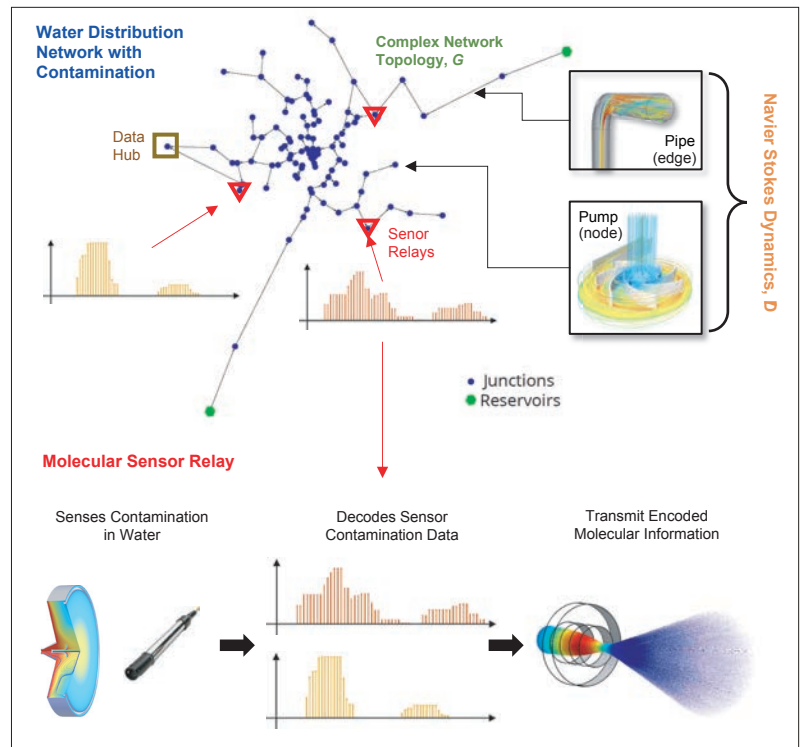


FIGURE 4. Monitoring contamination in a water distribution network (WDN) using molecular relay communication. Macro-scale simulations using EPANET2 and micro-simulations using COMSOL with CFD and particle tracing modules.

- 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.

Relay Placement Using Graph Fourier Transform (GFT) Operators: The relays should be strategically placed in accordance to the orthogonal components of the WDN (Fig. 4). There are two dimensions to consider in networks such as WDN:

1. The topology of the WDN
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 has 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 has 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.
- GFT can reveal the optimal smallest set of static relay locations. While 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 trans-

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mit MC signals to the destination data hub for analysis (Fig. 4). After that, the relay data can recover the WDN condition at each node [14].

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 EM 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 include 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, and 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.

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)
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 three 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 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 fails, we have identified that molecular signals are likely to succeed. They would have to propagate through complex environments involving vast fluid networks and 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
 3. Can last or persist for long periods in hostile environments

DNA encoded messages living in bacteria satisfy 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, toward 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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BIOGRAPHIES

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CHENGLIN ZHAO received the Bachelor's degree from Tianjin University in 1986, and the Master's degree from Beijing University of Posts and Telecommunications (BUPT) in 1993, and the Ph.D. degree from Beijing University of Posts and Telecommunications, in 1997. At present, he serves as a Professor in Beijing University of Posts and Telecommunications, Beijing, China. His research is focused on emerging technologies of short-range wireless communication, cognitive radios, 60GHz millimeter-wave communications