Experimental Results on the Open-Air Transmission of Macro-Molecular Communication using Membrane Inlet Mass Spectrometry

Daniel Tunç McGuiness, Stamatios Giannoukos, Alan Marshall, *Senior Member, IEEE* and Stephen Taylor

***Abstract*—Molecular communication (MC) is a method where the transmission of information involves the use of molecules rather than electromagnetic (EM) waves. In this paper an open-air transmission MC experiment is conducted to study signal behavior and the noise. A mass spectrometer is used as the detector and an in-house-built odor generator is used as transmitter. It is shown that the signal amplitude loss of the signal can be modelled by using advection-diffusion with decay equation. In addition, the noise of the system has shown to have similar characteristics to that of additive white Gaussian noise (AWGN).**

***Index Terms*—Molecular Communication; Mass Spectrometry; Open-air Transmission**

I. INTRODUCTION

TRANSMISSION of information using chemicals, Molecular Communication (MC), has been utilized by nature for many years [1]. However, as this communication can involve both very small scales (intercellular, DNA etc.) and large scales (bees, eels [2]), MC can be classified based on the transmission distance: micro- and macro-scale.

The first study of MC was done in the micro-scale, which can be defined as a system within the transmission range of nm - μm [3]. The antennae size poses a significant problem when shrinking an EM-based system to the micro-scale [4], and because of this, MC has been shown to be a good alternative for micro-scales. There have been numerous studies in micro-scale, such as transmission using diffusion [5], modulation [6] and channel capacity [7].

Using MC at the macro-scale (cm - m) [8] is a relatively new field of study compared to micro-scale. There have been a few practical [9]–[13] and theoretical [14] studies, which has shown the possibility macro-scale molecular communications. There are areas in which the use of macro-scale communications can be a better choice compare to EM. In [15] it was shown that signal attenuation per unit length in a copper pipe for MC was less than EM. There are several applications of macro-scale communications, such as infrastructure monitoring [16], a tool for studying biological communications [2] and odor transmission using digital media [17].

As mentioned, macro-scale MC is a new field with relatively few experimental studies done [10]–[13]. Some of the important aspects of communication systems; noise analysis, signal energy and signal amplitude analysis of open environment transmission have yet to be studied.

In this study the open-air transmission and the noise analysis of MC is investigated at the macro-scale. In the experiment, an in-house-built gas generator and a quadrupole mass analyzer were used. Noise analysis were undertaken and it is shown that the loss in signal amplitude and signal energy over distance can be modelled using advection-diffusion equation (ADE) with decay. The results show that the amplitude of the transmitted signal experiences a non-linear attenuation that differs significantly from EM-wave propagation channels.

II. EXPERIMENTAL SETUP

In order to test the open-air transmission of MC, two devices were employed. The generation and transmission of chemicals based on a message was made using an in-house-built odor generator [18], [19], and the detection of the chemical was made with a membrane inlet mass spectrometer (MIMS) having a quadrupole mass analyzer (QMA) [12], [18]. A QMA is an instrument capable of analyzing and distinguishing charged ions or sample molecules by their motion in an applied electric field. The analyzer of the MS allows the detection of ions with a particular mass-to-charge (m/z) ratio [12], [18], making it a useful tool for use in MC. The details of the experiment can be seen in [12], [18] with the major difference is the difference of the medium whereby the transmission environment is open space instead of a cylindrical pipe. The diagram for the experimental setup can be seen in Figure 1.

In this study, the open-air transmission of macro-MC is conducted. Here, open-air transmission, is defined as a boundary-less area where the space between the transmitter and the receiver is open to outside interference and not protected by a medium. This makes it challenging for the system as small disturbances from the ambient environment, in addition to the unwanted diffusion of the transmitted signal flow, can cause problems in retrieving the signal and the unguided medium can see a sudden shift in the concentration, producing lower signal amplitude and energy values with increasing distance. The parameters of the experiment are given in Table I.

III. MOLECULAR TRANSMISSION

Molecular propagation in a medium can be explained using the general convection-diffusion equation is shown below [20];

The research was funded from the Engineering and Physical Sciences Research Council (EPSRC) under the grant agreement: EP/M029425/1 'Creating a Stink - Investigating Olfactory Transport Streams'.

The authors are with the Department of Electrical Engineering & Electronics, University of Liverpool, L69 3GJ, UK (emails: danielmc@liverpool.ac.uk, stamgian@liverpool.ac.uk, alanm@liverpool.ac.uk, S.Taylor@liv.ac.uk)

Corresponding author: Daniel Tunç McGuiness

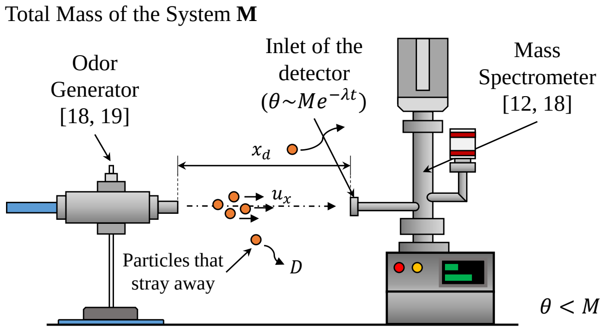

Fig. 1. A Diagram of the Experimental setup. The mass is transmitted from the odor generator (M) and sent through the open medium. Due to the nature of particle movements such as Brownian motion (D), some particles will stray from the sight of the detector. Because of this effect the amount of particles that are captured (θ) will be less than the particles that were introduced ($\theta < M$). Therefore a decay term (λ) is used to simulate this straying effect.

TABLE I
EXPERIMENTAL PARAMETERS

Parameter	Symbol	Value	Unit
Signal flow (Acetone)	q	8	ml/min
Tracked signal flow ion	m/z	43	Da
Carrier flow	Q	750	ml/min
Bit and Flush Duration	t_{bit}	60	s
Flush Duration	t_{flush}	60	s
Acetone detection time [18]	t_{d}	15	s
Carrier flow pressure	P_F	1	bar
Environment pressure	P	1.008 ± 0.002	bar
Environment temperature	K	293.5 ± 0.2	K
Diffusivity of Acetone in Air	D	0.124	cm^2/s

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C) - \nabla \cdot (\mathbf{u}C) + R \tag{1}$$

Where C is the concentration of the transferred gas (kg/m^3), D is the coefficient of diffusivity (m^2/s), $\mathbf{u}$ is the velocity vector (m/s), R is the source or sink of the system. However, because the system is has no defined boundary (i.e. pipe), the amount introduced by the system will not be equal to the amount detected by the receiver since some amount of particles will stray away from the path of the detector. This property can be modelled by introducing a sink ($R = -\lambda C$) to the equation. Since the transmission of information occurs in one-dimensional space (x-direction) and relative to the transmission distance (x) the area of the detector inlet is negligible and therefore can be considered a point in space, the 1-D equation can be simplified into;

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - u_x\frac{\partial C}{\partial x} - \lambda C \tag{2}$$

Where λ is the decay parameter of the function. The prototypical solution ($C(x = 0,\, t = 0) = M\delta(x)$) to the given expression in Eq. (2) is given in Eq. (3).

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-u_x t)^2}{4Dt} - \lambda t\right) \tag{3}$$

Where M is the amount of particles injected into the system (kg). The equation above represents the concentration of the introduced sample in a given time and space. By integrating the concentration function with respect to distance the particles that are present in the environment can be calculated. To calculate the chemicals absorbed by the detector, the integration function is substracted from the injected mass [14].

$$\theta(x,t) = M - \int_{-x_\epsilon}^{x_d} C(x,t)dx \tag{4}$$

Where x_d is the distance from the detector to the origin point and x_ϵ is the distance that particles travel against the flow. The solution to the above Eq. (4) for open distance transmission with decay is given in Eq. (5).

$$\theta_1(x,t) = M\exp(-\lambda t) \left[1 - \frac{1}{2}\left[\text{erf}\left(\frac{x_d - u_x t}{2\sqrt{Dt}}\right) + \text{erf}\left(\frac{x_\epsilon + u_x t}{2\sqrt{Dt}}\right)\right]\right] \tag{5}$$

The chemicals that are absorbed by the system (θ_1) in a given period of T is given in Eq. (6).

$$M_R = \theta_1(x, t = T) - \theta_1(x, t = 0) \tag{6}$$

Therefore, the removal of chemicals from the detector (θ_0) to the outside environment can be expressed by the following Eq. (7).

$$\theta_0(x,t) = M_R\exp(-\lambda t) \frac{1}{2}\left[\text{erf}\left(\frac{x_d - u_x t}{2\sqrt{Dt}}\right) + \text{erf}\left(\frac{x_\epsilon + u_x t}{2\sqrt{Dt}}\right)\right] \tag{7}$$

As can be seen from Eq (5) and (7) the mass parameter is different in each equation: former being the mass injected into the system (M) and the latter is the mass that is absorbed by the detector (M_R). This process of introduction/removal of particles can be seen in detail in [13]. To model the detrimental effects of open air transmission, the decay parameter (λ) with respect to transmission distance (x) is approximated using a power equation with a and b being fitting parameters [21], [22]. The parameters of the decay equation (a, b) can be influenced by numerous parameters, such as the temperature and the pressure of the environment, particles and eddies present in the transmission medium.

$$\lambda(x) = ax^b \quad a = 6.743 \times 10^{-5} \quad b = 2.616 \tag{8}$$

IV. RESULTS

A. Noise Analysis

To analyze the noise, the detector was left monitoring to the background noise. The background noise of the system can be caused by numerous parameters such as leftover chemicals within the MS vacuum chamber, pressure differences in the inlet of the MS or ambient chemicals in the air that produce a similar m/z ratio to the m/z ratio value of the signal chemical. The cumulative density function (cdf) of the observed

This article has been accepted for publication in a future issue of this journal, but has not been fully edited. Content may change prior to final publication. Citation information: DOI 10.1109/LCOMM.2018.2875445, IEEE Communications Letters

background noise can be seen in Figure 2 and to quantify the fitting of the distribution $F(x)$ to the empirical CDF $F_n(x)$ Kolmogorov-Smirnov test is used.

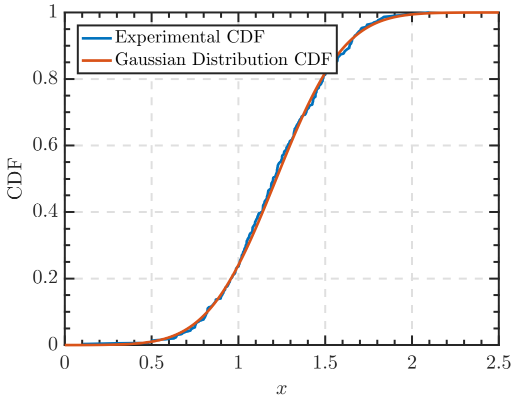

Fig. 2. Cumulative density function (CDF) of the noise from empirical data along with a Gaussian CDF fit (μ = 1.21, σ^2 = 0.096, D_n = 0.0284)

$$D_n = \sup_x |F_n(x) - F(x)| \tag{9}$$

As can be seen from the distribution fit of data, the results strongly suggest a Gaussian distribution for the noise in the system. Aside from having a DC offset value (caused by the particles present in the environment), the noise is behaving as white noise, where there is no dominant frequency component. Therefore, in a macro-scale molecular communication with a MIMS as a detector, the model of the noise can be defined as AWGN $\mathcal{N}(\mu, \sigma^2)$.

B. Open-air Transmission

The experiment was conducted by varying the transmission distance (x) from 2.5 cm to 15.0 cm. The transmission of the signal starts with 60s of flush (t_f). This is done by sending only the carrier flow (Q) and is used to clean up the sensor from the leftover chemicals by the signal flow (q). This is followed by a 60s pulse (t_bit) of chemicals ($Q + q$) and finally 60s of flush (Q) at the end of the experiment. Each transmission experiment was repeated 3 times and the average values of the experiments are taken.

To model the system, the equation derived in Section III are used. It is assumed that the noise is AWGN and present at the receiver. The results of the open-air transmission with comparison to the theoretical model can be seen in Figure 3 and the amplitude values compared to theoretical values for each distance in Figure 4. As it can be seen in Figures 3 and 4, the model shows agreement with experimental results. However, it should be noted that as distance increases the fluctuation in the signal sees a noticeable increase which can be seen in Figure 3 (e) and (f). It can also be seen that in the distance of 15 cm (Figure 3 (f)) the fluctuations caused by the noise start playing a bigger role in the signal which causes a decrease in the accuracy of the model.

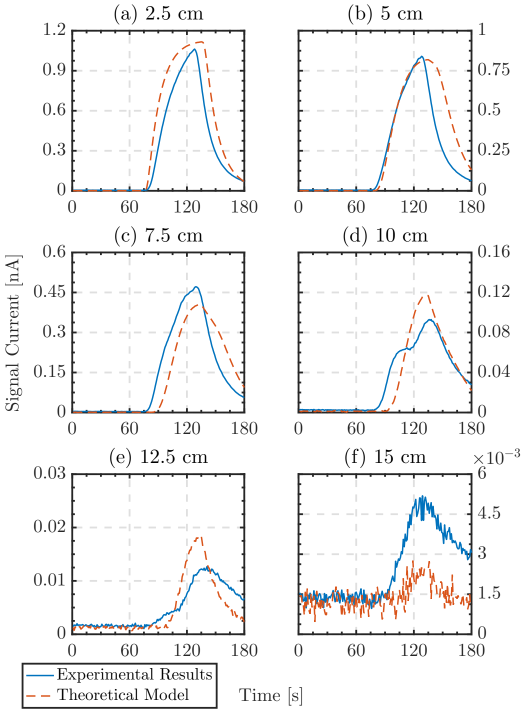

Fig. 3. Experimental results of the open-air transmission study along with comparison to the Theoretical model (u_x = 0.18 cm/s, D = 0.15 cm^2/s, M = 1.2 ng, T = 60 s, $x_\epsilon = x_d$)

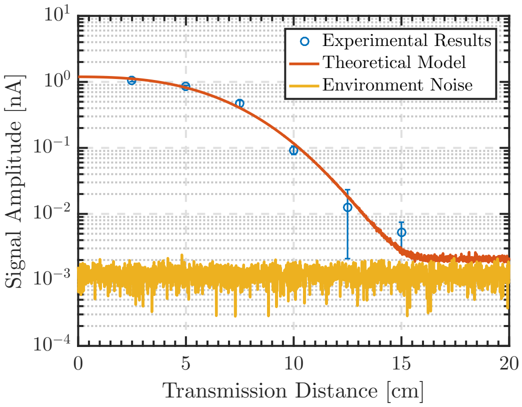

Fig. 4. Comparison of the maximum signal amplitude of the transmitted signal and the values generated by the theoretical model (u_x = 0.18 cm/s, D = 0.15 cm^2/s, M = 1.2 ng, T = 60s, ρ = 0.9961, $x_\epsilon = x_d$)

The signal sees increased distortion as the distance is increased. This distortion and the loss in the amplitude are due to outside interferences affecting the transmission (particle collisions in the medium or the diffusive properties causing the chemicals to miss the detector). When the transmission distance is increased further than 10 cm, the amplitudes of the retrieved signals are measured as 12.7×10^{-12} and 5.2×10^{-12} A for 12.5 cm and 15 cm respectively which compared to amplitude at 2.5 cm, 1.06×10^{-9} A is close to two orders or magnitude lower.

C. Signal Energy

Since a MS detects the samples introduced into the system by ionizing the samples and measuring the current from the ions hitting a detector, the energy of the transmitted signal (ϕ) is calculated as follows;

$$\phi_\gamma(x,t) = \int_{-\infty}^{+\infty} |\theta_\gamma(x,t)|^2 dt \quad \gamma = \{0,1\}$$

$$\phi(x) = \int_{t_{\text{flush}}}^{t_{\text{flush}}+t_{\text{bit}}} |\theta_1(x,t)|^2 dt + \int_{t_{\text{flush}}+t_{\text{bit}}}^{2t_{\text{flush}}+t_{\text{bit}}} |\theta_0(x,t)|^2 dt \tag{10}$$

Based on Eq. (10), the energy of the transmitted signal is calculated numerically and the comparison can be seen in Figure 5. As it can be seen, the theoretical model shows agreement to the experimental results and shows a non-linear behaviour as distance increases. It must also be noted that after a certain amount of distance ($x > 15$ cm) the energy of the transmitted signal dissipates and only the energy produced by the noise (N_0) remains which can be seen in Figure 5. Unlike an EM system where N_0 is defined as W/Hz, in molecular communications it can be defined as W/chemical or W/ion.

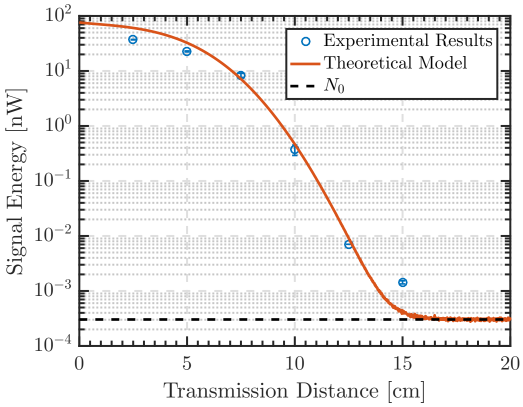

Fig. 5. Comparison of signal energy from experimental results with numerical results of the theoretical model (u_x = 0.18 cm/s, D = 0.15 cm^2/s, M = 1.2 ng, T = 60s, ρ = 0.9933, $x_\epsilon = x_d$)

V. CONCLUSION

An experiment was conducted to analyze the effects on a MC in an open-air environment. To generate the chemicals and the pulses of gas based on a given piece of information, an in-house built gas generator was used, and for detection of chemicals a MIMS is utilized. A noise analysis conducted on the system shows that the noise of the system exhibits a Gaussian distribution with equal intensity in frequency domain. The open-air experiment shows that the system, with MIMS as the receiver, can be modelled by using ADE with decay parameter (λ). However, the generality of the equation makes it possible for the model to be adaptable to system with different sensors that measure particles by absorption. The experiments along with the model shows that both signal amplitude and signal energy follows a nonlinear attenuation as distance increases and the decay parameter follows an exponential increase. This shows that the energy losses of the signal are higher that an EM system where the losses are inverse square proportional with the transmission distance.

REFERENCES

[1] T. D. Wyatt, *Pheromones and animal behaviour: communication by smell and taste*. Cambridge university press, 2003.
[2] W. C. Agosta, *Chemical communication: the language of pheromones*. Henry Holt and Company, 1992.
[3] T. Nakano, A. W. Eckford, and T. Haraguchi, *Molecular communication*. Cambridge University Press, 2013.
[4] N. Farsad, H. B. Yilmaz, A. Eckford, C.-B. Chae, and W. Guo, "A comprehensive survey of recent advancements in molecular communication," *IEEE Communications Surveys & Tutorials*, vol. 18, no. 3, pp. 1887–1919, 2016.
[5] S. Hiyama, Y. Moritani, T. Suda, R. Egashira, A. Enomoto, M. Moore, and T. Nakano, "Molecular communication," *Journal-Institute of Electronics Information and Communication Engineers*, vol. 89, no. 2, p. 162, 2006.
[6] M. S. Kuran, H. B. Yilmaz, T. Tugcu, and I. F. Akyildiz, "Modulation techniques for communication via diffusion in nanonetworks," in *Communications (ICC), 2011 IEEE International Conference on*. IEEE, 2011, pp. 1–5.
[7] N. Farsad, Y. Murin, A. Eckford, and A. Goldsmith, "On the capacity of diffusion-based molecular timing channels," in *Information Theory (ISIT), 2016 IEEE International Symposium on*. IEEE, 2016, pp. 1023–1027.
[8] L. P. Giné and I. F. Akyildiz, "Molecular communication options for long range nanonetworks," *Computer Networks*, vol. 53, no. 16, pp. 2753–2766, 2009.
[9] N. Farsad, W. Guo, and A. W. Eckford, "Tabletop molecular communication: Text messages through chemical signals," *PloS one*, vol. 8, no. 12, p. e82935, 2013.
[10] N. Farsad, D. Pan, and A. Goldsmith, "A novel experimental platform for in-vessel multi-chemical molecular communications," in *GLOBECOM 2017-2017 IEEE Global Communications Conference*. IEEE, 2017, pp. 1–6.
[11] H. Unterweger, J. Kirchner, W. Wicke, A. Ahmadzadeh, D. Ahmed, V. Jamali, C. Alexiou, G. Fischer, and R. Schober, "Experimental molecular communication testbed based on magnetic nanoparticles in duct flow," *arXiv preprint arXiv:1803.06990*, 2018.
[12] S. Giannoukos, D. Tunç McGuiness, A. Marshall, J. Smith, and S. Taylor, "A chemical alphabet for macromolecular communications." *Analytical chemistry*, 2018.
[13] D. T. McGuiness, S. Giannoukos, A. Marshall, and S. Taylor, "Parameter analysis in macro-scale molecular communications using advection-diffusion," *IEEE Access*, 2018.
[14] S. Wang, W. Guo, S. Qiu, and M. D. McDonnell, "Performance of macro-scale molecular communications with sensor cleanse time," in *Telecommunications (ICT), 2014 21st International Conference on*. IEEE, 2014, pp. 363–368.
[15] W. Guo, C. Mias, N. Farsad, and J.-L. Wu, "Molecular versus electromagnetic wave propagation loss in macro-scale environments," *IEEE Transactions on Molecular, Biological and Multi-Scale Communications*, vol. 1, no. 1, pp. 18–25, 2015.
[16] F. Stajano, N. Hoult, I. Wassell, P. Bennett, C. Middleton, and K. Soga, "Smart bridges, smart tunnels: Transforming wireless sensor networks from research prototypes into robust engineering infrastructure," *Ad Hoc Networks*, vol. 8, no. 8, pp. 872–888, 2010.
[17] R. C. Araneda, A. D. Kini, and S. Firestein, "The molecular receptive range of an odorant receptor," *Nature neuroscience*, vol. 3, no. 12, p. 1248, 2000.
[18] S. Giannoukos, A. Marshall, S. Taylor, and J. Smith, "Molecular communication over gas stream channels using portable mass spectrometry," *Journal of The American Society for Mass Spectrometry*, vol. 28, no. 11, pp. 2371–2383, 2017.
[19] M. Statheropoulos, G. Pallis, K. Mikedi, S. Giannoukos, A. Agapiou, A. Pappa, A. Cole, W. Vautz, and C. P. Thomas, "Dynamic vapor generator that simulates transient odor emissions of victims entrapped in the voids of collapsed buildings," *Analytical chemistry*, vol. 86, no. 8, pp. 3887–3894, 2014.
[20] C. E. Baukal Jr, V. Gershtein, and X. J. Li, *Computational fluid dynamics in industrial combustion*. CRC press, 2000.
[21] J. M. Stockie, "The mathematics of atmospheric dispersion modeling," *Siam Review*, vol. 53, no. 2, pp. 349–372, 2011.
[22] M. Çağlar, "Velocity fields with power-law spectra for modeling turbulent flows," *Applied mathematical modelling*, vol. 31, no. 9, pp. 1934–1946, 2007.