On the Effect of Flow and Degradation on Hitting Rate of Mobile Nano Sensors in Diffusive Molecular Communication Systems

GAURAV SHARMA

Department of Electrical and Electronics Engineering Atal Bihari Vajpayee Indian Institute of Information Technology and Management Gwalior, Madhya Pradesh, 474015

INDIA

Abstract: In the paper, an analysis regarding the effect of drift and molecular degradation on the average number of molecules received at the fusion center (FC) for a diffusive log-normal molecular communication (MC) system is undertaken. The effect of drift and molecular degradation simultaneously on molecular reception has not been examined exhaustively in MC literature. Therefore, by utilizing the log-normal distribution of the number of molecules hitting FC, we calculated the closed-form expressions for the average number of molecules received in a drift and molecular degradation-free scenario. Subsequently, we also analytically calculated the closed-form expressions for the average number of molecules received at FC for a drift-only scenario, and a drift with molecular degradation scenario, respectively. Numerical results highlight lower average molecular receptions at FC when the transmission media neither experiences drift nor molecular degradation. The drift introduction in the molecular degradation-free system significantly increases the average molecular receptions at FC. On the contrary, with the simultaneous introduction of molecular degradation, the average number of molecular receptions at FC is significantly higher. Finally, all the numerical results corroborate the derived analytical findings.

Key-Words: Biomarkers, diffusive molecular communication, drift, fusion-center, log-normal molecular channel, mobile nano-sensors, molecular degradation.

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1 Introduction

Molecular communication (MC) is a natureinspired communication phenomenon, where the information transfer from transmitting nanomachine to receiving nanomachine is accomplished through molecules [1]. The information transfer between transmitter and receiver through chemical exchange makes the MC link highly reliable in environments where conventional electromagnetic (EM) spectrum-based cannot provide reliable communication [2], [3]. In the last decade, the MC systems have experienced steady growth, wherein numerous synthetic MC-based systems have been proposed with the primary objective of observing, analysing, and interpreting the communication process at the nanoscale [4]. Unlike conventional communication systems, where the EM spectrum is utilized in MC modulation is accomplished by utilizing certain physical characteristic features such as concentration [5], type [6], or time of release [7]. In addition to the information modulation, in MC, the molecular propagation from the source towards the destination is achieved through pure diffusion, drift, molecular motors, etc. [8], [9]. The diffusive MC systems are widely employed

because of their practical implementation and economical energy requirement in the shipment of the information molecules between source and destination. However, to facilitate the movement of information molecules, in recent times, diffusion processes along with drift mechanisms are being utilized for information propagation from transmitter to receiver [8].

The favoured attribute of MC lies in its installation in the biochemical and biophysical applications [8]. Therefore, many nano-scale networks have been developed primarily to expedite the revolutionary applications in health care and biomedical fields [10]. Out of these approaches, some of the most widespread entities widely employed in biomedical applications are the Mobile Nano-Sensors (MNSs) [11]. The rapid advancements in nanotechnology have encouraged the deployment of these MNSs in complex environments. One such challenging aspect experienced in most biomedical and health care scenarios is the problem of early and timely detection of abnormalities, especially cancer inside the human cardiovascular system [12]. Therefore, systems that can identify the presence of an anomaly become imperative to em-

ployment.

Nowadays, the MNSs play a pivotal role in nanomedicine and target drug delivery systems as they are majorly hired for shipping and dispensing imaging probes, therapeutic agents and biological materials to the target locations such as specific organs, tissue, and cells [13]. This inherent feature of the MNSs to smartly release, move, observe and read the anomaly inside the cardiovascular system fosters the utilization of MNSs as a potential candidate for anomaly detection. The MNSs are injected into the human circulatory system with the help of an injection. These MNSs navigate to the target site with the assistance of the bloodstream (having a defined flow) [14] and activate themselves wherever there is a high concentration of the biomarkers. After interaction with the biomarkers, these MNSs are eventually transformed into secondary (Type C) molecules, ultimately absorbed at the fusion center (FC). The Type C molecules, on reaching the FC exhibit log-normal distribution.

In MC literature, for any real-world physical process, channel modeling is done by assuming the Gaussian behaviour of the system. However, many practical phenomena are analytically measured using various skewed distributions. The skewed distributions are usually employed for low average values, with higher variances, and values cannot be negative. For example, for modeling the lengths of latent periods of infectious diseases, the log-normal distributions are employed as such skewed distribution processes often closely fit the log-normal distribution [15]. Further, many practical case scenarios from the medical field also fit the log-normal distributions [16].

Since log-normal distribution is one of the bestsuited distributions for modeling in vivo channel behaviour, in this manuscript, we have assumed the distribution of secondary (Type C) molecules to exhibit log-normal distribution. To the best of our knowledge, log-normal channel behaviour has not been reported anywhere in the MC literature. The main contributions of this manuscript are as follows:

- To calculate the average number of information molecules reaching the FC, the expression of the Type C (secondary biomarker) molecules exhibiting the log-normal distribution is calculated.
- The closed-form expression of the average number of molecules received at FC when the information molecules experience neither drift (flow velocity) nor molecular degradation in the media is also calculated.

- The closed-form expression for the average number of molecules received at FC is analyt-ically calculated for the scenario when the information molecules experience drift only.
- Lastly, we calculated the closed-form expression for the average number of molecules received at FC in those environments where the information molecules experience both drift and molecular degradation simultaneously.

The rest of the paper has been organized as follows: Section II highlights the current state of the art in MC literature. Section III illustrates the proposed system model used for incorporating the design structures. Section IV depicts the performance analysis of the system model under consideration. Section V discusses the numerical results and the graphical validation of the analysis, and finally, Section VI concludes the manuscript.

2 Related Work

The dearth of relevant research laid the groundwork for carrying out substantial research in diffusive log-normal MC. In [17], the authors highlighted the systems' development that would effectively perform communication at the nano-scale level. Besides, the use of biological entities such as pheromones, light transduction and neurons for long-range communication over long-range nanonetworks was discussed by authors in [3]. Meanwhile, an architectural design of MC systems at a macro-scale level was implemented in [9], wherein static target and mobile nano-sensors were considered. Similarly, in [18], the architectural facet of the nano-networks was discussed, while in [1], an extensive study about the MC systems was carried out. Furthermore, [4] proposed the mathematical modeling for the channel in the diffusive MC scenario, where log-normal distribution was employed for the approximate modeling of the medium. Correspondingly, the characterization of the MNSs in the field of nanochemistry was highlighted in [19] and [11].

In [12], the technique of plasma proteome mining was underlined. However, in [13], a twotier network for abnormality detection was emphasized. Authors in [20] asserted the use of MNSs to disclose cancerous tissues by utilizing the concepts of reaction-diffusion, advection-diffusion, and degradation equations. More substantial work on biomarkers was carried out in [21]. Alternatively, in [14], the authors scripted the usage of multiple biological devices known as cooperative biological nano-machines (CN) to unveil any anomaly inside the Internet of Bio-things (IoBT) system by assuming the mobility of the FC. Simultaneously, the cooperation of molecules that help form a certain critical number of biological particles was highlighted by authors in [22].

Based on the aforementioned literature, one can say that the physical characteristics of the MC channel play a pivotal role in the modeling of MC systems. The role of molecular degradation is significant, especially in molecular biology. In molecular biology, analyzing molecular degradation enables understanding cellular functionality and maintaining cellular hemostasis. Various cellular structures, such as proteasomes and lysosomes, are responsible for the degradation of proteins. Analyzing molecular degradation would facilitate the early detection of various cancers and neurodegenerative diseases. Moreover, in the existing MC literature, flow velocity and molecular degradation effects are studied separately. Further, molecular degradation removes stray molecules from the environment to prevent inter-symbol interference (ISI). However, in many practical biological processes, the collective effect of flow velocity and molecular degradation has severe implications on cellular dynamics. For example, molecular degradation, such as proteolysis, is crucial in regulating proteins' lifetime. So, changes in flow velocity influence the activity and distribution of proteolytic enzymes. Therefore, in this paper, we have tried to calculate the number of molecules received at the receiver while considering the effect of degradation and flow velocity (drift) distinctly and collectively.

3 System Model

The system model for diffusive log-normal MC comprises the cartesian coordinate system confined in a semi-infinite structure. The system model characteristic features are limited to spatial and temporal components of the aqueous environment inside which the MNSs are injected with the help of an injection site. These MNSs (Type A molecules) propagate through the media at constant flow velocity (v_f) . These Type A molecules contact the primary biomarkers secreted by the target cells, and the healthy cells are transformed into Type C molecules. These Type C molecules propagate through the media and are eventually absorbed at the FC. Fig. 1, highlights the pictorial representation of the system model, and the complete diffusive molecular communication environment is based on certain assumptions, given as:

• The whole communication environment functions as spatial and temporal components with aqueous media experiencing no temperature and viscosity changes.



Figure 1: System Model.

- The information molecules are identical, and the transmission time slot is large enough to counter ISI (Inter Symbol Interference).
- The transmission starts at x=0 and t=0, with the FC acting as a fully absorbing receiver, hypersensitive to only Type C molecules.

These assumptions highlight two primary elements (molecular density and molecular flux) of the Fickian theory. The concentration density f(s, t) represents the average number of molecules diffused per unit volume for both the particles (Type A and Type C). The molecular flux (J(s,t)), being a vector component, denotes the average number of diffused molecules crossing a unit cross-sectional area per unit time. MNSs undergoing a reaction with the Type B biomarkers yield Type C molecules. Due to molecular degradation and flow velocity (drift), (v_f), the Type C molecules are received at the FC. Mathematically the molecular degradation as given in [23] is expressed as:

$$C(t) = C_0 e^{-k_d t},$$
 (1)

where C_0 is the initial molecular concentration and k_d is the molecular degradation rate of the environment. In many practical environments, such as in the blood flow mechanism, the MNSs travel by diffusion process and undergo drift and molecular degradation. Therefore, the Type C molecules reaching FC not only arrive because of the degradation process but also undergo drift in the environment. So, for accurate measurement of the average number of molecules received by the FC, it becomes imperative to collectively analyze the effect of drift and molecular degradation in the system. The subsequent section will provide an analytical framework for our system model.

4 Performance Analysis

The mathematical expression which gives the relationship between molecular density f(s, t), and

molecular flux $\Phi(s, t)$ is given as [24]:

$$[f(s, t + dt) * dxdy] - [f(s, t) * dxdy] = [\Phi_x(s, t) * dydz * dt - \Phi_x(s + \vec{x}dx, t) * dydz * dt] + [\Phi_y(s, t) * dxdz * dt - \Phi_y(s + \vec{y}dy, t) * dxdz * dt] + [\Phi_z(s, t) * dxdy * dt - \Phi_z(s + \vec{z}dz, t) * dxdy * dt].$$
(2)

The above expression derived its basis from the fact that: "There is a sense of equality between the average net increase in the number of diffused molecules contained inside a diminutive volume at a specific time and the average net influx of diffused molecules also contained inside the same diminutive volume at the same time". Thus, by putting the differential terms in the above mathematical expression equal to zero, the more generalized version of the continuity equation is obtained as [8]:

$$\frac{\partial f(s,t)}{\partial t} = -\left(\frac{\partial \Phi_x(s,t)}{\partial x} + \frac{\partial \Phi_x(s,t)}{\partial y} + \frac{\partial \Phi_z(s,t)}{\partial z}\right) \quad (3)$$

Moreover, the mathematical liaison between the concentration density and the flux as represented by Fick's Ist diffusion law is given as [8]:

$$\Phi_{S}(s,t) = -D \frac{\partial f(s,t)}{\partial s} \quad (\text{for} \quad s = x, y, z), \quad (4)$$

where *D* is the diffusion coefficient and the negative sign indicates the inward flow of the flux with respect to (w.r.t.) concentration density f(s, t). The value of *D* is independent of the information molecules' temperature, viscosity, velocity and radius. By mathematical substitutions, the resultant Fick's II^{*nd*} Diffusion Law is expressed as [1]:

$$\frac{\partial f(s,t)}{\partial t} = D \nabla^2 (f(s,t)), \tag{5}$$

where ∇^2 is the Laplacian operator. The whole of the environment is assumed to be a semi-infinite volume with reflecting surfaces. Therefore, there is no transmission at $x = 0^-$ instant and the expression of (5) becomes [1]:

$$\frac{\partial f(s,t)}{\partial t} = D\left(\frac{\partial^2 f(x,t)}{\partial x^2}\right).$$
 (6)

The solution of (6) gives the distribution of Type A molecules which is expressed as:

$$f(s,t) = \frac{2N_{Tx}}{\sqrt{4\pi Dt}} \exp\left(-\frac{X^2}{4Dt}\right) \quad \text{for} \quad t \ge 0; 0 \le X < \infty,$$
(7)

where N_{Tx} is the number of molecules injected at the injection site, $\mu = 0$ is the mean of the Type A molecules and $\sigma^2 = 2Dt$ is the variance. The Type A molecules, during the course of propagation inside the semi-infinite structure, are transformed into Type C log-normal distributed molecules undergoing reaction with the primary biomarkers. The Type C molecules are mathematically expressed as:

$$f(y_{Tr}, t) = \frac{1}{2Y_{Tr}} \frac{2N_{Tx}}{\sqrt{4\pi Dt}} \exp\left(-\frac{(\ln Y_{Tr})^2}{4Dt}\right)$$
(8)
for $t \ge 0; 0 < Y_{Tr} < \infty$,

where ln(.) is the natural logarithmic function and Y_{Tr} is the transformed random variable. The mean (μ) of Type C molecules showing log-Normal distribution is 0 and Variance (σ^2) is 2Dt.

The Type C molecules on reaching FC without degradation and flow velocity are collected, and the concentration of the molecules received is given as:

$$F_{hit} = \int_0^T \frac{1}{2Y_{Tr}} \frac{2N_{Tx}}{\sqrt{4\pi Dt}} \exp\left(-\frac{(\ln Y_{Tr})^2}{4Dt}\right) dt, \quad (9)$$

where F_{hit} is the number of molecules hitting the FC without drift (v_f) and degradation (k_d) . Thus, the closed-form expression of the above numerical expression is obtained by first substituting $\frac{\ln(Y_{Tr})}{\sqrt{4Dt}} = u$. The resultant expression of the average number of molecules reaching the FC without degradation and without drift is obtained as:

$$F_{hit} = \frac{N_{Tx} \ln(Y_{Tr})}{4DY_{Tr}\sqrt{\pi}} \left(-\sqrt{\pi}Q(u) + \frac{e^{-u^2}}{u}\right), \qquad (10)$$

where Q(.) is the standard *Q*-function. By incorporating molecular degradation the expression (9) gets modified as:

$$F_{hit,deg} = \int_{0}^{T} \frac{1}{2Y_{Tr}} \frac{2N_{Tx}}{\sqrt{4\pi Dt}} \\ \exp\left(-\left\{\frac{(\ln Y_{Tr})^{2}}{4Dt} + k_{d}t\right\}\right) dt, \\ = \int_{0}^{T} \frac{1}{Y_{Tr}} \frac{N_{Tx}}{\sqrt{4\pi Dt}} \exp\left(-\frac{(\ln Y_{Tr})^{2}}{4Dt}\right) dt \\ + \int_{0}^{T} \frac{1}{Y_{Tr}} \frac{N_{Tx}}{\sqrt{4\pi Dt}} \exp(-k_{d}t) dt, \quad (11)$$

where $F_{hit,deg}$ and k_d are the average number of molecules hitting the FC and the degradation parameter, respectively. Therefore, by utilizing integral properties, the closed-form expression of the integral in (11) is given as:

$$F_{hit,deg} = \frac{N_{Tx}(Y_{Tr})^{\left(\sqrt{\frac{k_d}{D}} - 1\right)} \ln(Y_{Tr})}{4D\sqrt{\pi}} \left\{ -\sqrt{\pi}Q(u + \sqrt{Tk_d}) + \frac{e^{-\left(u + \sqrt{Tk_d}\right)^2}}{u + \sqrt{Tk_d}} \right\},$$
(12)

where k_d is obtained as

$$k_d = \frac{\ln(2)}{\Lambda(1/2)},\tag{13}$$

where $\Lambda(1/2)$ is the half-life of the information molecules. Furthermore, if the effect of flow velocity (v_f) and degradation parameter (k_d) is taken into account, then the mathematical expression of (9), used for obtaining the average number of molecules hitting the FC, is modified into a new expression given as:

$$F_{hit,flow} = \int_{0}^{T} \frac{2N_{Tx}}{2Y_{Tr}\sqrt{4\pi Dt}} \\ \exp\left(-\frac{(\ln Y_{Tr} - v_{f}t)^{2}}{4Dt} - k_{d}t\right) dt, \\ = \int_{0}^{T} \frac{N_{Tx}}{Y_{Tr}\sqrt{4\pi Dt}} \exp\left(-\frac{(\ln Y_{Tr} - v_{f}t)^{2}}{4Dt}\right) dt \\ + \int_{0}^{T} \frac{N_{Tx}}{Y_{Tr}\sqrt{4\pi Dt}} \exp(-k_{d}t) dt,$$
(14)

where $F_{hit,flow}$ represents the average number of molecules hitting the FC surface under the effect of flow and degradation. Thus, the closed-form expression of (14) is obtained as:

$$F_{hit,flow} = \frac{2N_{Tx}Y_{Tr}^{(c-1)}}{\sqrt{\left(v_f^2 + 4Dk_d\right)}} \operatorname{erfc}\left(\frac{\sqrt{T(v_f^2 + 4Dk_d)}}{2\sqrt{D}} + \frac{\ln(Y_{Tr})}{2\sqrt{DT}}\right), \quad (15)$$

where $c = \frac{v_f + \sqrt{v_f^2 + 4Dk_d}}{2D}$.

Remark 1: From (12), increasing degradation $k_d \to \infty$ causes the argument inside *Q*-function and the exponential function to approach to very high values, i.e., $(u + \sqrt{Tk_d}) \to \infty$. Therefore, with $(u + \sqrt{Tk_d}) \to \infty$, the $Q(u + \sqrt{Tk_d}) \to 0$ and $\exp(-u + \sqrt{Tk_d}) \to 0$. Since the average number of molecules hitting the FC, is directly proportional to the $Q(u + \sqrt{Tk_d})$ and $\exp(-u + \sqrt{Tk_d})$, so $F_{hit,deg} \to 0$.

Remark 2: According to (15), for high flow velocities v_f values, i.e., as $v_f \to \infty$, due to extensive molecular collisions, the average number of molecules hitting the FC surface decreases such that $F_{hit,flow} \to 0$. Simultaneously, as $k_d \to \infty$, the argument $\sqrt{T(v_f^2 + 4Dk_d)} \to \infty$, which leads to $\operatorname{erfc}\left(\sqrt{T(v_f^2 + 4Dk_d)}/2\sqrt{D}\right) \to 0$ and $c \to 0$. Since





Figure 2: Number of molecules observed at Fusion Center with different degradation parameter (k_d) values and no flow velocity.

 $F_{hit,flow}$ is directly proportional to erfc(.) and *c*, so for $k_d \rightarrow \infty F_{hit,flow} \rightarrow 0$.

Remark 3: In many practical scenarios, specific enzymes, such as acetylcholinesterase (AChE), break down the information molecules in the environment. Therefore, the degradation process caused by these AChE molecules inhibits the propagation of molecules and hampers molecular reception. Thus, the employment of degradation (k_d) in the molecular reception process signifies the severity of molecular reception at FC. Simultaneously, flow velocity in the diffusive environment facilitates molecular motion, thereby enhancing the molecular reception process.

5 Numerical Results

Based on the mathematical analysis done in the previous section, the plots representing the average number of molecules received at FC for different physical environments are shown in Fig. 2, Fig. 3 and Fig. 4 respectively. The number of molecules injected is 1,00,000, while $D = 79.4 \mu m^2/sec$. The distance the Type C molecules travel until FC absorbs them is $15\mu m$. Note that for all the simulation results presented in this paper, we have used Monte Carlo simulations, where the results are averaged over 60,000 independent realizations of the system.

Fig. 2 illustrates the graphical representation of the average number of molecules received at the fusion center (FC) versus time duration for different molecular degradation and no drift. The figure shows that the average number of molecules received at the FC in a no-drift environment first increases with time and then decreases,



Figure 3: Number of molecules received at FC with different flow velocities and without molecular degradation.

respectively. Moreover, the effect of molecular degradation on the molecular reception at FC also plays an important role. With increasing k_d , the average number of molecules decreases rapidly. Therefore, increasing k_d negatively impacts the overall system's efficiency. Moreover, increasing k_d corresponds to a scenario where the half-lifetime of the information molecules is short. A decrease in the half-lifetime results in a decrease in the information molecules' activation energy, resulting in fewer molecular reception at FC. Further, due to the absence of flow velocity, there is a significant drop in the molecular absorption at FC. This can also be observed from the plot, where for $k_d = 1 \text{ sec}^{-1}$ out of 1,00,000 molecules, around 150 molecules are received at FC.

Fig. 3 shows the pictorial representation of the average number of molecules received at the FC versus time in a drift-only environment. The figure shows that introducing drift into the MC environment facilitates the molecular reception at FC. The drift phenomenon positively impacts the reception probability at FC, i.e., increasing v_f increases the reception probability of the molecules at FC. Increasing the drift velocity enhances the overall activation energy of the molecules. However, due to the stochastic nature of the media, increasing the drift velocity results in collisions among molecules. This collision is responsible for the overall decay in the activation energy of the molecules. Decaying in the molecules' activation energy due to molecular collisions is primarily responsible for making the molecule unrecognizable at the FC. The plot can further validate this; increasing flow velocities from



Figure 4: Number of molecules received at FC with different flow velocities and with molecular degradation ($k_d = 1 sec^{-1}$).

 $25 \ \mu m/sec$ to $75 \ \mu m/sec$ subsequently causes a decay in the average number of molecular reception at FC from around 4500 to around 1500.

Fig. 4 gives the pictorial representation of the average number of received molecules at FC versus time for different values of v_f and $k_d = 1sec^{-1}$. From the figure, it can be easily inferred that, compared to the scenario of no degradation, the average number of molecules reaching the FC in the degradation case is less, subsequently decreasing with the increasing values of time. The decrease in the average number of molecules received at FC is primarily because most molecules travelling inside the fluid die out due to molecular degradation even before reaching the FC. An increase in k_d corresponds to a decrease in the half-life of the information molecules. A decrease in the half-lifetime of the information molecules leads to a simultaneous decrease in the molecular activation energy, subsequently reducing the overall molecular reception at FC. Moreover, v_f has a positive impact on the molecular reception, whereas k_d has a negative impact, with v_f overshadowing the effect of k_d . However, for high flow velocities due to the phenomena of molecular collisions, the average number of molecules received at FC decreases.

From the plot, it can be concluded that there is always a tradeoff in choosing the different values of the flow velocities. Higher flow velocities result in molecular collisions, subsequently reducing the activation energy of the information molecules, which inherently reduces the reception rate at FC.

6 Conclusion

In this paper, we provided a detailed analysis of the effect of drift and molecular degradation on the reception of the average number of molecules at FC in diffusive molecular communication. By utilizing the log-normal distribution of the Type C information molecules, we first analytically calculated the closed-form expression of the average number of received molecules at FC when the information molecules experience neither molecular degradation nor any drift in the media. Subsequently, to analyze the effect of molecular degradation in the diffusive log-normal channels, we calculated the closed-form expression of the average number of received molecules at FC when the information molecules experience drift without molecular degradation in the environment. Further, we also calculated the closed-form expression of the average number of received molecules at FC when the information molecules simultaneously experience drift and molecular degradation in the environment. Based on the mathematical analysis, we observed that the average number of molecules received at FC is less when there is neither drift nor molecular degradation in the environment. However, the average number of molecules received at FC increases with the introduction of drift (by employing flow velocity) only into the media. Subsequently, for an environment where information molecules experience both drift and molecular degradation simultaneously, the average number of molecules received at FC is comparatively less, signifying that the net effect of physical environments affects the molecular reception at FC. Finally, the plots also highlight the dependence of molecular reception on the time parameter. The analysis presented in this manuscript would bridge the gap between the analytical and practical systems, and help understand how flow and molecular degradation conditions impact cellular behavior. Further, the collective study of flow velocity and molecular degradation presented in this article would pave the path for future research in the design of biomaterials.

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Please visit Contributor Roles Taxonomy (CRediT) that contains several roles: The problem formulation, numerical analysis and final findings were done by Gaurav Sharma.

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Conflicts of Interest

The author have no conflict of interest.

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