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# Stochastic Modeling for the Formation of Activated Carbons: Non-linear Approach

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# APPENDIXES

## Appendix A. Derivation of the Master Equation of a Pure-Death Process

Suppose that a system comprising a population of particulate or discrete entities in a given space is to be stochastically modeled as a pure-death process. The random variable characterizing this process is denoted by N(t) with realization n; moreover, the intensity of death is denoted by $\mu_n(t)$. Thus, one of the following two events is considered to occur during time interval $(t, t+\Delta t)$. First, the number of entities decreases by one, which is a death event, with a conditional probability of $\{[\mu_n(t)]\Delta t + o(\Delta t)\}$. Second, the number of entities changes by a number other than one with a conditional probability of o(Δt), which is defined such that

$$\lim_{\Delta t \to 0} \frac{o(\Delta t)}{\Delta t} = 0 \tag{A.1}$$

Naturally, the conditional probability of no change in the number of entities during this time interval is $(1 - \{[\mu_n(t)]\Delta t + o(\Delta t)\})$.

Let the probability that exactly n entities are present at time t be denoted as $p_n(t) = \Pr[N(t) = n]$, where $n \in (n_0, n_0 - 1, ..., 2, 1, 0)$; $n_0$ is the initial number of entities in the system. For the two adjacent time intervals, (0, t) and $(t, t+\Delta t)$, the occurrence of exactly n entities being present at time $(t + \Delta t)$ are realized according to the following mutually exclusive events; see Figure A.1.

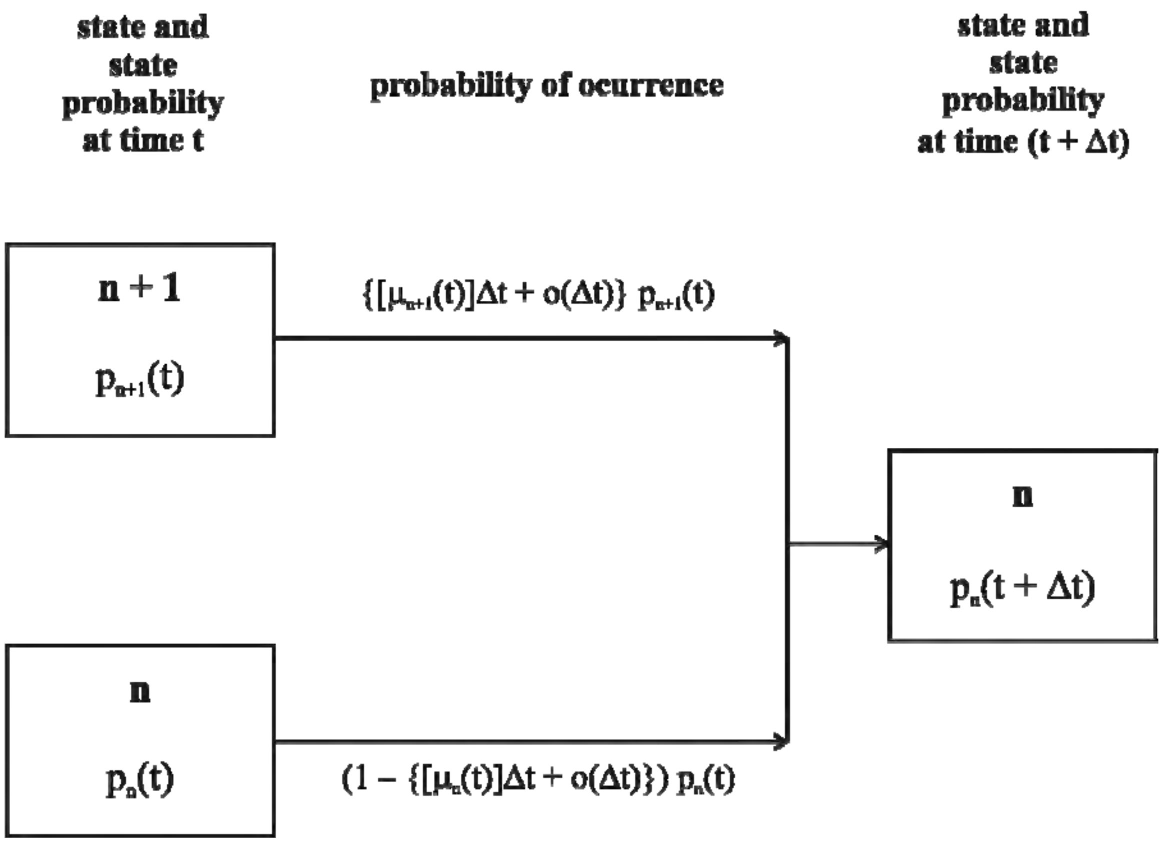


**Figure A.1. Probability balance for the pure-death process involving the mutually exclusive events in the time interval, (t, t + Δt).**

(1) With a probability of $\{[\mu_{n+1}(t)]\Delta t + o(\Delta t)\}p_{n+1}(t)$, the number of entities will decrease by one during time interval $(t, t+\Delta t)$, provided that exactly $(n+1)$ entities are present at time t.

(2) With a probability of o(Δt), the number of entities will change by exactly j entities during time interval $(t, t+\Delta t)$, provided that exactly $(n-j)$ entities are present at time t, where $2 \le j \le n_0$.

(3) With a probability of $(1-\{[\mu_n(t)]\Delta t + o(\Delta t)\})p_n(t)$, the number of entities will remain unchanged during time interval $(t, t+\Delta t)$, provided that n entities are present at time t.

Summing all these probabilities and consolidating all quantities of o(Δt) yield

$$p_n(t+\Delta t) = \{[\mu_{n+1}(t)]\Delta t\}\, p_{n+1}(t) + \{1-[\mu_n(t)]\Delta t\}\, p_n(t) + o(\Delta t) \tag{A.2}$$

Rearranging this equation, dividing it by Δt, and taking the limit as Δt → 0 give rise to the master equation of the pure-death process as[{19 Oppenheim, I. 1977; 27 van Kampen, N. G. 1992 }]

$$\frac{d}{dt} p_n(t) = \mu_{n+1}(t)\, p_{n+1}(t) - \mu_n(t)\, p_n(t) \tag{A.3}$$

This is Eq. (3) in the text. For convenience, the intensity function, $\mu_n(t)$, of the pure-death process of interest, Eq. (2) in the text, is rewritten as

$$\mu_n(t) = -\frac{dn}{dt} = \alpha\, n^2 \tag{A.4}$$

Inserting the right-hand side of the above expression into the right-hand side of the master equation, Eq. (A.3), gives rise to

$$\frac{d}{dt}p_n(t) = \left[\alpha\left(n+1\right)^2\right]p_{n+1}(t) - \left[\alpha n^2\right]p_n(t)\,, \quad n = n_0, n_0 - 1, \ldots, 2, 1, 0 \qquad \text{(A.5)}$$

This is Eq. (5) in the text.

## Appendix B. Expansion of the Master Equation

The master equation of the process, Eq. (3) in the text, is

$$\frac{d}{dt}p_n(t) = \mu_{n+1}p_{n+1}(t) - \mu_n p_n(t)\,, \quad n = n_0, n_0 - 1, \ldots, 2, 1, 0 \tag{B-1}$$

The one-step operator, **E**, is defined by its effect on an arbitrary function, f(n), as follows:[18]

$$\mathbf{E}f(n) = f(n+1) \quad \text{and} \quad \mathbf{E}^{-1}f(n) = f(n-1)$$

With the aid of this operator, Eq. (B-1) is reduced to

$$\frac{d}{dt}p_n(t) = \left(\mathbf{E} - 1\right)\mu_n p_n(t)\,, \quad n = n_0, n_0 - 1, \ldots, 2, 1, 0 \tag{B-2}$$

The intensity of death, $\mu_n$, in this expression is given in Eq. (2) in the text as

$$\mu_n(t) = -\frac{dn}{dt} = \alpha n^2 \tag{B-3}$$

where $\alpha$ is a proportionality constant. Thus, the master equation, Eq. (B-2), can be rewritten as

$$\frac{d}{dt}p_n(t) = \left(\mathbf{E} - 1\right)\left(\alpha n^2\right)p_n(t) \tag{B-4}$$

It is expected that at later time t, the probability distribution of N(t), $p_n(t)$ or p(n;t), exhibits a sharp peak at some position of order $\Omega$, while its width will be of order $\Omega^{½}$ (see Figure A-1); the symbol, $\Omega$, is the system's size, which is $n_0$ in the current work. To formulate this formally, N(t) is expressed as the sum of the macroscopic term, $\Omega\varphi(t)$, and the fluctuation term, $\Omega^{½}\Xi(t)$. Thus,

$$N(t) = n_0\varphi(t) + n_0^{1/2}\Xi(t) \tag{B-5}$$

whose realization is

$$n = n_0\varphi(t) + n_0^{1/2}\xi \tag{B-6}$$

The function, $\varphi(t)$, in these two equations is adjusted so as to follow the motion of the peak in time. Accordingly, $p(n;t)$ is transformed into function $\pi(\xi;t)$ depending on the realization of $\Xi(t)$, $\xi$, as

$$p(n;t) = \Pr[N(t) = n] = \Pr[\Xi(t) = \xi] = \pi(\xi;t) \tag{B-7}$$

From Eq. (B-6), we have

$$\xi = n(n_0^{-1/2}) - n_0^{1/2}\varphi(t) \tag{B-8}$$

With n fixed, the time derivative of the above expression is given by

$$\frac{d\xi}{dt} = -n_0^{1/2}\frac{d\varphi}{dt} \tag{B-9}$$

Differentiating Eq. (B-7) with respect to time t leads to

$$\frac{d}{dt}p(n;t) = \frac{\partial\pi}{\partial t} + \frac{\partial\pi}{\partial\xi}\left(\frac{d\xi}{dt}\right) \tag{B-10}$$

By inserting Eq. (B-9) into this equation, we obtain

$$\frac{d}{dt}p(n;t) = \frac{\partial\pi}{\partial t} - n_0^{1/2}\left(\frac{d\varphi}{dt}\right)\frac{\partial\pi}{\partial\xi} \tag{B-11}$$

In light of the one-step operator, **E**, we obtain, from Eq. (B-6)

$$\begin{aligned}\mathbf{E}n = n+1 &= [n_0\varphi(t) + n_0^{1/2}\xi] + 1 \\ &= [n_0\varphi(t) + n_0^{1/2}\xi] + n_0^{1/2}n_0^{-1/2} \\ &= n_0\varphi(t) + n_0^{1/2}(\xi + n_0^{-1/2})\end{aligned}$$

In other words, **E** transforms n into (n+1), and therefore, $\xi$ into ($\xi + n_0^{-1/2}$); as a result, from Eq. (B-7),

$$\mathbf{E}p(n;t) = p(n+1;t)$$

or

$$\mathbf{E}\pi(\xi;t) = \pi(\xi + n_0^{-1/2};t) \tag{B-12}$$

The Taylor expansion of $\pi(\xi + n_0^{-1/2}; t)$ about ξ, is given by

$$\pi(\xi + n_0^{-1/2}; t) = \pi(\xi; t) + n_0^{-1/2} \frac{\partial}{\partial \xi} \pi(\xi; t) + \frac{1}{2!} (n_0^{-1/2})^2 \frac{\partial^2}{\partial \xi^2} \pi(\xi; t) + ...$$

or

$$\pi(\xi + n_0^{-1/2}; t) = \left( 1 + n_0^{-1/2} \frac{\partial}{\partial \xi} + \frac{1}{2} n_0^{-1} \frac{\partial^2}{\partial \xi^2} + ... \right) \pi(\xi; t) \tag{B-13}$$

In view of Eq. (B-12), the above expression can be transformed to

$$p(n+1; t) = \mathbf{E} p(n; t) = \left( 1 + n_0^{-1/2} \frac{\partial}{\partial \xi} + \frac{1}{2} n_0^{-1} \frac{\partial^2}{\partial \xi^2} + ... \right) p(n; t)$$

Thus, we have

$$\mathbf{E} = 1 + n_0^{-1/2} \frac{\partial}{\partial \xi} + \frac{1}{2} n_0^{-1} \frac{\partial^2}{\partial \xi^2} + ... \tag{B-14}$$

Substituting Eqs. (B-6), (B-7), (B-11), and (B-13) into the master equation, Eq. (B-2), leads to

$$\frac{\partial \pi}{\partial t} - n_0^{1/2} \left( \frac{d\varphi}{dt} \right) \frac{\partial \pi}{\partial \xi}$$

$$= n_0 \left( n_0^{-1/2} \frac{\partial}{\partial \xi} + \frac{1}{2} n_0^{-1} \frac{\partial^2}{\partial \xi^2} + ... \right) \left[ \alpha n_0 (\varphi + n_0^{-1/2} \xi)^2 \right] \pi \tag{B-15}$$

Absorbing the system's size, $n_0$, into the time variable, t, as

$$n_0 t = \gamma$$

and truncating the terms after the second-order derivative for large $n_0$ give

$$\frac{\partial \pi}{\partial \gamma} - n_0^{1/2} \left( \frac{d\varphi}{d\tau} \right) \frac{\partial \pi}{\partial \xi}$$

$$= \left( n_0^{-1/2} \frac{\partial}{\partial \xi} + \frac{1}{2} n_0^{-1} \frac{\partial^2}{\partial \xi^2} \right) \left[ \alpha n_0 (\varphi + n_0^{-1/2} \xi)^2 \right] \pi \tag{B-16}$$

By expanding the right-hand side of this equation and collecting the resultant terms of orders $n_0^{1/2}$ and $n_0^0$ separately, we have

$$\begin{aligned}
&\frac{\partial \pi}{\partial \gamma} - n_0^{1/2}\left(\frac{d\varphi}{d\tau}\right)\frac{\partial \pi}{\partial \xi} \\
&= n_0^0\left[2\alpha\varphi\frac{\partial}{\partial \xi}(\xi\pi) + \frac{1}{2}\alpha\varphi^2\frac{\partial^2 \pi}{\partial \xi^2}\right] - n_0^{1/2}\left(-\alpha\varphi^2\right)\frac{\partial \pi}{\partial \xi} \\
&\quad + n_0^{-1/2}\left[\alpha\varphi\frac{\partial^2}{\partial \xi^2}(\xi\pi) + \alpha\frac{\partial}{\partial \xi}\left(\xi^2\pi\right) + \frac{1}{2}\alpha n_0^{-1/2}\frac{\partial^2}{\partial \xi^2}\left(\xi^2\pi\right)\right] \qquad \text{(B-17)}
\end{aligned}$$

Comparing both sides of the above expression gives rise to

$$\frac{d\varphi}{d\gamma} = -\alpha\varphi^2 \qquad \text{(B-18)}$$

and

$$\frac{\partial \pi}{\partial \gamma} = 2\alpha\varphi\frac{\partial}{\partial \xi}(\xi\pi) + \frac{1}{2}\alpha\varphi^2\frac{\partial^2 \pi}{\partial \xi^2} \qquad \text{(B-19)}$$

Of these two equations, the former is the macroscopic equation governing the overall behavior of the process, and the latter is a linear Fokker-Plank equation governing the fluctuations of the process around the macroscopic values and whose coefficients depend on t through φ(t).

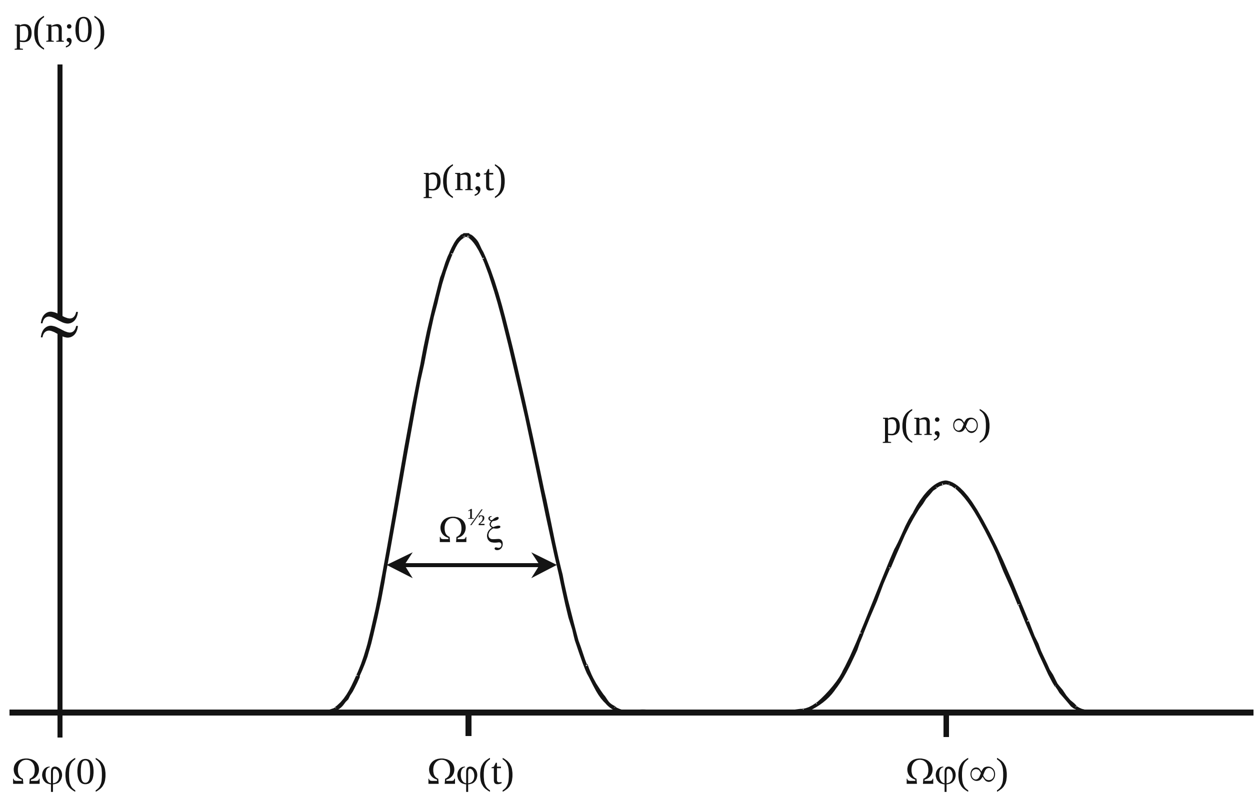


**Figure B-1.** Temporal evolution of the probability distribution, p(n;t).

## Appendix C. Derivation of Mean and Variance

Random variable N(t) in terms of φ(t) is given by Eq. (B-5) as

$$N(t) = n_0\varphi(t) + n_0^{1/2}\Xi(t) \tag{C-1}$$

whose realization, n, is given by Eq. (B-6) as

$$n = n_0\varphi(t) + n_0^{1/2}\xi \tag{C-2}$$

At t = 0, n = $n_0$ and ( $n_0^{1/2}\xi$ ) = 0, i.e., no fluctuations around $n_0$ exist. Hence, from Eq. (C-2),

$$\varphi(0) = 1 \tag{C-3}$$

For convenience, Eq. (B-18) for φ(t) is rewritten below.

$$\frac{d\varphi}{d\gamma} = -\alpha\varphi^2 \tag{C-4}$$

where $\gamma = n_0 t$. Integrating this equation with the initial condition given by Eq. (C-3) leads to

$$\varphi(\gamma) = \frac{1}{\alpha\gamma + 1}$$

In terms of t, this equation can be rewritten as

$$\varphi(t) = \frac{1}{(\alpha n_0)t + 1} \tag{C-5}$$

For any arbitrary functions f and g which take integers, the following expression holds (van Kampen, 1992)

$$\sum_{n=0}^{n_0-1}[g(n)\mathbf{E}f(n)] = \sum_{n=1}^{n_0}[f(n)\mathbf{E}^{-1}g(n)] \tag{C-6}$$

For the case where

$$g(-1) = f(0) = g(n_0) = g(n_0 + 1) = 0,$$

Equation (C-6) becomes

$$\sum_{n=0}^{n_0}[g(n)\mathbf{E}f(n)] = \sum_{n=0}^{n_0}[f(n)\mathbf{E}^{-1}g(n)] \quad \text{(C-7)}$$

When functions f and g take real numbers, the central-difference approximation gives

$$\frac{\partial}{\partial x}f(x) \approx \frac{f(x+\Delta x)-f(x)}{\Delta x} \quad \text{(C-8)}$$

and

$$\frac{\partial^2}{\partial x^2}f(x) \approx \frac{f(x+\Delta x)-2f(x)+f(x-\Delta x)}{(\Delta x)^2} \quad \text{(C-9)}$$

Hence,

$$\begin{aligned}
&\sum_x\left[g(x)\frac{\partial}{\partial x}f(x)\right] \\
&\approx \sum_x\left[g(x)\frac{f(x+\Delta x)-f(x)}{\Delta x}\right] \\
&\approx \frac{1}{\Delta x}\left\{\sum_x\left[g(x)f(x+\Delta x)\right]-\sum_x\left[g(x)f(x)\right]\right\} \quad \text{(C-10)}
\end{aligned}$$

In view of the property of the one-step operator, Eq. (C-7), the right-hand side of the above expression can be transformed to

$$\begin{aligned}
&\frac{1}{\Delta x}\left\{\sum_x\left[g(x)f(x+\Delta x)\right]-\sum_x\left[g(x)f(x)\right]\right\} \\
&= \frac{1}{\Delta x}\left\{\sum_x\left[g(x)\mathbf{E}f(x)\right]-\sum_x\left[g(x)f(x)\right]\right\} \\
&= \frac{1}{\Delta x}\left\{\sum_x\left[f(x)\mathbf{E}^{-1}g(x)\right]-\sum_x\left[g(x)f(x)\right]\right\} \\
&= \frac{1}{\Delta x}\left\{\sum_x\left[f(x)g(x-\Delta x)\right]-\sum_x\left[f(x)g(x)\right]\right\}
\end{aligned}$$

$$= \sum_x \left[ f(x) \frac{g(x-\Delta x) - g(x)}{\Delta x} \right]$$

$$= -\sum_x \left[ f(x) \frac{g(x) - g(x-\Delta x)}{\Delta x} \right]$$

$$\approx -\sum_x \left[ f(x) \frac{\partial}{\partial x} g(x) \right] \tag{C-11}$$

Thus,

$$\sum_x \left[ g(x) \frac{\partial}{\partial x} f(x) \right] = -\sum_x \left[ f(x) \frac{\partial}{\partial x} g(x) \right] \tag{C-12}$$

Similarly,

$$\sum_x \left[ g(x) \frac{\partial^2}{\partial x^2} f(x) \right]$$

$$\approx \sum_x \left[ g(x) \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} \right]$$

$$\approx \frac{1}{(\Delta x)^2} \left\{ \sum_x \left[ g(x) f(x+\Delta x) \right] - 2\sum_x \left[ g(x) f(x) \right] + \sum_x \left[ g(x) f(x-\Delta x) \right] \right\} \tag{C-13}$$

In light of Eq. (C-7), the right-hand side of the above expression can be rewritten as

$$\frac{1}{(\Delta x)^2} \left\{ \sum_x \left[ g(x) f(x+\Delta x) \right] - 2\sum_x \left[ g(x) f(x) \right] + \sum_x \left[ g(x) f(x-\Delta x) \right] \right\}$$

$$= \frac{1}{(\Delta x)^2} \left\{ \sum_x \left[ g(x) \mathbf{E} f(x) \right] - 2\sum_x \left[ g(x) f(x) \right] + \sum_x \left[ g(x) \mathbf{E}^{-1} f(x) \right] \right\}$$

$$= \frac{1}{(\Delta x)^2} \left\{ \sum_x \left[ f(x) \mathbf{E}^{-1} g(x) \right] - 2\sum_x \left[ g(x) f(x) \right] + \sum_x \left[ f(x) \mathbf{E} g(x) \right] \right\}$$

$$= \frac{1}{(\Delta x)^2} \left\{ \sum_x \left[ f(x) g(x-\Delta x) \right] - 2\sum_x \left[ f(x) g(x) \right] + \sum_x \left[ f(x) g(x+\Delta x) \right] \right\}$$

$$= \sum_x \left[ f(x) \frac{g(x+\Delta x) - 2g(x) + g(x-\Delta x)}{(\Delta x)^2} \right]$$

$$\approx \sum_x \left[ f(x) \frac{\partial^2}{\partial x^2} g(x) \right]$$

Thus,

$$\sum_x \left[ g(x) \frac{\partial^2}{\partial x^2} f(x) \right] = \sum_x \left[ f(x) \frac{\partial^2}{\partial x^2} g(x) \right] \tag{C-14}$$

The linear Fokker-Plank equation governing the fluctuations of the process around the macroscopic values is given by Eq. (B-19) as

$$\frac{\partial \pi}{\partial \gamma} = 2\alpha\varphi \frac{\partial}{\partial \xi}(\xi\pi) + \frac{1}{2}\alpha\varphi^2 \frac{\partial^2 \pi}{\partial \xi^2} \tag{C-15}$$

Because $\gamma = n_0 t$, this equation can be rewritten as

$$\frac{\partial \pi}{\partial t} = 2(\alpha n_0)\varphi \frac{\partial}{\partial \xi}(\xi\pi) + \frac{1}{2}(\alpha n_0)\varphi^2 \frac{\partial^2 \pi}{\partial \xi^2} \tag{C-16}$$

Multiplying both sides of the above equation by $\xi$ and summing over all values of $\xi$ yield

$$\sum_\xi \xi \frac{\partial \pi}{\partial t} = 2(\alpha n_0)\varphi \left[ \sum_\xi \xi \frac{\partial(\xi\pi)}{\partial \xi} \right] + \frac{1}{2}(\alpha n_0)\varphi^2 \left[ \sum_\xi \xi \frac{\partial^2 \pi}{\partial \xi^2} \right] \tag{C-17}$$

By virtue of Eqs. (C-12) and (C-14), the right-hand side of this expression can be transformed to

$$\sum_\xi \xi \frac{\partial \pi}{\partial t} = 2(\alpha n_0)\varphi \left[ -\sum_\xi \xi\pi \frac{\partial \xi}{\partial \xi} \right] + \frac{1}{2}(\alpha n_0)\varphi^2 \left[ \sum_\xi \pi \frac{\partial^2 \xi}{\partial \xi^2} \right]$$

or

$$\sum_\xi \xi \frac{\partial \pi}{\partial t} = -\left[ 2(\alpha n_0)\varphi \right] \left[ \sum_\xi \xi\pi \right] \tag{C-18}$$

The first moment of random variable $\Xi(t)$, i.e., $E[\Xi(t)]$, is defined as

$$E[\Xi(t)] = \sum_\xi \xi\pi(\xi; t)$$

or

$$E[\Xi(t)] = \sum_{\xi} \xi \pi \tag{C-19}$$

and thus,

$$\frac{d}{dt} E[\Xi(t)] = \sum_{\xi} \xi \frac{\partial \pi}{\partial t} \tag{C-20}$$

In light of Eqs. (C-19) and (C-20), Eq. (C-18) reduces to

$$\frac{d}{dt} E[\Xi(t)] = -\left[2\left(\alpha n_0\right)\varphi\right] E[\Xi(t)] \tag{C-21}$$

Inserting Eq. (C-5) for φ(t) into this equation and integrating the resulting expression yield

$$E[\Xi(t)] = \frac{c_1}{\left[\left(\alpha n_0\right)t + 1\right]^2} \tag{C-22}$$

From the initial conditions for the transformed probability distribution, π(ξ;t),

$$\pi(\xi; 0) = \begin{cases} 1 & \text{if} \quad \xi = 0 \\ \\ 0 & \text{elsewhere} \end{cases} \tag{C-23}$$

and the definition of E[Ξ(t)], as given by Eq. (C-19), we have

$$E[\Xi(0)] = 0 \tag{C-24}$$

thereby indicating that

$$c_1 = 0 \tag{C-25}$$

Hence,

$$E[\Xi(t)] = 0 \tag{C-26}$$

Similarly, multiplying both sides of Eq. (C-16) by $\xi^2$ and summing over all values of $\xi$ yield

$$\sum_{\xi} \xi^2 \frac{\partial \pi}{\partial t} = 2(\alpha n_0)\varphi\left[\sum_{\xi} \xi^2 \frac{\partial(\xi\pi)}{\partial \xi}\right] + \frac{1}{2}(\alpha n_0)\varphi^2\left[\sum_{\xi} \xi^2 \frac{\partial^2 \pi}{\partial \xi^2}\right] \tag{C-27}$$

By virtue of Eqs. (C-12) and (C-14), the right-hand side of the above expression can be transformed to

$$\sum_{\xi} \xi^2 \frac{\partial \pi}{\partial t} = 2(\alpha n_0)\varphi\left[-\sum_{\xi} \xi\pi \frac{\partial \xi^2}{\partial \xi}\right] + \frac{1}{2}(\alpha n_0)\varphi^2\left[\sum_{\xi} \pi \frac{\partial^2 \xi^2}{\partial \xi^2}\right]$$

or

$$\sum_{\xi} \xi^2 \frac{\partial \pi}{\partial t} = -4(\alpha n_0)\varphi\left[\sum_{\xi} \xi^2 \pi\right] + (\alpha n_0)\varphi^2\left[\sum_{\xi} \pi\right] \tag{C-28}$$

For the transformed probability distribution, $\pi(\xi;t)$, the following property must hold

$$\sum_{\xi} \pi(\xi;t) = 1$$

or

$$\sum_{\xi} \pi = 1 \tag{C-29}$$

In view of this equation, Eq. (C-28) can be rewritten as

$$\sum_{\xi} \xi^2 \frac{\partial \pi}{\partial t} = -4(\alpha n_0)\varphi\left[\sum_{\xi} \xi^2 \pi\right] + (\alpha n_0)\varphi^2 \tag{C-30}$$

The second moment of random variable $\Xi(t)$, i.e., $E[\Xi^2(t)]$, is defined as

$$E[\Xi^2(t)] = \sum_{\xi} \xi^2 \pi(\xi;t)$$

or

$$E[\Xi^2(t)] = \sum_{\xi} \xi^2 \pi \tag{C-31}$$

and thus,

$$\frac{d}{dt}E[\Xi^2(t)] = \sum_{\xi}\xi^2\frac{\partial\pi}{\partial t} \tag{C-32}$$

In view of Eqs. (C-31) and (C-32), Eq. (C-30) reduces to

$$\frac{d}{dt}E[\Xi^2(t)] = -4(\alpha n_0)\varphi\, E[\Xi^2(t)] + (\alpha n_0)\varphi^2$$

or

$$\frac{d}{dt}E[\Xi^2(t)] + 4(\alpha n_0)\varphi\, E[\Xi^2(t)] = (\alpha n_0)\varphi^2 \tag{C-33}$$

By substituting Eq. (C-5) for φ(t) into this equation and integrating the resulting expression,

$$E[\Xi^2(t)] = \frac{1}{3\left[(\alpha n_0)t+1\right]} + \frac{c_2}{\left[(\alpha n_0)t+1\right]^4} \tag{C-34}$$

From the aforementioned initial conditions for the transformed probability distribution, π(ξ;t), Eq. B-23, and the definition of $E[\Xi^2(t)]$, Eq. (C-31), we have

$$E[\Xi^2(0)] = 0, \tag{C-35}$$

thereby indicating that

$$c_2 = -\frac{1}{3} \tag{C-36}$$

Hence,

$$E[\Xi^2(t)] = \frac{1}{3}\left\{\frac{1}{\left[(\alpha n_0)t+1\right]} - \frac{1}{\left[(\alpha n_0)t+1\right]^4}\right\} \tag{C-37}$$

The mean, E[N(t)] or m(t), is the expected value (first moment) of random variable N(t). From Eq. (C-1), m(t) can be obtained as

$$m(t) = E[N(t)] = n_0\varphi(t) + n_0^{1/2}E[\Xi(t)] \tag{C-38}$$

Substituting Eqs. (C-5) and (C-26) into the above expression gives rise to

$$m(t) = \frac{n_0}{(\alpha n_0)t + 1} \tag{C-39}$$

This is Eq. (7) in the text. Note that $(\alpha n_0)$ is a constant. By lumping $[(\alpha n_0)t]$ as dimensionless time $\tau$, we have

$$m(\tau) = \frac{n_0}{\tau + 1} \tag{C-40}$$

The normalized, or dimensionless, form of the mean, $\bar{m}(\tau)$, is obtained from this expression as

$$\bar{m}(\tau) = \frac{m(\tau)}{n_0} = \frac{1}{\tau + 1} \tag{C-41}$$

This is Eq. (9) in the text.

The variance, Var[N(t)] or $\sigma^2(t)$, is the second moment of N(t) about the mean, m(t). Thus,

$$\sigma^2(t) = \mathrm{Var}[N(t)] = E[(N(t) - E[N(t)])^2] = E[N^2(t)] - m^2(t) \tag{C-42}$$

In view of Eq. (C-1) and the above expression, we have

$$\sigma^2(t) = n_0 \mathrm{Var}[\Xi(t)] = n_0 E[\{\Xi(t) - E[\Xi(t)]\}^2] = n_0(E[\Xi^2(t)] - \{E[\Xi(t)]\}^2) \tag{C-43}$$

Substituting Eqs. (C-26) and (C-37) into this equation yields

$$\sigma^2(t) = \frac{n_0}{3[(\alpha n_0)t + 1]}\left\{1 - \frac{1}{[(\alpha n_0)t + 1]^3}\right\}$$

This is Eq. (10) in the text. In terms of $\tau$, this equation becomes

$$\sigma^2(\tau) = \frac{n_0}{3(\tau+1)}\left[1 - \frac{1}{(\tau+1)^3}\right] \tag{C-44}$$

This is Eq. (11) in the text. The standard deviation, $\sigma(\tau)$, is the square root of the variance, $\sigma^2(\tau)$.

Hence, from the above equation,

$$\sigma(\tau) = \left[\sigma^2(\tau)\right]^{1/2} = \left[\frac{n_0}{3(\tau+1)}\right]^{1/2}\left[1 - \frac{1}{(\tau+1)^3}\right]^{1/2} \tag{C-45}$$

The normalized form of the standard deviation, $\bar{\sigma}(\tau)$, is given by

$$\bar{\sigma}(\tau) = \frac{\sigma(\tau)}{n_0} = \frac{1}{\left[3n_0(\tau+1)\right]^{1/2}}\left[1 - \frac{1}{(\tau+1)^3}\right]^{1/2} \tag{C-46}$$

This is Eq. (13) in the text.

## Appendix D. Estimation of $n_0$

For convenience, the order of magnitude estimate of the total number of obtainable pores, $n_0$, that could form open pores on the carbonaceous substrate's internal surfaces per unit weight of the activated susbtrate is obtained by dividing the total volume of open pores per unit weight of ACs by the volume of a single open pore. The former can be recovered from the experimental characterization of ACs produced from a carbonaceous substrate under specific activation conditions, and the latter can be computed under the assumption that the shape of the pore is perfectly cylindrical. For illustration, the total volume of open pores for ACs prepared at 873 K is 0.96 $cm^3$ per gram of ACs.[28] Moreover, the volume of a single pore is given by

$$v_p = \pi(\bar{r})^2 \ell \tag{D-1}$$

where $\bar{r}$ and $\ell$ are the pore's average radius and length, respectively. For a perfectly cylindrical pore, $\bar{r}$ can be expressed as[37]

$$\bar{r} = \frac{2\varepsilon_s}{\rho_s S_g} \tag{D-2}$$

In the above expression, $\varepsilon_s$, $\rho_s$, and $S_g$ are structural properties of ACs, which are specifically, their porosity, apparent density, and surface area per unit weight of ACs, respectively. For ACs prepared at 873 K,[28] the corresponding values of these properties are 0.66, 0.69 $g \cdot cm^{-3}$, and 1,366 $m^2 \cdot g^{-1}$,[28] thereby yielding $\bar{r}$ as 1.40 nm. By changing $\ell$ from 1 nm to 50 nm, the volume of a single pore, $v_p$, varies from $6.16 \cdot 10^{-21}$ $cm^3$ to $3.08 \cdot 10^{-19}$ $cm^3$ as computed from Eq. (D-1).

Thus, the order of magnitude estimate of $n_0$ falls within the range between $3.12 \cdot 10^{15}$ and $1.56 \cdot 10^{17}$ pores per milligram of ACs.