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The solution of an infinite set of differential-difference equations occurring in polymerization and queueing problems

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Abstract. The time-dependent solutions of an infinite set of differential-difference equations arising from queueing theory and models of 'living' polymer are expressed in terms of modified Bessel functions. Explicit solutions are available for constant values of a parameter describing the arrival rate or monomer concentration; for time-dependent parameter a formal solution is obtained in terms of a function which satisfies a Volterra type integral equation of the second kind. These results are used as the basis of a numerical method of solving the infinite set of differential equations when the time-dependent parameter itself satisfies a differential equation.

1. *Introduction.* Menčik (7) and Brown and Szwarc (3) discuss a model of 'living' polymers for which the initial polymerization will eventually be compensated by a step-by-step depolymerization. The process is described mathematically by the following equations for the molecular concentrations P_n of n-mers, the concentration P_0 of water and the concentration M of monomer,

$$\frac{dM}{dT} = -k_+ M \sum_{n=0}^{\infty} P_n + k_- \sum_{n=1}^{\infty} P_n, \tag{1}$$

$$\frac{dP_0}{dT} = -k_+ MP_0 + k_- P_1, \tag{2}$$

$$\frac{dP_n}{dT} = k_+ MP_{n-1} - \{k_+ M + k_-\}P_n + k_- P_{n+1} \quad (n \geqslant 1). \tag{3}$$

Here k_+ is the rate constant of polymerization and k_- is the rate constant of depolymerization.

(2) and (3) also arise from the stochastic model of single server queues, if $k_+ M$ is interpreted as the arrival rate and k_- as the service rate (1).

The initial conditions, corresponding to no polymer present, associated with (1), (2) and (3) are

$$T = 0, \quad M = M_0, \quad P_0 = A, \quad P_n = 0 \quad \text{for} \quad n \geqslant 1.$$

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In order to simplify the equations, the following changes of variable can be made (8),

$$Q_n = P_n + P_{n+1} + \ldots,$$

i.e.
$$P_n = Q_n - Q_{n+1},$$

and
$$Q_n = \frac{k_-}{k_+} q_n, \quad M = \frac{k_-}{k_+} m, \quad T = \frac{1}{k_-} t.$$

(1), (2) and (3) now become

$$\frac{dm}{dt} = -q_0 m + q_1, \tag{4}$$

$$q_0 = \frac{k_+}{k_-} A, \tag{5}$$

$$\frac{dq_n}{dt} = m q_{n-1} - (m+1) q_n + q_{n+1} \quad (n \geqslant 1), \tag{6}$$

where q_0 is now a constant and the initial conditions are

$$t = 0, \quad m = \frac{k_+}{k_-} M_0 = a, \quad q_0 = \frac{k_+}{k_-} A = b, \quad q_n = 0 \quad \text{for} \quad n \geqslant 1.$$

(5), which is equivalent to
$$P_0 + P_1 + \ldots = A,$$

expresses the physical fact that the total number of molecules of water in the system at any time t is equal to the number at $t = 0$. In the queueing problem, where the P_n represent probabilities, the value of A would be unity.

The steady-state solution of (6) is obtained by equating the derivatives in (6) to zero, and is well known to correspond to a geometric distribution ((2), p. 101; (3, 7)).

The time-dependent solution of (6), for constant m and general boundary conditions, was first given by Ledermann and Reuter (6), using the spectral theory of birth and death processes. Other methods of solution have been given by Bailey (1), using generating functions and Laplace transforms, by Champernowne (4) using a series method, and by Clarke (5). Clarke considers the more general problem of solving (6) when m is a function of time and introduces a generating function which satisfies a hyperbolic partial differential equation. The solution of this equation involves a Volterra type integral equation, which is solved explicitly by Clarke for the case of constant m.

In § 2 of the present paper the solution of (6) for constant m satisfying the specified initial conditions is deduced from the standard recurrence relations for Bessel functions. The solution for constant m is used in § 3 to reduce the general problem to that of solving an integral equation somewhat similar to Clarke's, but trivial for constant m. The need for a numerical treatment of the problem, when m satisfies the differential equation (4), is discussed in § 4. In § 5 an iterative method of solving (4), simultaneously with the integral equation, is given, and various practical points arising from the method are discussed in § 6.

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2. *Solution of the equations with constant coefficients.* As a guide to the general solution of (4) and (6), with the initial conditions stated, m can be taken as constant and (6) solved under this assumption. Introducing new variables x_n defined by

$$x_n = \exp\{(m+1)t\}\frac{dq_n}{dt}$$

(6) becomes
$$\frac{dx_n}{dt} = mx_{n-1} + x_{n+1} \quad (n \geqslant 1), \tag{7}$$

with x_0 identically zero, and initial conditions

$$t = 0, \quad x_1 = mq_0, \quad x_n = 0 \quad \text{for} \quad n \geqslant 2.$$

Writing
$$x_n = v^n X_n, \quad t = \frac{1}{w}t', \tag{8}$$

(7) becomes
$$w\frac{dX_n}{dt'} = \frac{m}{v}X_{n-1} + vX_{n+1}. \tag{9}$$

If $v = m^{\frac{1}{2}}$, $w = 2m^{\frac{1}{2}}$, i.e. $t' = 2m^{\frac{1}{2}}t$, then (9) reduces to

$$2\frac{dX_n}{dt'} = X_{n-1} + X_{n+1}.$$

This is now the standard recurrence relation for I_{n+r}, $(-1)^r K_{n+r}$ ((9), p. 79). The initial conditions that $X_1 = m^{\frac{1}{2}}q_0$, $X_n = 0$ for $n > 1$, rule out the K_{n+r} for all n, and $X_0 \equiv 0$ limits the solution to

$$X_n = \sum_r \alpha_r I_{n+r},$$

where n is integral and $\alpha_{-r} = -\alpha_r$ since $I_{-r}(t') = I_r(t')$. This is further restricted by the initial conditions to

$$X_n = m^{\frac{1}{2}}q_0\{I_{n-1}(t') - I_{n+1}(t')\}.$$

Changing variables, the solution of (6), for constant m, is

$$q_n = q_0 m^{\frac{1}{2}(n+1)}\int_0^t \{I_{n-1}(2\tau\sqrt{m}) - I_{n+1}(2\tau\sqrt{m})\}\exp\{-(m+1)\tau\}\,d\tau \quad (n \geqslant 1). \tag{10}$$

This is a special case of the result first obtained by Ledermann and Reuter (6).†

3. *Solution of the equations with time-dependent coefficients.* Even when m is a function of time, the variables $\exp\left\{\int_0^t m(y)\,dy + t\right\}q_n$ still satisfy recurrence relations like (7), but with different boundary conditions. The exponential factor in t can be introduced into (10) simply by replacing τ by $t-\tau$, which suggests generalizing the constants v and w used in (8) to obtain the form

$$q_n = \int_0^t [I_{n-1}\{w(t,\tau)\}\,m(\tau)\{v(t,\tau)\}^{n-1} - I_{n+1}\{w(t,\tau)\}\{v(t,\tau)\}^{n+1}] \times \exp[-\{u(t,\tau) + (t-\tau)\}]\,G(\tau)\,d\tau, \tag{11}$$

where
$$u(t,\tau) = \int_\tau^t m(y)\,dy$$

† I am indebted to the referee for pointing out this simple approach, which is similar to a method given by Sack (8).

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for the solution of (6) when m is a given function of time. Substitution in (6) gives

$$[I_{n-1}\{w(t,t)\}m(t)\{v(t,t)\}^{n-1}-I_{n+1}\{w(t,t)\}\{v(t,t)\}^{n+1}]G(t)$$
$$+\int_0^t\left[(n-1)\,I_{n-1}\{w(t,\tau)\}\,m(\tau)\,\{v(t,\tau)\}^{n-2}\frac{\partial v}{\partial t}+\frac{dI_{n-1}(w)}{dw}\frac{\partial w}{\partial t}m(\tau)\{v(t,\tau)\}^{n-1}\right.$$
$$\left.-(n+1)\,I_{n+1}\{w(t,\tau)\}\{v(t,\tau)\}^{n}\frac{\partial v}{\partial t}-\frac{dI_{n+1}(w)}{dw}\frac{\partial w}{\partial t}\{v(t,\tau)\}^{n+1}\right]\exp[-\{u(t,\tau)+(t-\tau)\}]\,G(\tau)\,d\tau$$
$$=m(t)\int_0^t[I_{n-2}\{w(t,\tau)\}m(\tau)\{v(t,\tau)\}^{n-2}-I_n\{w(t,\tau)\}\{v(t,\tau)\}^n]\exp[-\{u(t,\tau)+(t-\tau)\}]\,G(\tau)\,d\tau$$
$$+\int_0^t[I_n\{w(t,\tau)\}m(\tau)\{v(t,\tau)\}^n-I_{n+2}\{w(t,\tau)\}\{v(t,\tau)\}^{n+2}]\exp[-\{u(t,\tau)+(t-\tau)\}]\,G(\tau)\,d\tau. \quad (12)$$

Using the standard recurrence relations ((9), p. 79)

$$\frac{dI_n(w)}{dw}=\tfrac{1}{2}\{I_{n-1}(w)+I_{n+1}(w)\},\quad nI_n(w)=\frac{w}{2}\{I_{n-1}(w)-I_{n+1}(w)\}$$

to eliminate the terms containing $I_{n-1}(w)$ and $I_{n+1}(w)$, it can be seen that the coefficients of $I_{n-2}(w)$, $I_n(w)$ and $I_{n+2}(w)$ occurring under the integral sign in (12) will vanish, provided that

$$\left.\begin{aligned} w\frac{\partial v}{\partial t}+v\frac{\partial w}{\partial t}-2m(t)&=0,\\ w\frac{\partial v}{\partial t}-v\frac{\partial w}{\partial t}+2v^2&=0,\end{aligned}\right\}$$

i.e.

$$\left.\begin{aligned} vw&=2\int_0^t m(y)\,dy+\psi_1(\tau),\\ \frac{w}{v}&=2t+\psi_2(\tau).\end{aligned}\right\} \quad (13)$$

If $w(t,t)$ is chosen to be zero, then $I_n\{w(t,t)\}$ is zero for $n \geqslant 1$ and (12) is satisfied identically except for $n=1$. Putting τ equal to t in (13) to determine the arbitrary functions ψ_1 and ψ_2, the required solution of (13) is

$$v(t,\tau)=\left\{\frac{u(t,\tau)}{t-\tau}\right\}^{\frac{1}{2}}$$

and

$$w(t,\tau)=2\{(t-\tau)\,u(t,\tau)\}^{\frac{1}{2}}.$$

The formal solution is completed by simplifying the only equation not satisfied identically, to give the following integral equation for $G(t)$,

$$G(t)+\int_0^t\left\{\frac{m(\tau)}{v(t,\tau)}-v(t,\tau)\right\}I_1\{w(t,\tau)\}\exp[-\{u(t,\tau)+(t-\tau)\}]\,G(\tau)\,d\tau=q_0. \quad (14)$$

This is somewhat similar to the integral equation obtained by Clarke (5), using quite different methods. However, the kernel is simpler than that of Clarke's, becoming identically zero when $m(\tau)$ is constant, so that (14) becomes $G(t)=q_0$ and (11) reduces immediately to (10).

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4. *Discussion of the numerical treatment.* It is feasible that the results of § 3 may be of use if m is a prescribed function of time, but in the original formulation m is itself defined by a differential equation. This being so, numerical methods have to be used to obtain a solution. When it has been decided to treat the problem numerically, it may, at first sight, seem reasonable to solve (4) and (6) as a set of simultaneous differential equations. However, in the chemical problem, thousands rather than hundreds of equations are involved, so that this approach would be extremely tedious with present-day computers. Also, if a particular set of variables is of interest, it is necessary to solve all the equations, whereas using the results developed in § 3, it is only necessary to find the functions $m(t)$, $G(t)$ and $q_1(t)$ satisfying (4), (14) and (11) with $n = 1$. Particular values of q_n can then be found from (11), using quadrature, enabling the determination of the concentration P_n of any n-mer at any time during the reaction.

A knowledge of $m(t)$, $G(t)$ and $q_1(t)$ is also sufficient to determine the moments of the distribution, which are of considerable importance in both the chemical and queueing problems. The first moment μ_1' is obtained by putting

$$r_n = q_n + q_{n+1} + \dots$$

and substituting from (6) to give
$$\frac{dr_1}{dt} = mq_0 - q_1 \tag{15}$$

and
$$\frac{dr_n}{dt} = mr_{n-1} - (m+1)r_n + r_{n+1} \quad (n \geqslant 1). \tag{16}$$

A comparison of (15) and (4) shows that

$$r_1 = a - m,$$

and therefore
$$\mu_1' = \sum_{n=1}^{\infty} nP_n$$
$$= \frac{k_-}{k_+} r_1,$$

i.e.
$$\mu_1' = M_0 - M. \tag{17}$$

In the chemical problem, the interpretation of (17) is that the total number of molecules of monomer in the system remains constant.

Putting
$$s_n = r_n + r_{n+1} + \dots$$

and using (16) gives
$$\frac{ds_1}{dt} = mr_0 - r_1,$$

therefore
$$s_1 = \int_0^t \{m(\tau) r_0(\tau) - r_1(\tau)\} d\tau, \quad \text{where} \quad r_0(\tau) = q_0 + r_1(\tau).$$

But
$$s_1 = \sum_{n=1}^{\infty} \frac{n(n+1)}{2} p_n,$$

therefore the second moment μ_2' is given by

$$\mu_2' = \frac{2k_-}{k_+} s_1 - \mu_1'.$$

Higher moments can be obtained in a similar fashion.

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5. *Iterative method of solution.* In the numerical treatment it is convenient to introduce and evaluate the function

$$\chi(t) = \int_0^t m(y)\,dy.$$

When $m(t_0), \ldots, m(t_n)$; $\chi(t_0), \ldots, \chi(t_n)$; $G(t_0), \ldots, G(t_n)$; $q_1(t_0), \ldots, q_1(t_n)$ are known, the values of $m(t_{n+1})$, $\chi(t_{n+1})$, $G(t_{n+1})$ and $q_1(t_{n+1})$ can be determined by the following iterative scheme:

(i) estimate $m(t_{n+1})$ from

$$m(t_{n+1}) = m(t_n)\{1 - hq_0\} + hq_1(t_n),$$

where h is the time interval between t_n and t_{n+1},

(ii) evaluate $\chi(t_{n+1})$ from

$$\chi(t_{n+1}) = \chi(t_n) + \tfrac{1}{2}h\{m(t_n) + m(t_{n+1})\};$$

here, and in the succeeding steps, the trapezoidal rule is used merely to illustrate the method and simplify the written expressions,

(iii) evaluate $u(t_{n+1}, t_r)$, $v(t_{n+1}, t_r)$, $w(t_{n+1}, t_r)$ and $z(t_{n+1}, t_r)$ from

$$u(t_{n+1}, t_r) = \chi(t_{n+1}) - \chi(t_r),$$

$$v(t_{n+1}, t_r) = \left\{\frac{u(t_{n+1}, t_r)}{t_{n+1} - t_r}\right\}^{\frac{1}{2}},$$

$$w(t_{n+1}, t_r) = 2(t_{n+1} - t_r)\, v(t_{n+1}, t_r),$$

$$z(t_{n+1}, t_r) = h \exp\left[-\{u(t_{n+1}, t_r) + (t_{n+1} - t_r)\}\right] G(t_r)$$

for $0 \leqslant r \leqslant n$,

(iv) evaluate $G(t_{n+1})$ from

$$G(t_{n+1}) = q_0 - \sum_{r=0}{}' \left\{\frac{m(t_r)}{v(t_{n+1}, t_r)} - v(t_{n+1}, t_r)\right\} I_1\{w(t_{n+1}, t_r)\}\, z(t_{n+1}, t_r),$$

where Σ' indicates that the first term is to be halved,

(v) evaluate $q_1(t_{n+1})$ from

$$q_1(t_{n+1}) = \tfrac{1}{2}h\, m(t_{n+1})\, G(t_{n+1}) + \sum_{r=0}^{n}{}' \left[I_0\{w(t_{n+1}, t_r)\}\, m(t_r) - I_2\{w(t_{n+1}, t_r)\}\{v(t_{n+1}, t_r)\}^2\right] z(t_{n+1}, t_r),$$

(vi) obtain a revised estimate of $m(t_{n+1})$ from

$$m(t_{n+1}) = \frac{1}{1 + \frac{1}{2}hq_0}\left[\{1 - \tfrac{1}{2}hq_0\}\, m(t_n) + \tfrac{1}{2}h\{q_1(t_n) + q_1(t_{n+1})\}\right]$$

and continue the iteration until the required degree of precision is obtained.

6. *Notes on the numerical method.* Values of

$$m(t_0), \ldots, m(t_s); \quad \chi(t_0), \ldots, \chi(t_s); \quad G(t_0), \ldots, G(t_s); \quad q_1(t_0), \ldots, q_1(t_s)$$

can be found from Taylor series expansions of $m(t)$, $\chi(t)$, $G(t)$ and $q_1(t)$ about $t = t_0 = 0$.

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The series for $m(t)$ and $q_1(t)$ are obtained in an obvious way by differentiating (4) and (6) to give

$$m(t) = a - abt + ab(1+b)\frac{t^2}{2!} - ab(1+a+2b+b^2)\frac{t^3}{3!} + ab(1+3a+3b+4ab+a^2+3b^2+b^3)\frac{t^4}{4!} - \ldots, \quad (18)$$

$$q_1(t) = abt - ab(1+a+b)\frac{t^2}{2!} + ab(1+3a+2b+3ab+a^2+b^2)\frac{t^3}{3!} - ab(1+6a+3b+15ab+6a^2+3b^2+7ab^2+6a^2b+a^3+b^3)\frac{t^4}{4!} + \ldots. \quad (19)$$

Integration of (18) will give the expansion of $\chi(t)$. The series for $G(t)$ is obtained by differentiating the integral equation (14). To facilitate this, the kernel of the equation can be expressed as

$$K(t,\tau) = \{m(\tau)\,A(t,\tau) - B(t,\tau)\}\exp[-\{u(t,\tau)+(t-\tau)\}],$$

where
$$A(t,\tau) = (t-\tau) + \frac{(t-\tau)^2\,u(t,\tau)}{1!\,2!} + \frac{(t-\tau)^3\,\{u(t,\tau)\}^2}{2!\,3!} + \ldots$$

and
$$B(t,\tau) = u(t,\tau) + \frac{(t-\tau)\,\{u(t,\tau)\}^2}{1!\,2!} + \frac{(t-\tau)^2\,\{u(t,\tau)\}^3}{2!\,3!} + \ldots.$$

This leads to
$$G(t) = b - ab^2\frac{t^3}{3!} + ab^2(5+3a+2b)\frac{t^4}{4!} - \ldots. \quad (20)$$

The importance of (18), (19) and (20) is that they enable the functions $m(t)$, $\chi(t)$, $G(t)$ and $q_1(t)$ to be evaluated, without iteration, over the initial interval (t_0, t_s), where $m(t)$ varies most rapidly. A study of these initial values also enables an accurate estimate to be made of the time step h necessary for a given precision.

As pointed out in § 5, the trapezoidal rule was used to simplify the written expressions, but the quadrature necessary in the numerical approach can be effected using any Newton–Cotes type integration formula.

To save computing time, it is essential to double the time interval whenever possible. A method of doing this, which has been found convenient in practice, is to evaluate and store a fixed number of function values with their associated time interval and then examine their central differences to see if the correction term in the quadrature formula would have been negligible if a larger interval had been used. The modification to the calculation of $z(t_{n+1}, t_r)$ when the time interval is not constant is trivial with this arrangement.

To reduce storage problems on the computer it is also convenient to carry out steps (iii), (iv) and (v) of § 5 concurrently so that consecutive values of $u(t_{n+1}, t_r)$, $v(t_{n+1}, t_r)$, $w(t_{n+1}, t_r)$ and $z(t_{n+1}, t_r)$ can be stored in the same locations.

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