

## SUPPLEMENTARY MATERIAL

### APPENDIX A: BASIC CONCEPT OF NEW HOMOTOPY PETURBATION METHOD

To explain this method, let us consider the following function:

$$D_o(u) - f(r) = 0, \quad r \in \Omega \quad (\text{A1})$$

with the boundary conditions of

$$B_o(u, \frac{\partial u}{\partial n}) = 0, \quad r \in \Gamma \quad (\text{A2})$$

where  $D_o$  is a general differential operator,  $B_o$  is a boundary operator,  $f(r)$  is a known analytical function and  $\Gamma$  is the boundary of the domain  $\Omega$ . In general, the operator  $D_o$  can be divided into a linear part  $L$  and a non-linear part  $N$ . The eqn. (A.1) can therefore be written as

$$L(u) + N(u) - f(r) = 0 \quad (\text{A3})$$

By the homotopy technique, we construct a homotopy  $v(r, p) : \Omega \times [0,1] \rightarrow \mathfrak{R}$  that satisfies

$$H(v, p) = (1-p)[L(v) - L(u_0)] + p[D_o(v) - f(r)] = 0. \quad (\text{A4})$$

$$H(v, p) = L(v) - L(u_0) + pL(u_0) + p[N(v) - f(r)] = 0. \quad (\text{A5})$$

where  $p \in [0, 1]$  is an embedding parameter, and  $u_0$  is an initial approximation of eqn. (A1) that satisfies the boundary conditions. From eqns. (A4) and (A5), we have

$$H(v, 0) = L(v) - L(u_0) = 0 \quad (\text{A6})$$

$$H(v, 1) = D_o(v) - f(r) = 0 \quad (\text{A7})$$

When  $p=0$ , the eqns. (A4) and (A5) become linear equations. When  $p=1$ , they become non-linear equations. The process of changing  $p$  from zero to unity is that of  $L(v) - L(u_0) = 0$  to  $D_o(v) - f(r) = 0$ . We first use the embedding parameter  $p$  as a “small parameter” and assume that the solutions of eqns. (A.4) and (A.5) can be written as a power series in  $p$ :

$$v = v_0 + pv_1 + p^2v_2 + \dots \quad (\text{A8})$$

Setting  $p=1$  results in the approximate solution of the eqn. (A1):

$$u = \lim_{p \rightarrow 1} v = v_0 + v_1 + v_2 + \dots \quad (\text{A9})$$

This is the basic idea of the HPM.

### APPENDIX B: SOLUTION OF EQNS. (11) and (13) USING NEW HOMOTOPY PERTURBATION METHOD

In this appendix, we indicate how Eqns. (18) and (20) in this paper are derived. Furthermore, a new Homotopy approach was constructed to determine the solution of Eqns. (11) and (13) as follows:

$$(1-l) \left[ \frac{\partial r}{\partial T} - \frac{\partial^2 r}{\partial X^2} - k_0 r N(T=0) \right] - l \left[ \frac{\partial r}{\partial T} - \frac{\partial^2 r}{\partial X^2} - k_0 r N \right] = 0 \quad (\text{B1})$$

$$(1-l) \left[ \frac{\partial N}{\partial T} - \xi \frac{\partial^2 N}{\partial X^2} - k_0 r(T=0) N \right] - l \left[ \frac{\partial N}{\partial T} - \xi \frac{\partial^2 N}{\partial X^2} - k_0 r N \right] = 0 \quad (\text{B2})$$

where  $l$  is the impeding parameter and  $l \in [0,1]$ .

The initial and boundary conditions are,

$$T = 0, \quad r = 1, \quad N = 1 \quad (\text{B3})$$

$$X = 0, \quad \frac{\partial r}{\partial X} = 0, \quad N = \frac{n_0}{R_0} \quad (\text{B4})$$

$$X = 1, \quad r = 1, \quad \frac{\partial N}{\partial X} = 0 \quad (\text{B5})$$

The approximate solutions of (B1) - (B2) are

$$r = r_0 + l r_1 + l^2 r_2 + l^3 r_3 + \dots \quad (\text{B6})$$

$$N = N_0 + l N_1 + l^2 N_2 + l^3 N_3 + \dots \quad (\text{B7})$$

Substituting the Eqns. (B6) and (B7) into Eqns. (B1) - (B2) and comparing the coefficients of like powers  $l$  we get

$$l^0 : \frac{\partial r_0}{\partial T} - \frac{\partial^2 r_0}{\partial X^2} - k_0 r_0 = 0 \quad (\text{B8})$$

$$l^0 : \frac{\partial N_0}{\partial T} - \xi \frac{\partial^2 N_0}{\partial X^2} - k_0 N_0 = 0 \quad (\text{B9})$$

Solving Eqns. (B8) – (B9), and using the boundary conditions

$$T = 0, \quad r_0 = 1, \quad N_0 = \frac{n_0}{R_0} \quad (\text{B10})$$

$$X = 0, \quad \frac{\partial r_0}{\partial X} = 0, \quad N_0 = \frac{n_0}{R_0} \quad (\text{B11})$$

$$X = 1, \quad r_0 = 1, \quad \frac{\partial N_0}{\partial X} = 0 \quad (\text{B12})$$

We can obtain the following results.

$$r_0(X, T) = \frac{\cosh\left(\sqrt{\frac{k_0 n_0}{R_0}} X\right)}{\cosh\sqrt{\frac{k_0 n_0}{R_0}}} + 16 \frac{k_0 n_0}{R_0} \sum_{n=0}^{\infty} \frac{\cos\left[\frac{\pi(2n+1)X}{2}\right] \exp\left[-\left(\frac{k_0 n_0}{R_0} + \frac{\pi^2(2n+1)^2}{4}\right) T\right]}{\sin\left[\frac{\pi(2n+1)}{2}\right] [(2n+1)\pi] \left[4 \frac{k_0 n_0}{R_0} + (2n+1)^2 \pi^2\right]}$$

(B13)

$$N_0(X, T) = \frac{n_0}{R_0} \left[ \cosh\left[\sqrt{\frac{k_0}{\xi}} X\right] + \tanh\left[\sqrt{\frac{k_0}{\xi}}\right] \sinh\left[\sqrt{\frac{k_0}{\xi}} X\right] \right] \\ + \frac{4n_0\xi\pi}{R_0} \sum_{n=1}^{\infty} \frac{1}{[4k_0 + \pi^2(2n+1)^2\xi]} \sin\left[\frac{\pi(2n+1)X}{2}\right] \exp\left[-\left[k_0 + \frac{\pi^2(2n+1)^2}{4}\right] T\right] \\ - 4\xi \sum_{n=1}^{\infty} \frac{1}{[\pi(2n+1)]} \sin\left[\frac{\pi(2n+1)X}{2}\right] \exp\left[-\left[k_0 + \frac{\pi^2(2n+1)^2}{4}\right] T\right]$$

(B14)

According to the HPM, we can conclude that

$$r(x) = \lim_{p \rightarrow 1} r(x) \approx r_0 \quad (\text{B15})$$

$$N(x) = \lim_{p \rightarrow 1} N(x) \approx N_0 \quad (\text{B16})$$

Using Eqn. (B13) in Eqn. (B15), Eqn. (B14) in (B16) we obtain the final results as described in Eqns.(18) and (20) in the text.

Also using the relation

$$p(X, T) = [1 - r(X, T)] \quad (\text{B17})$$

we can obtain  $p(X, T)$ .

### APPENDIX C: NUMERICAL VALUES OF THE PARAMETER USED IN THE WORK AND [1, 2]:

Parameter	Dimension	Numerical value
$d$ (thickness of film )	(m)	$10^{-6}$ , $10^{-5}$ , $10^{-4}$
$D$ (diffusion coefficient for reactant and product)	(m <sup>2</sup> /s)	$10^{-9}$
$D_n$ (diffusion coefficient for charge carrier within film)	(m <sup>2</sup> /s)	$10^{-9}$ , $10^{-8}$ , $10^{-7}$
$k$ (second –order reaction rate constant)	(m <sup>3</sup> ×mol/s)	$10^1$ , $10^0$ , $10^{-1}$ , $10^{-2}$
$R_0$ (concentration of reactant in the bulk of solution)	(mol/m <sup>3</sup> )	$10^2$ , $10^1$ , $10^0$

$n_0$ (initial concentration of charge carriers within film)	(mol/m <sup>3</sup> )	$4 \times 10^3$
$\xi = Dn/D$ (ratio of diffusion coefficient)	none	0.01,0.1, 1
$k_0$ (Dimensionless rate constant)	none	0.2, 0.6, 1.2, 2, 3

#### APPENDIX D: THE SCILAB PROGRAM FOR THE NUMERICAL SIMULATION OF THE EQNS. (11) and (13) AND EQNS. (18) and (20).

```

function pdex4
m = 0;
x = linspace(0,1);
t = linspace(0,1);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
% Extract the first solution component as u.
u1 = sol (:,:,1);
u2 = sol (:,:,2);
figure
plot(x,u1(end,:))
xlabel ('Distance x')
ylabel ('u1(x, 2)')
% -----
figure
plot(x,u2(end,:))
xlabel ('Distance x')
ylabel ('u2(x, 2)')
% -----
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1];
f = [1;1].*DuDx;
k=1;a=10^(-9);r0=1;n=1;d=10^(-4);
F1 =-(k*n*d^2*u(1))/a;
F2 =-(k*r0*d^2*u(2))/a;
s=[F1; F2];
% -----
function u0 = pdex4ic(x)
u0 = [1; 1];
% -----
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = [0; ul(2)-1];
ql = [1; 0];
pr = [ur(1)-1; 0];
qr = [0; 1];

```