第 43 卷 第 13 期/2023 年 7 月/光学学报 研究论文

光学学报

光在两层平板介质中传输的时域P3方程

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摘要 生物表面组织是多层介质，目前只有光在单层介质中传输的P3方程，本文给出了光在两层平板介质中传播的P3方程的时域解，编写蒙特卡罗模拟进行验证。结果表明P3时域方程与蒙特卡罗模拟符合很好，说明双层平板介质的P3方程正确地反映了光子在介质中的迁移。与扩散时域方程相比，在峰值位置附近，P3时域方程测量的反射率和透射率更加准确，在远离峰值时，P3方程与扩散方程结果一致。双层平板介质的P3时域方程扩展了P3方程的应用范围，可以替代扩散方程，也可以代替单层平板介质的P3方程，可以更好地研究光在生物组织中的传播过程。

关键词 光子迁移；P3近似；扩散方程；蒙特卡罗模拟

中图分类号 O439 **文献标志码** A **DOI**：10.3788/AOS222049

1 引 言

研究生物组织的光学特性，模拟计算光在组织中的分布，对光治疗和诊断有着重要的意义，因此需要确定光学特性的理论模型[1]。目前，生物组织常用的模型是辐射传输方程[2]，最广泛使用的是辐射传输模型的一阶近似-扩散方程。但在探测距离小和吸收大的情况下，扩散方程不准确。因此有相关人员研究辐射传输模型的三阶近似P3方程[2-6]。和扩散方程相比，P3方程更加准确，应用范围更广，但也更加复杂，难以建立数学模型。

目前已经有几种光在生物组织中传播的P3方程。Boas等[2]建立了P3频域方程。Hull等[3]研究了具有简化边界条件的P3近似。高宗慧等[4]在半无限厚介质中也进行P3方程研究。Liemert等[5]建立了光在平板介质中传输的P3方程。使用傅里叶变换方法，建立了半无限厚介质的P3方程的稳态和时域解[6]，也建立了单层平板介质的稳态和时域方程[7]。目前的几种P3方程都是研究光在单层介质中进行传播内容的。实际上，生物组织是个多层介质，需要建立多层组织的理论模型。目前的多层介质理论几乎都是扩散方程理论。Dayan等[8]求解两层扩散方程。然而，为了得到解析解，在傅里叶变换中引入了几种近似方法。Kienle等[9-10]利用傅里叶逆变换，得到了光在两层半无限厚介质中传输的稳态、频率和时域的扩散方程精确解。Martelli等[11-12]使用本征函数方法结合分离变量技术，求解两层和三层的时域扩散方程。

虽然有很多人研究光在两层介质中的传输，这些研究都是对扩散方程的研究，对两层的P3方程的研究鲜有报道，因此本文使用傅里叶变换的方法，建立了光在两层平板介质中传播的P3时域方程，计算了时域方程的时间分辨漫反射与透射率。蒙特卡罗模拟作为一种实验验证手段，使用蒙特卡罗模拟进行验证。与扩散方程进行比较，结果表明，时域P3方程正确地反映了光子的迁移，时域P3方程比扩散方程更加精确。

2 理论模型

假设一无限细的光束垂直照射到两层平板介质中，如图1所示，平板介质在横坐标上是无限大的，第一层的厚度为L_1，吸收系数为μ_{1a}，散射系数为μ_{1s}，各项异性因子为g_1，第二层的厚度为L_2，吸收系数为μ_{2a}，散射系数为μ_{2s}，各项异性因子为g_2，两层介质的总厚度为$d=L_1+L_2$。当光垂直照射时，被深度为$z=z_0=1/(\mu'_{1s}+\mu_{1a})$的第一层介质散射。其中$\mu'_{is}=\mu_{is}(1-g_i)$，$\mu'_{is}$为第$i$层介质的约化散射系数。坐标系的原点是光入射到介质中的位置，入射方向是z轴，x轴和y轴是介质的表面，探测位置为$\rho=(x^2+y^2)^{1/2}$，ω是入射光的频率，c为光在介质中传播的速度。

可以由辐射传输理论推导P近似方程，第一层介质和第二层介质的P3方程为

$$\begin{cases} D_{11}\nabla^2\Phi_{10}-\mu_{1a}\Phi_{10}+2D_{11}\nabla^2\Phi_{12}=-\delta(x,y,z-z_0) \\ 2D_{12}\nabla^2\Phi_{11}-\mu_{1t}^{(3)}\Phi_{13}+3D_{12}\nabla^2\Phi_{13}=0 \\ D_{21}\nabla^2\Phi_{20}-\mu_{2a}\Phi_{20}+2D_{21}\nabla^2\Phi_{22}=0 \\ 2D_{22}\nabla^2\Phi_{21}-\mu_{2t}^{(3)}\Phi_{23}+3D_{22}\nabla^2\Phi_{23}=0 \end{cases}, \tag{1}$$

收稿日期：2022-11-24；**修回日期**：2023-02-13；**录用日期**：2023-02-26；**网络首发日期**：2023-03-09

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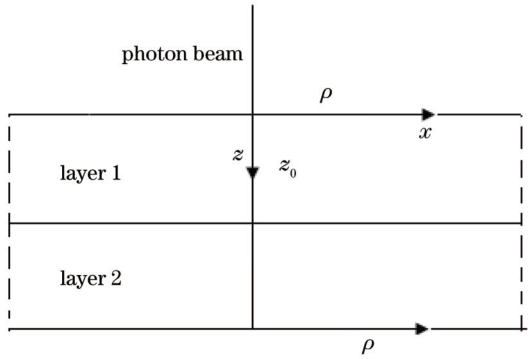

图1　光在两层平板介质中传输的模型

Fig. 1　Light transport model in a two-layer slab medium

式中：$\Phi_{ij}(x,y,z)$是P3方程的四个解，i表示层数，j表示第几个解。在扩散方程中，只有前两个解。如果采用Henyey-Greenstein相位函数，则可求出i层的所有高阶矩g_{il}[4]。式(1)中，$\mu_{it}^{(l)}$可以写为

$$\begin{cases}\mu_{it}^{(l)}=\mu_{ia}+\mu_{is}(1-g_{il})+\mathrm{j}\dfrac{\omega}{c}\\ \mu_{it}^{(0)}=\mu_{ia}+\mathrm{j}\dfrac{\omega}{c}\end{cases}。\tag{2}$$

式(1)中的D_{i1}是第i层介质的扩散方程的扩散系数，D_{i2}是另一个扩散系数，公式为

$$D_{i1}=\frac{1}{3\mu_{it}^{(1)}},D_{i2}=\frac{3}{35\mu_{it}^{(2)}}。\tag{3}$$

一些研究人员使用傅里叶变换方法求解扩散方程[5]，得到辐射传输模型的前两个解$\Phi_0(\rho,z)$和$\Phi_1(\rho,z)$，$\Phi_0(\rho,z)$是通量率，$\Phi_1(\rho,z)$是光通量。使用傅里叶变换方法，得到辐射传输模型的前四个解，也就是P3方程的四个解$\Phi_{ij}(\rho,z)$。对式(1)进行傅里叶变换，傅里叶变换表达式为

$$\varphi_{ij}(z,s_1,s_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Phi_{ij}(x,y,z,s)\exp\left[-\mathrm{j}(s_1x+s_2y)\right]\mathrm{d}x\mathrm{d}y。\tag{4}$$

式(1)的傅里叶变换可以写为

$$\begin{cases}D_{11}\nabla^2\varphi_{10}-(\mu_{1a}+D_{11}s^2)\varphi_{10}+2D_{11}\nabla^2\varphi_{12}-2D_{11}s^2\varphi_{12}=-\delta(z-z_0)\\ 3D_{12}\nabla^2\varphi_{13}-(\mu_{1t}^{(3)}+3D_{12}s^2)\phi_{13}+2D_{12}\nabla^2\varphi_{11}-2D_{12}s^2\varphi_{11}=0\\ D_{21}\nabla^2\varphi_{20}-(\mu_{2a}+D_{21}s^2)\varphi_{20}+2D_{21}\nabla^2\varphi_{22}-2D_{21}s^2\varphi_{22}=0\\ 3D_{22}\nabla^2\varphi_{23}-(\mu_{2t}^{(3)}+3D_{22}s^2)\phi_{23}+2D_{22}\nabla^2\varphi_{21}-2D_{22}s^2\varphi_{21}=0\end{cases},\tag{5}$$

式中：$s^2=\sqrt{s_1^2+s_2^2}$。在第一层中，当$z<z_0$时，$\varphi_{ij}(z,s)$写为

$$\begin{cases}\phi_{10}=A_1'\exp(-z\nu_1^-)+B_1'\exp(z\nu_1^-)+C_1'\exp(-z\nu_1^+)+E_1'\exp(z\nu_1^+)\\ \phi_{11}=A_1'h_{11}(v)(-\nu_1^-)\exp(-z\nu_1^-)+B_1'h_{11}(\nu_1^-)\exp(+z\nu_1^-)+C_1'h_{11}(-\nu_1^+)\exp(-z\nu_1^+)+E_{11}'h_1(\nu_1^+)\exp(z\nu_1^+)\\ \phi_{12}=A_1'h_{12}(-\nu_1^-)\exp(-z\nu_1^-)+B_1'h_{12}(\nu_1^-)\exp(+z\nu_1^-)+C_1'h_{12}(-\nu_1^+)\exp(-z\nu_1^+)+E_{11}'h_2(\nu_1^+)\exp(z\nu_1^+)\\ \phi_{13}=A_1'h_{13}(-\nu_1^-)\exp(-z\nu_1^-)+B_1'h_{13}(\nu_1^-)\exp(+z\nu_1^-)+C_1'h_{13}(-\nu_1^+)\exp(-z\nu_1^+)+E_{11}'h_3(\nu_1^+)\exp(z\nu_1^+)\end{cases}。\tag{6}$$

第一层中，当$z>z_0$时，$\varphi_{ij}(z,s)$写为

$$\begin{cases}\phi_{10}=A_1\exp(-z\nu_1^-)+B_1\exp(z\nu_1^-)+C_1\exp(-z\nu_1^+)+E_1\exp(z\nu_1^+)\\ \phi_{11}=A_1h_{11}(-\nu_1^-)\exp(-z\nu_1^-)+B_1h_{11}(\nu_1^-)\exp(z\nu_1^-)+C_1h_{11}(-\nu_1^+)\exp(-z\nu_1^+)+E_1h_{11}(\nu_1^+)\exp(z\nu_1^+)\\ \phi_{12}=A_1h_{12}(-\nu_1^-)\exp(-z\nu_1^-)+B_1h_{12}(\nu_1^-)\exp(z\nu_1^-)+C_1h_{12}(-\nu_1^+)\exp(-z\nu_1^+)+E_1h_{12}(\nu_1^+)\exp(z\nu_1^+)\\ \phi_{13}=A_1h_{13}(-\nu_1^-)\exp(-z\nu_1^-)+B_1h_{13}(\nu_1^-)\exp(z\nu_1^-)+C_1h_{13}(-\nu_1^+)\exp(-z\nu_1^+)+E_1h_{13}(\nu_1^+)\exp(z\nu_1^+)\end{cases}。\tag{7}$$

第二层中，$\varphi_{ij}(z,s)$写为

$$\begin{cases}\phi_{20}=A_2\exp(-zv^-)+B_2\exp(zv^-)+C_2\exp(-zv^+)+E_2\exp(zv^+)\\ \phi_{21}=A_2h_{21}(-v^-)\exp(-zv^-)+B_2h_{21}(v^-)\exp(zv^-)+C_2h_{21}(-v^+)\exp(-zv^+)+E_2h_{21}(v^+)\exp(zv^+)\\ \phi_{22}=A_2h_{22}(-v^-)\exp(-zv^-)+B_2h_{22}(v^-)\exp(zv^-)+C_2h_{22}(-v^+)\exp(-zv^+)+E_2h_{22}(v^+)\exp(zv^+)\\ \phi_{23}=A_2h_{23}(-v^-)\exp(-zv^-)+B_2h_{23}(v^-)\exp(zv^-)+C_2h_{23}(-v^+)\exp(-zv^+)+E_2h_{23}(v^+)\exp(zv^+)\end{cases}。\tag{8}$$

其中，每层的v可以表达为

$$\begin{cases}v_i^+=\sqrt{\dfrac{-b_i+\sqrt{b_i^{\,2}-4a_ic_i}}{2a_i}},v_i^-=\sqrt{\dfrac{-b_i-\sqrt{b_i^{\,2}-4a_ic_i}}{2a_i}}\\ a_i=27\mu_{it}^{(1)}\\ b_i=-\left[27\mu_{it}^{(1)}(\alpha_{i0}^2+\alpha_{i3}^2)-28\mu_{it}^{(3)}(\alpha_{i2}^2-\alpha_{i0}^2)\right]\\ c_i=27\mu_{it}^{(1)}\alpha_{i0}^2\alpha_{i3}^2+28\mu_{it}^{(3)}(\alpha_{i0}^2\alpha_{i1}^2-\alpha_{i2}^2\alpha_{i1}^2)\end{cases},\tag{9}$$

$\alpha_{i0}^2=(\mu_{ia}+D_i s^2)/D_{i1}, \alpha_{i1}^2=\alpha_{i2}^2=s^2, \alpha_{i3}^2=(\mu_{it}^{(3)}+3D_{i2}s^2)/3D_{i2}$ 。 (10)

假设 $s=0$，式(9)与文献[3]中的公式完全相同。在式(6)～(8)中，$h_i(v)$可以表达为

$$\begin{cases} h_{i1}(v)=\dfrac{3(v_i^2-\alpha_{i3}^2)}{2(v_i^2-\alpha_{i1}^2)}\dfrac{3v_i}{7\mu_{it}^{(3)}}\dfrac{v_i^2-\alpha_{i0}^2}{2(v_i^2-\alpha_{i2}^2)} \\ h_{i2}(v)=-\dfrac{v_i^2-\alpha_{i0}^2}{2(v_i^2-\alpha_{i2}^2)} \\ h_{i3}(v)=+3v_i/7\mu_{it}^{(3)}\dfrac{v_i^2-\alpha_{i0}^2}{2(v_i^2-\alpha_{i2}^2)} \end{cases} 。 \tag{11}$$

在式(7)中，系数A_1、B_1、C_1、E_1为

$$\begin{cases} B_1=(c_1a_{22}-c_2a_{12})/(a_{11}a_{22}-a_{12}a_{21}) \\ E_1=(c_2a_{11}-c_1a_{21})/(a_{11}a_{22}-a_{12}a_{21}) \\ A_1=k_0+(k_1-B_1)\exp(-2zb_{11}v^-)=k_0+k_1\exp(-2zb_{11}v^-)-B_1\exp(-2zb_{11}v^-) \\ C_1=k_2+k_3\exp(-2zb_{12}v^+)-E_1\exp(-2zb_{12}v^+) \end{cases}, \tag{12}$$

其中a_{11}、a_{12}、c_1表示为

$$\begin{cases} a_{11}=\left[h_{22}(v^-)-h_{22}(v^+)\right]l_{22}\left[h_{23}(v^-)h_{11}(v_1^-)-h_{21}(v^-)h_{13}(v_1^-)\right]m_{11}- \\ \quad \left[-h_{23}(v^-)h_{21}(v^+)+h_{21}(v^-)h_{23}(v^+)\right]m_{22}\left[h_{22}(v^-)-h_{12}(v_1^-)\right]l_{11} \\ a_{12}=\left[h_{22}(v^-)-h_{22}(v^+)\right]l_{22}\left[h_{23}(v^-)h_{11}(v_1^+)-h_{21}(v^-)_1h_{13}(v_1^+)\right]m_{12}- \\ \quad \left[-h_{23}(v^-)h_{21}(v^+)+h_{21}(v^-)h_{23}(v^+)\right]m_{22}\left[h_{22}(v^-)-h_{12}(v_1^+)\right]l_{12} \\ c_1=\left[-h_{23}(v^-)h_{21}(v^+)+h_{21}(v^-)h_{23}(v^+)\right]m_{22}\left\{p_{22}\left[h_{22}(v^-)-h_{12}(v_1^-)\right]+p_{12}\left[h_{22}(v^-)-h_{12}(v_1^+)\right]\right\}- \\ \quad \left[h_{22}(v^-)-h_{22}(v^+)\right]\times l_{22}\left\{p_{11}\left[-h_{23}(v^-)h_{11}(v_1^-)+h_{21}(v^-)h_{13}(v_1^-)\right]+p_{12}\left[-h_{23}(v^-)h_{11}(v_1^+)+h_{21}(v^-)h_{13}(v_1^+)\right]\right\} \end{cases}, \tag{13}$$

其中l、m、p的公式为

$$\begin{cases} l_{11}=\exp(L_1v_1^-)-\exp(-2zb_{11}v_1^-)\exp(-L_1v_1^-) \\ l_{12}=\exp(L_1v_1^+)-\exp(-2zb_{12}v_1^+)\exp(-L_1v_1^+) \\ m_{11}=\exp(L_1v_1^-)+\exp(-2zb_{11}v_1^-)\exp(-L_1v_1^-) \\ p_{11}=\left[k_0+k_1\exp(-2zb_{11}v_1^-)\right]\exp(-L_1v_1^-) \\ p_{12}=\left[k_2+k_3\exp(-2zb_{12}v_1^+)\right]\exp(-L_1v_1^+) \end{cases}, \tag{14}$$

$$\begin{cases} l_{21}=\exp(-L_1v_2^-)-\exp\left[-2(d+zb_{12})v_2^-\right]\exp(L_1v_2^-) \\ l_{22}=\exp(-L_1v_2^+)-\exp\left[-2(d+zb_{22})v_2^+\right]\exp(L_1v_2^+) \\ m_{21}=\exp(-L_1v_2^-)+\exp\left[-2(d+zb_{12})v_2^-\right]\exp(L_1v_2^-) \\ m_{22}=\exp(-L_1v_2^-)+\exp\left[-2(d+zb_{12})v_2^-\right]\exp(L_1v_2^-) \end{cases}, \tag{15}$$

式中：$d=L_1+L_2$。在式(12)中，有

$$\begin{cases} k_0=\left[-1/2h_{13}(v_1^+)-1/3h_{11}(v_1^+)\right]\exp(z_0v_1^-)/\left[h_{13}(v_1^+)h_1(v_1^-)-h_{13}(v_1^-)h_1(v_1^+)\right] \\ k_2=\left[1/3h_{11}(v_1^-)+1/2h_{13}(v_1^-)\right]\exp(z_0v_1^+)/h_{13}(v_1^+)h_{11}(v_1^-)-h_{13}(v_1^-)h_{11}(v_1^+) \\ k_1=-\left[-1/2h_{13}(v_1^+)-1/3h_{11}(v_1^+)\right]\exp(-z_0v_1^-)/\left[h_{13}(v_1^+)h_{11}(v_1^-)-h_{13}(v_1^-)h_{11}(v_1^+)\right] \\ k_3=-\left[1/3h_{11}(v_1^-)+1/2h_{13}(v_1^-)\right]\exp(-z_0v_1^+)/h_{13}(v_1^+)h_{11}(v_1^-)-h_{13}(v_1^-)h_{11}(v_1^+) \end{cases}。 \tag{16}$$

式(6)中的系数A_1'、B_1'、C_1'、E_1'的表达式为

$$A'=A-k_0,\ B'=B-k_1,\ C'=C-k_2,\ E'=E-k_3 。 \tag{17}$$

式(8)中的系数A_2、B_2、C_2、E_2为

$$\begin{cases} A_2=(c_3a_{42}-c_4a_{32})/(a_{31}a_{42}-a_{32}a_{41}) \\ C_2=(c_4a_{31}-c_3a_{41})/(a_{31}a_{42}-a_{32}a_{41}) \\ B_2=-A_2\exp\left[-2(d_2+zb_{21})v^-\right] \\ E_2=-C_2\exp\left[-2(d_2+zb_{22})v^+\right] \end{cases}, \tag{18}$$

其中a_{31}、a_{32}、a_{41}、a_{42}、c_3、c_4表示为

$$\begin{cases} a_{31}=\left[h_{12}(v_1^-)-h_{12}(v_1^+)\right]l_{12}\left[-h_{13}(v_1^-)h_{21}(v_2^-)+h_{11}(v_1^-)h_{23}(v_2^-)\right]m_{21}- \\ \quad\left[h_{13}(v_1^-)h_{11}(v_1^+)-h_{11}(v_1^-)h_{13}(v_1^+)\right]m_{12}\left[h_{12}(v_1^-)-h_{22}(v_2^-)\right]l_{21} \\ a_{32}=\left[h_{12}(v_1^-)-h_{12}(v_1^+)\right]l_{12}\left[-h_{13}(v_1^-)h_{21}(v_2^+)-h_{11}(v_1^-)h_{23}(v_2^+)\right]m_{22}- \\ \quad\left[h_{13}(v_1^-)h_{11}(v_1^+)-h_{11}(v_1^-)h_{13}(v_1^+)\right]m_{12}\left[h_{12}(v_1^-)-h_{22}(v_2^+)\right]l_{22} \\ c_3=\left[h_{13}(v_1^-)h_{11}(v_1^+)-h_{11}(v_1^-)h_{13}(v_1^+)\right]\left[h_{12}(v_1^-)-h_{12}(v_1^+)\right]\left[-m_{12}p_{12}-l_{12}p_{12}\right] \end{cases}, \tag{19}$$

$$\begin{cases} a_{41}=\left[h_{12}(v_1^+)-h_{12}(v_1^-)\right]l_{11}\left[-h_{13}(v_1^+)h_{21}(v_2^-)+h_{11}(v_1^+)h_{23}(v_2^-)\right]m_{21}- \\ \quad\left[h_{13}(v_1^+)h_{11}(v_1^- -h_{11}(v_1^+)h_{13}(v_1^-)\right]m_{11}\left[h_{12}(v_1^+)-h_{22}(v_2^-)\right]l_{21} \\ a_{42}=\left[h_{12}(v_1^+)-h_{12}(v_1^-)\right]l_{11}\left[-h_{13}(v_1^+)h_{21}(v_2^+)+h_{11}(v_1^+)h_{23}(v_2^+)\right]m_{22}- \\ \quad\left[h_{13}(v_1^+)h_{11}(v_1^-)-h_{11}(v_1^+)h_{13}(v_1^-)\right]m_{11}\left[h_{12}(v_1^+)-h_{22}(v_2^+)\right]l_{22} \\ c_4=\left[h_{13}(v_1^+)h_{11}(v_1^-)-h_{11}(v_1^+)h_{13}(v_1^-)\right]\left[h_{12}(v_1^+)-h_{12}(v_1^-)\right](-m_{11}p_{11}-l_{11}p_{11}) \end{cases}。 \tag{20}$$

在式(12)和式(18)中，外推边界条件为

$$\begin{cases} zb_{i1}=-2\dfrac{1+R_{\mathrm{eff}}}{1-R_{\mathrm{eff}}}\dfrac{\mu_{\mathrm{a}}}{v_{i-}^2(0)} \\ zb_{i2}=-2\dfrac{1+R_{\mathrm{eff}}}{1-R_{\mathrm{eff}}}\dfrac{\mu_{\mathrm{a}}}{v_{i+}^2(0)} \end{cases}, \tag{21}$$

式中：R_{eff}是与折射率有关的常数，如果生物介质的折射率为1.4，$R_{\mathrm{eff}}=0.493$[9-10]。这样，得到$\varphi_{ij}(z,s)$的解，通过Hankel变换，得到$\Phi_{ij}(\rho,z)$的解：

$$\Phi_{ij}(\rho,z)=\frac{1}{2\pi}\int_0^{\infty}\phi_{ij}(z,s)s\mathrm{J}_0(s\rho)\mathrm{d}s, \tag{22}$$

式中：J_0是0阶贝塞尔函数；s是积分变量。式(12)是Hankel变换，它可以通过傅里叶逆变换得到。每一层的$\varphi_{ij}(z,s)$写成指数形式，这样就得到频域解，通过计算不同频率的解，对其进行傅里叶变换，得到时域方程。本文中，采用$\omega=100\times10^9\times2\times\pi/1024$的整数倍，使用快速傅里叶变换，则得到时域解法，采用的方法与相关文献[9-10]一致。在式(9)和式(10)中，假设$s=0$，式(9)和式(10)与文献[2]中的公式完全一致，也就是文献[3]的相关方程是本文方程的特殊形式。

在两层平板介质的上表面$z=0$，可以计算反射率，P_3近似稳态方程的空间分辨漫反射的解为

$$R(\rho)=k_0\Phi_0(\rho,z)+k_1\Phi_1(\rho,z)+k_2\Phi_2(\rho,z)+k_3\Phi_3(\rho,z), \tag{23}$$

式中：系数k_0、k_1、k_2、k_3是与折射率有关的常数，如果生物组织的折射率为1.4，$k_0=0.1177$、$k_1=-0.3056$、$k_2=0.4444$、$k_3=-0.5487$。在扩散方程中，只是采用了前2项。

两层平板介质的下表面$z=d$，可以按照相关的方法计算透过率[7,13-14]：

$$T(\rho)=\Phi_1(\rho,z=d)。 \tag{24}$$

至此，得到了光在两层介质中传播的时域P3方程，给出了反射率和透射率的计算。

3 两层平板介质的P3时域方程与扩散时域方程的比较

蒙特卡罗模拟作为各种理论的验证方法和实验手段，因此使用蒙特卡罗模拟[15-16]来验证建立的P3方程的正确性。对不同参数的平板进行蒙特卡罗模拟，同时使用P3方程与扩散方程进行比较。本文使用Liemert等建立的多层平板介质的时域方程和扩散方程[13-14]。

3.1 时域反射率的比较

首先，对P3方程计算的时域反射率与蒙特卡罗模拟的结果进行比较，比较了相同厚度不同光学参数的两种介质时域方程。假设两种介质折射率$n=1.4$，$g=0.9$，上表面$z=0$，探测距离$\rho=5.5$ mm。一种介质的参数为$\mu_{1\mathrm{s}}=\mu_{2\mathrm{s}}=10\ \mathrm{mm}^{-1}$，$\mu_{1\mathrm{a}}=0.0001\ \mathrm{mm}^{-1}$，$\mu_{2\mathrm{a}}=0.001\ \mathrm{mm}^{-1}$。另一种介质的光学参数为$\mu_{1\mathrm{s}}=\mu_{2\mathrm{s}}=10\ \mathrm{mm}^{-1}$，$\mu_{1\mathrm{a}}=0.001\ \mathrm{mm}^{-1}$，$\mu_{2\mathrm{a}}=0.01\ \mathrm{mm}^{-1}$。两种介质的厚度分别为$L_1=3$ mm，$L_2=7$ mm，两种介质的区别是第二种介质的吸收系数是第一种介质的10倍，结果如图2(a)所示。从图2(a)可以看出，不同光学参数下，时域P3方程和蒙特卡罗模拟符合很好，说明时域P3方程正确地表述了光子的迁移。同时进行不同探测距离的比较，结果都显示时域P3方程和蒙特卡罗模拟高度符合。

将P3时域方程与扩散时域方程比较，主要比较峰值附近的结果。假设介质折射率为$n=1.4$，$g=0.9$，$d=10$ mm，探测距离$\rho=5.5$ mm，$\mu_{1\mathrm{s}}=\mu_{2\mathrm{s}}=10\ \mathrm{mm}^{-1}$，$\mu_{1\mathrm{a}}=0.0001\ \mathrm{mm}^{-1}$，$\mu_{2\mathrm{a}}=0.001\ \mathrm{mm}^{-1}$。P3时域方程与扩散方程、蒙特卡罗模拟的结果如图2(b)所示，可以看出，在时域图形的峰值处，P3方程更加符合蒙特卡罗模拟，因此P3时域方程比扩散时域方程更准确。为了进一步比较P3方程与扩散方程，计算P3方程、扩散方程与蒙特卡罗模拟的相对误差，光学参数与图2(b)相同，结果如图2(c)所示，可以进一步看出，P3时域方程在峰值附近的精度高于扩散方程。图2(b)和图2

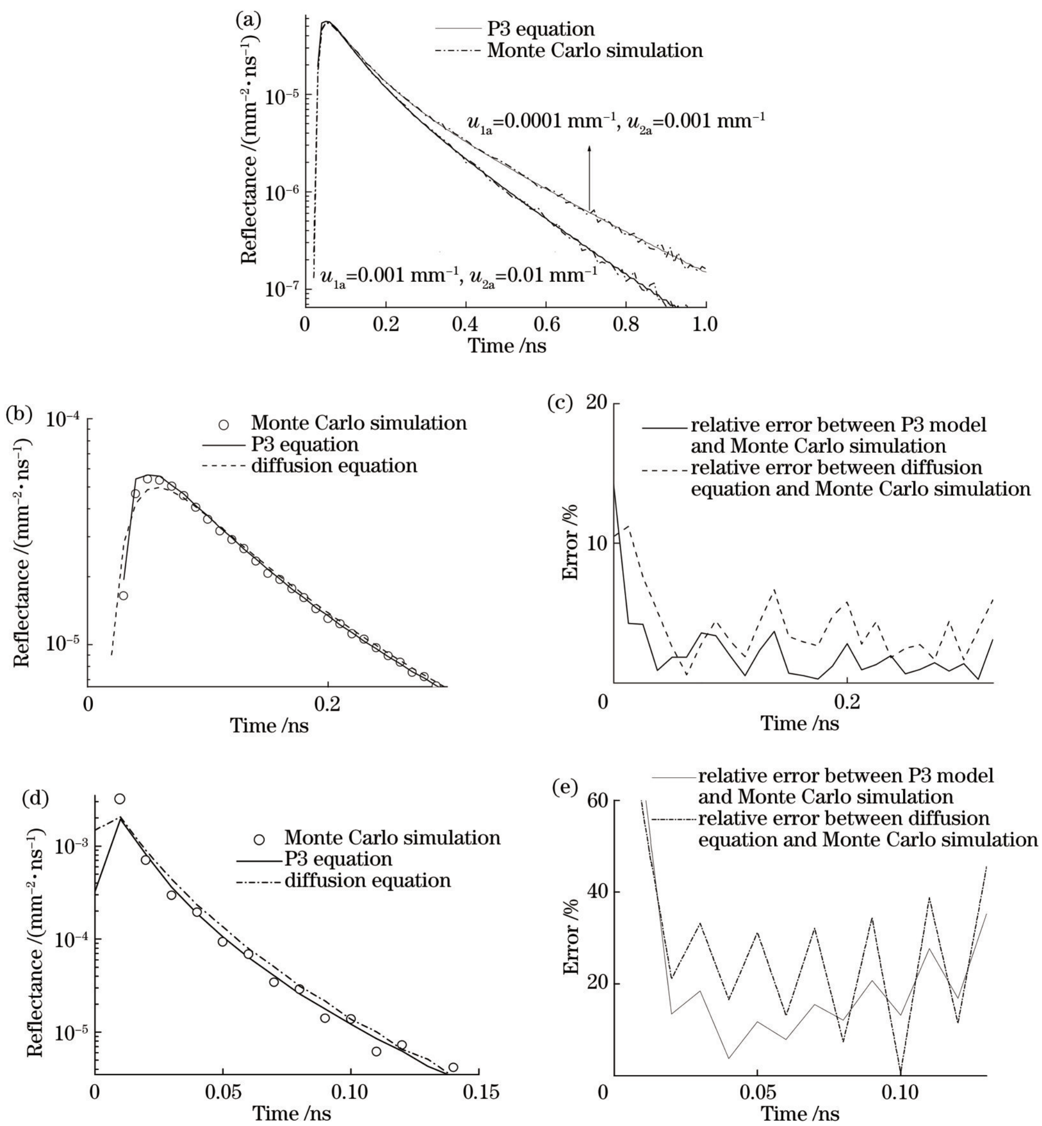

图2 P3近似模型、蒙特卡罗模拟、扩散近似的反射率比较。(a)相同厚度、不同吸收系数下P3方程与蒙特卡罗模拟的比较;(b)在峰值附近、远离光源、低吸收系数时,P3方程、扩散方程、蒙特卡罗模拟的比较;(c)远离光源、低吸收系数时,P3方程、扩散方程、蒙特卡罗模拟的相对误差;(d)近源处、高吸收系数时,P3方程、扩散方程、蒙特卡罗模拟的比较;(e)近源处、高吸收系数时,P3方程、扩散方程、蒙特卡罗模拟的相对误差

Fig. 2 Reflectance comparison of P3 approximation model with Monte Carlo simulation and diffusion approximation. (a) Comparison of P3 equation with Monte Carlo simulation with the same thickness and different absorption coefficients; (b) comparison of the P3 equation with the Monte Carlo simulation and the diffusion equation near the peak, at low absorption coefficient, away from light source; (c) relative error of P3 equation, diffusion equation, and Monte Carlo simulation at low absorption coefficient, away from light source; (d) comparison of the P3 equation with the Monte Carlo simulation and the diffusion equation near the peak, at high absorption coefficient, near light source; (e) relative error of P3 equation, diffusion equation, and Monte Carlo simulation at high absorption coefficient, near light source

(c)都是在远离光源处和吸收系数满足扩散方程时的结果,也就是在满足扩散方程时,在峰值附近,P3方程比扩散方程更加准确。

为了比较在近源处、吸收系数较大的情况,此时扩散方程不准确,假设介质折射率$n=1.4$,$g=0.9$,$d=10$ mm,探测距离$\rho=1.5$ mm,$\mu_{1s}=\mu_{2s}=10$ mm^{-1},$\mu_{1a}=0.1$ mm^{-1},$\mu_{2a}=0.05$ mm^{-1}。P3时域方程计算的反射率与扩散方程、蒙特卡罗模拟的结果如图2(d)所示,相对误差如图2(e)所示。从图2(d)和图2(e)可以看出:吸收系数较大时,曲线衰减特别快;P3方程与蒙特卡罗模拟比较符合,扩散方程与蒙特卡罗模拟有较大误差。进一步说明,在近源处和吸收系数较大时,P3方程更加准确。比较图2(c)和图2(e)可以看出:满足扩散方程时,也就是低吸收、远离光源时,P3方程误差在3%左右,扩散方程误差在7%左右;近距离探测、高吸收时,峰值附近,P3方程的误差在15%左右,而扩散

方程的误差在30%左右。因此在近光源处和吸收系数较大时，P3时域方程的反射率比扩散方程更有优势。

3.2 时域透射率的比较

对P3方程计算的时域透射率与蒙特卡罗模拟的结果进行比较。下表面中$z=d=L_1+L_2$，比较光学参数相同、厚度不同的两种介质的时域方程，假设两种介质折射率$n=1.4$，$g=0.9$，探测距离为$\rho=5.5$ mm。一种介质的参数为$\mu_{1s}=\mu_{2s}=10\ \text{mm}^{-1}$，$\mu_{1a}=0.0001\ \text{mm}^{-1}$，$\mu_{2a}=0.001\ \text{mm}^{-1}$，介质的厚度分别为$L_1=3$ mm，$L_2=7$ mm，另一种介质的光学参数与上面相同，厚度不同，其厚度为$L_1=3$ mm，$L_2=17$ mm，结果如图3(a)所示。从图3(a)可以看出，不同厚度情况下，时域P3方程的透射率与蒙特卡罗模拟的反射率很好符合，说明P3时域方程的透射率正确描述了光子的迁移。

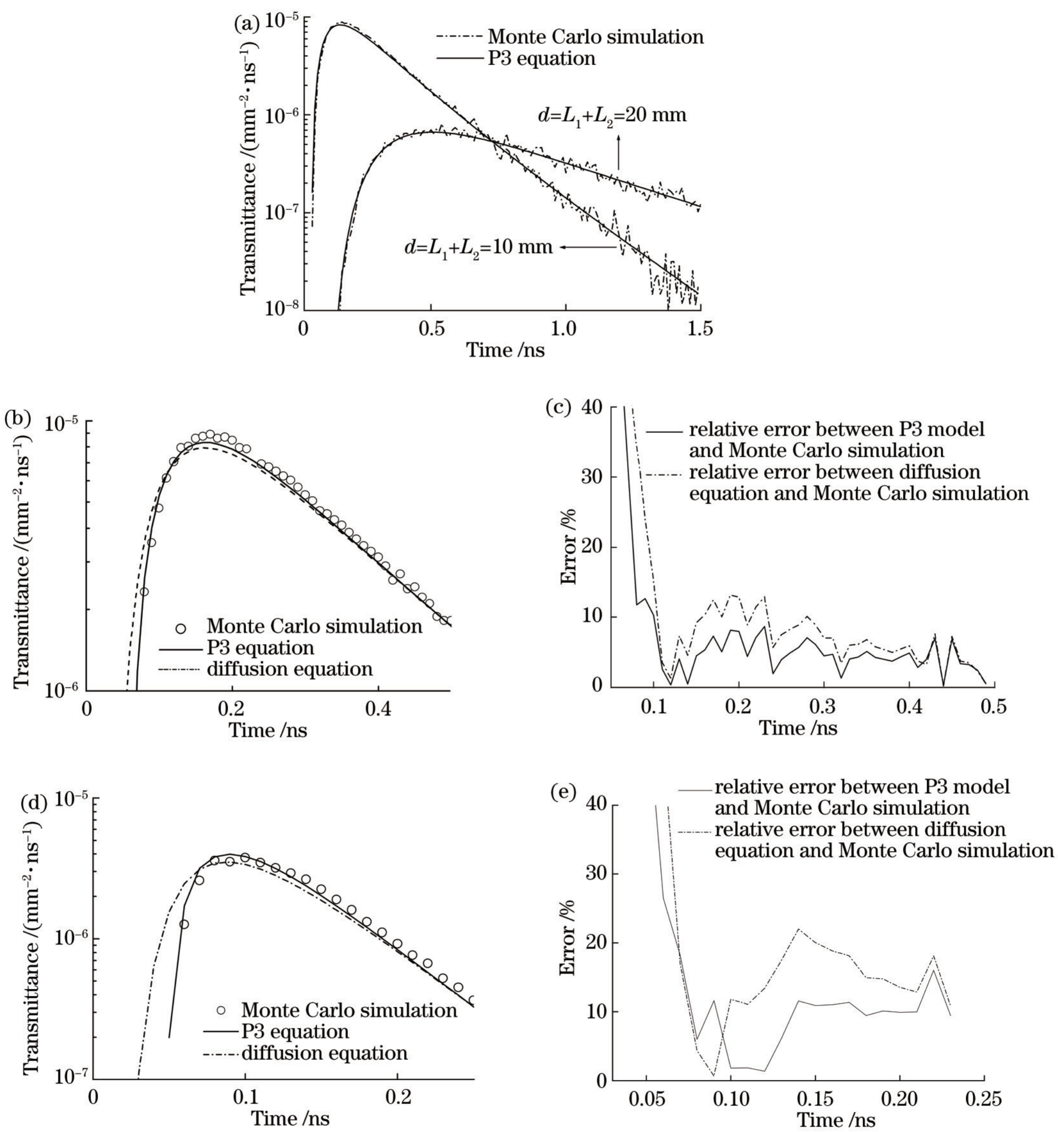

图3 P3近似模型、蒙特卡罗模拟、扩散近似的透射率比较。(a)相同参数、不同厚度下P3方程与蒙特卡罗模拟的比较；(b)在峰值附近、远离光源、低吸收系数时，P3方程、扩散方程、蒙特卡罗模拟的比较；(c)远离光源、低吸收系数时，P3方程、扩散方程、蒙特卡罗模拟的相对误差；(d)近源处，高吸收系数时，P3方程、扩散方程、蒙特卡罗模拟的比较；(e)近源处、高吸收系数时，P3方程、扩散方程、蒙特卡罗模拟的相对误差

Fig. 3 Transmittance comparison of P3 approximate model with Monte Carlo simulation and diffusion approximation. (a) Comparison of P3 equation with Monte Carlo simulation with the same parameters and different thickness; (b) comparison of P3 equation with diffusion equation and Monte Carlo simulation near the peak, at low absorption coefficient, away from light source; (c) relative error of P3 equation, diffusion equation, and Monte Carlo simulation at low absorption coefficient, away from light source; (d) comparison of P3 equation with diffusion equation and Monte Carlo simulation at high absorption coefficient, near light source; (e) relative error of P3 equation, diffusion equation, and Monte Carlo simulation at high absorption coefficient, near light source

对P3方程计算的时域透射率和扩散方程的结果进行比较。使用的光学参数与图3(a)的光学参数相同,两层介质的总厚度为d=3+7=10 mm。P3方程的结果与扩散方程和蒙特卡罗模拟的结果如图3(b)所示,相对误差如图3(c)所示。结果表明,在峰值附近,P3时域方程计算的透过率比扩散方程更加符合蒙特卡罗模拟。

为了比较在近源处、吸收系数较大的时域透射率,采用与图2(d)相同的参数,只是在下表面测量$z=d=L_1+L_2=10$ mm,$\rho=1.5$ mm。P3时域方程的透过率与扩散方程、蒙特卡罗模拟的结果如图3(d)所示,相对误差如图3(e)所示。从图3(d)和图3(e)可以看出:P3方程与蒙特卡罗模拟比较符合,而扩散方程与蒙特卡罗模拟有较大误差;满足扩散方程时,也就是低吸收、远离光源探测时,P3方程的透过率误差在7%左右,扩散方程误差在13%左右;而近距离探测、高吸收时,峰值附近,P3方程的透过率的误差在10%左右,而扩散方程的误差在20%左右。进一步说明,在近源处和吸收系数较大时,P3方程的透过率比扩散方程准确。通过比较图3(c)和图3(e)可以进一步看出,P3时域方程的透过率比扩散方程准确。

4 结 论

在生物医学光学的研究中,人体组织通常由多层组成,很多人建立两层或多层介质的扩散方程,但是扩散方程适用于高散射和低吸收的介质。因此有人研究了辐射模型的P3方程。目前的P3方程都是研究光在同一介质中进行传输的,有科研人员甚至给出了单一介质的P5方程[17]。而实际上,生物组织是多层的不同介质,需要建立多层介质P3方程,因此建立了光在两层平板介质进行传播的频域方程,通过频域解的傅里叶变换,给出时域解,计算时域方程的时间分辨漫反射率和透射率。通过和蒙特卡罗模拟比较,证明P3时域方程正确地反映了光子迁移的结论。通过和扩散方程的比较,P3时域方程在峰值附近更加符合蒙特卡罗模拟,远离峰值时,P3时域方程与扩散时域方程数值几乎相同。近源处和吸收系数较大时,发现扩散方程具有较大的误差,而P3方程误差较小,说明两层平板介质的时域方程比扩散方程更具有优势。当两层介质光学参数相同时,可以推导出两层介质的平板介质模型与单层平板介质模型[7]相同。因此两层平板介质的P3方程不仅包含能解决单层平板的P3方程,更为建立任意多层平板介质的P3方程打下基础。有科研人员使用单层介质的P3方程提取生物组织的光学参数[18],因此双层介质的P3时域扩散方程也可以用来提取多层介质的光学参数。

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Time-Domain P3 Equation for Light Transmission in Two-Layer Slab Medium

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Abstract

Objective It is of great significance to study the optical properties of biological tissue and simulate the distribution of light in tissue for light therapy and diagnosis. Therefore, a theoretical model of optical properties needs to be determined. Currently, the model commonly used in biological tissue is the radiative transfer equation. The most widely used one is the first-order approximation of the radiative transfer model, namely the diffusion equation. However, in the case of small detection distance and large absorption, the diffusion equation is not accurate. Therefore, some people have studied the third-order approximation P3 equation of the radiative transfer model. Compared with the diffusion equation, the P3 equation is more accurate and more widely applied, but it is more complicated to establish a mathematical model. At present, several P3 equation models are studied in one layer medium. In fact, biological tissue is a multilayer medium, so it is necessary to establish the P3 model of multilayer tissue. At present, there are several models in the diffusion equation that can solve the problem in a multilayer medium. In particular, Kienle *et al*. obtained the exact solutions of the diffusion equation in the steady state and frequency and time domains of light transmission in two semi-infinite thick media through the inverse Fourier transform. It is necessary to establish the P3 equation of light transmission in two or more layers. In this paper, the P3 time domain equation of light transmission in a two-layer slab medium is given and compared with Monte Carlo simulation and diffusion equation.

Methods On the basis of the radiative transfer theory, the P3 equation is given. According to Fourier transform method, the frequency domain solution is established. Based on the Fourier transform in the frequency domain, the time domain solution of the P3 equation in a two-layer slab medium is given. Monte Carlo simulation is a statistical verification method, which can replace experiments to verify the correctness of the theoretical model. The P3 time domain equation and diffusion equation are calculated, and the Monte Carlo simulation program for the multi-layer medium is written. The P3 time domain equation of light transmission in a two-layer slab medium is verified by Monte Carlo simulation. The advantages of the P3 time domain equation and the diffusion equation in the case of low absorption coefficient at a long distance and high absorption coefficient at a short distance are compared.

Results and Discussions The P3 time domain equation of the two-layer slab medium is compared with the Monte Carlo simulation. The results show that the reflectance and transmittance of the P3 time domain equation for light transmission in the two-layer slab medium are in good agreement with the Monte Carlo simulation results, which indicates that the P3 time domain equation for light transmission in the two-layer slab medium correctly reflects the light migration in the medium. The P3 time domain equation is compared with the time domain diffusion equation of a multi-layer medium. When the absorption coefficient is low, and the detection distance is large, the results of the P3 equation are consistent with those of the diffusion equation. Near the peak value, the reflectance error of the P3 equation is about 3%, and that of the diffusion equation is about 7%. The transmittance error of the P3 equation is about 7%, and that of the diffusion equation is about 13%. In other words, when the diffusion equation is satisfied, the P3 equation is more accurate than the diffusion equation at the peak value. When the absorption coefficient is high, and the detection distance is small, the reflectance error of the diffusion equation is about 30%. The transmittance error of the P3 equation is about 10%, and that of the diffusion equation is about 20%. It is further indicated that the reflectance and transmittance of the P3 equation are more accurate than those of the diffusion equation when the absorption coefficient is larger near the source. So the P3 time domain equation in a two-layer medium has an advantage over the diffusion equation.

Conclusions The P3 time domain equation of light transmission in a two-layer slab medium is given. The P3 time domain equation is consistent with the Monte Carlo simulation results and is more accurate than the diffusion equation. So the diffusion equation of the two-layer medium can be replaced by the P3 time domain equation. When the optical parameters of the two layers are the same, a one-layer model can be derived. Therefore, the P3 equation in a two-layer slab medium not only includes the P3 equation in a one-layer slab medium but also lays the foundation for the P3 equation in a multi-layer slab medium. At present, the diffusion equation is used to extract the optical parameters of biological tissue, and the P3 equation in the one-layer medium is used to extract the optical parameters of biological tissue. Therefore, the P3 time domain diffusion equation in a two-layer medium can be used to extract the optical parameters of multi-layer media.

Key words photo migration; P3 approximation; diffusion equation; Monte Carlo simulation